# Package 'nimble'

December 17, 2024

Title MCMC, Particle Filtering, and Programmable Hierarchical Modeling

**Description** A system for writing hierarchical statistical models largely compatible with 'BUGS' and 'JAGS', writing nimbleFunctions to operate models and do basic R-style math, and compiling both models and nimbleFunctions via custom-generated C++. 'NIMBLE' includes default methods for MCMC, Laplace Approximation, Monte Carlo Expectation Maximization, and some other tools. The nimbleFunction system makes it easy to do things like implement new MCMC samplers from R, customize the assignment of samplers to different parts of a model from R, and compile the new samplers automatically via C++ alongside the samplers 'NIMBLE' provides. 'NIMBLE' extends the 'BUGS'/'JAGS' language by making it extensible: New distributions and functions can be added, including as calls to external compiled code. Although most people think of MCMC as the main goal of the 'BUGS'/'JAGS' language for writing models, one can use 'NIMBLE' for writing arbitrary other kinds of model-generic algorithms as well. A full User Manual is available at <https://r-nimble.org>.

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BugReports https://github.com/nimble-dev/nimble/issues

SystemRequirements GNU make

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Note For convenience, the package includes the necessary header files for the Eigen distribution. (This is all that is needed to use that functionality.) You can use an alternative installation of Eigen on your system or the one we provide. The license for the Eigen code is very permissive and allows us to distribute it with this package. See <http://eigen.tuxfamily.org/index.php? title=Main\_Page> and also the License section on that page.

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Collate config.R all\_utils.R options.R distributions\_inputList.R distributions processInputList.R distributions\_implementations.R BUGS\_BUGSdecl.R BUGS\_contexts.R BUGS\_nimbleGraph.R BUGS\_modelDef.R BUGS\_model.R BUGS\_graphNodeMaps.R BUGS\_readBUGS.R BUGS\_macros.R BUGS\_testBUGS.R BUGS\_getDependencies.R BUGS\_utils.R BUGS mathCompatibility.R externalCalls.R genCpp exprClass.R genCpp\_operatorLists.R genCpp\_RparseTree2exprClasses.R genCpp\_initSizes.R genCpp\_buildIntermediates.R genCpp\_processSpecificCalls.R genCpp\_sizeProcessing.R genCpp\_toEigenize.R genCpp\_insertAssertions.R genCpp\_maps.R genCpp liftMaps.R genCpp eigenization.R genCpp addDebugMarks.R genCpp generateCpp.R RCfunction core.R RCfunction compile.R nimbleFunction util.R nimbleFunction core.R nimbleFunction nodeFunction.R nimbleFunction nodeFunctionNew.R nimbleFunction Rderivs.R nimbleFunction Rexecution.R nimbleFunction compile.R nimbleFunction keywordProcessing.R nimbleList\_core.R types\_util.R types\_symbolTable.R types\_modelValues.R types\_modelValuesAccessor.R types\_modelVariableAccessor.R types\_nimbleFunctionList.R types\_nodeFxnVector.R types\_numericLists.R cppDefs\_utils.R cppDefs\_variables.R cppDefs\_core.R cppDefs\_namedObjects.R cppDefs\_ADtools.R cppDefs\_BUGSmodel.R cppDefs\_RCfunction.R cppDefs\_nimbleFunction.R cppDefs\_nimbleList.R cppDefs modelValues.R cppDefs cppProject.R cppDefs\_outputCppFromRparseTree.R cppInterfaces\_utils.R cppInterfaces models.R cppInterfaces modelValues.R cppInterfaces\_nimbleFunctions.R cppInterfaces\_otherTypes.R nimbleProject.R initializeModel.R parameterTransform.R CAR.R Laplace.R MCMC utils.R MCMC configuration.R MCMC build.R MCMC\_run.R MCMC\_samplers.R MCMC\_conjugacy.R MCMC\_autoBlock.R MCMC RJ.R MCMC WAIC.R MCEM build.R crossValidation.R BNP\_distributions.R BNP\_samplers.R NF\_utils.R miscFunctions.R makevars.R setNimbleInternalFunctions.R registration.R nimble-package.r QuadratureGrids.R zzz.R

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ADbreak

NIMBLE language function to break tracking of derivatives

# Description

This function is used in a method of a nimbleFunction that has derivatives enabled. It returns its value but breaks tracking of derivatives.

# Usage

ADbreak(x)

# Arguments

x scalar value

# Details

This function only works with scalars.

ADNimbleList

# Description

nimbleList definition for the type of nimbleList returned by nimDerivs.

# Usage

ADNimbleList

# Format

An object of class list of length 1.

# Fields

value The value of the function evaluated at the given input arguments. jacobian The Jacobian of the function evaluated at the given input arguments. hessian The Hessian of the function evaluated at the given input arguments.

## See Also

nimDerivs

ADproxyModelClass-class

create an ADproxyModelClass object

# Description

create an ADproxyModelClass object. For internal use.

#### Arguments

Rmodel The name of an uncompiled model

# Details

This is a proxy model for model\_AD. The class needs just enough pieces to be used like a model for purposes of nodeFunction compilation. The model will contain an ADproxyModel and then the nodeFunction setup code will extract it. The model interface will population the proxy model's CobjectInterface

# Author(s)

NIMBLE development team

any\_na

# Description

NIMBLE language functions that can be used in either compiled or uncompiled nimbleFunctions to detect if there are any NA or NaN values in a vector.

#### Usage

any\_na(x)

any\_nan(x)

# Arguments ×

vector of values

# Author(s)

NIMBLE Development Team

as.carAdjacency Convert CAR structural parameters to adjacency, weights, num format

# Description

This will convert alternate representations of CAR process structure into (adj, weights, num) form required by dcar\_normal.

#### Usage

```
as.carAdjacency(...)
```

#### Arguments

```
. . .
```

Either: a symmetric matrix of unnormalized weights, or two lists specifying adjacency indices and the corresponding unnormalized weights.

#### Details

Two alternate representations are handled:

A single matrix argument will be interpreted as a matrix of symmetric unnormalized weights.

Two lists will be interpreted as (the first) a list of numeric vectors specifying the adjacency (neighboring) indices of each CAR process component, and (the second) a list of numeric vectors giving the unnormalized weights for each of these neighboring relationships.

# as.carCM

## Author(s)

Daniel Turek

# See Also

CAR-Normal

as.carCM

Convert weights vector to parameters of dcar\_proper distributio

# Description

Convert weights vector to C and M parameters of dcar\_proper distribution

#### Usage

as.carCM(adj, weights, num)

# Arguments

adj	vector of indices of the adjacent locations (neighbors) of each spatial location. This is a sparse representation of the full adjacency matrix.
weights	vector of symmetric unnormalized weights associated with each pair of adjacent locations, of the same length as adj. This is a sparse representation of the full (unnormalized) weight matrix.
num	vector giving the number of neighbors of each spatial location, with length equal to the total number of locations.

#### Details

Given a symmetric matrix of unnormalized weights, this function will calculate corresponding values for the C and M arguments suitable for use in the dcar\_proper distribution. This function can be used to transition between usage of dcar\_normal and dcar\_proper, since dcar\_normal uses the adj, weights, and num arguments, while dcar\_proper requires adj, num, and also the C and M as returned by this function.

Here, C is a sparse vector representation of the row-normalized adjacency matrix, and M is a vector containing the conditional variance for each region. The resulting values of C and M are guaranteed to satisfy the symmetry constraint imposed on C and M, that  $M^{-1}C$  is symmetric, where M is a diagonal matrix and C is the row-normalized adjacency matrix.

#### Value

A named list with elements C and M. These may be used as the C and M arguments to the dcar\_proper distribution.

#### asRow

#### Author(s)

Daniel Turek

#### See Also

CAR-Normal, CAR-Proper

asRow

*Turn a numeric vector into a single-row or single-column matrix* 

# Description

Turns a numeric vector into a matrix that has 1 row or 1 column. Part of NIMBLE language.

#### Usage

asRow(x)

asCol(x)

# Arguments

x Numeric to be turned into a single row or column matrix

#### Details

In the NIMBLE language, some automatic determination of how to turn vectors into single-row or single-column matrices is done. For example, in A %\*% x, where A is a matrix and x a vector, x will be turned into a single-column matrix unless it is known at compile time that A is a single column, in which case x will be turned into a single-row matrix. However, if it is desired that x be turned into a single row but A cannot be determined at compile time to be a single column, then one can use A %\*% asRow(x) to force this conversion.

## Author(s)

Perry de Valpine

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autoBlock

# Description

The automated parameter blocking algorithm is no longer actively maintained. In some cases, it may not operate correctly with more recent system features and/or distributions.

# Usage

```
autoBlock(
   Rmodel,
   autoIt = 20000,
   run = list("all", "default"),
   setSeed = TRUE,
   verbose = FALSE,
   makePlots = FALSE,
   round = TRUE
)
```

# Arguments

Rmodel	A NIMBLE model object, created from nimbleModel.
autoIt	The number of MCMC iterations to run intermediate MCMC algorithms, through the course of the procedure. Default 20,000.
run	List of additional MCMC algorithms to compare against the automated blocking MCMC. These may be specified as: the character string 'all' to denote blocking all continuous-valued nodes; the character string 'default' to denote NIMBLE's default MCMC configuration; a named list element consisting of a quoted code block, which when executed returns an MCMC configuration object for comparison; a custom-specificed blocking scheme, specified as a named list element which itself is a list of character vectors, where each character vector specifies the nodes in a particular block. Default is c('all', 'default').
setSeed	Logical specificying whether to call set.seed(0) prior to beginning the blocking procedure. Default TRUE.
verbose	Logical specifying whether to output considerable details of the automated block procedure, through the course of execution. Default FALSE.
makePlots	Logical specifying whether to plot the hierarchical clustering dendrograms, through the course of execution. Default FALSE.
round	Logical specifying whether to round the final output results to two decimal places. Default TRUE.

## Details

Runs NIMBLE's automated blocking procedure for a given model object, to dynamically determine a blocking scheme of the continuous-valued model nodes. This blocking scheme is designed to produce efficient MCMC sampling (defined as number of effective samples generated per second of algorithm runtime). See Turek, et al (2015) for details of this algorithm. This also (optionally) compares this blocked MCMC against several static MCMC algorithms, including all univariate sampling, blocking of all continuous-valued nodes, NIMBLE's default MCMC configuration, and custom-specified blockings of parameters.

This method allows for fine-tuned usage of the automated blocking procedure. However, the main entry point to the automatic blocking procedure is intended to be through either buildMCMC(..., autoBlock = TRUE), or configureMCMC(..., autoBlock = TRUE).

# Value

Returns a named list containing elements:

- summary: A data frame containing a numerical summary of the performance of all MCMC algorithms (including that from automated blocking)
- autoGroups: A list specifying the parameter blockings converged on by the automated blocking procedure
- conf: A NIMBLE MCMC configuration object corresponding to the results of the automated blocking procedure

#### Author(s)

Daniel Turek

#### References

Turek, D., de Valpine, P., Paciorek, C., and Anderson-Bergman, C. (2015). Automated Parameter Blocking for Efficient Markov-Chain Monte Carlo Sampling. <arXiv:1503.05621>.

# See Also

configureMCMC buildMCMC

BUGSdeclClass-class BUGSdeclClass contains the information extracted from one BUGS declaration

# Description

BUGSdeclClass contains the information extracted from one BUGS declaration

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buildAGHQGrid

# Description

Create quadrature grid for use in AGHQuad methods in Nimble.

#### Arguments

d	Dimension of quadrature grid being requested.
nQuad	Number of quadrature nodes requested on build.

#### Details

This function is used by used by buildOneAGHQuad1D and buildOneAGHQuad create the quadrature grid using adaptive Gauss-Hermite quadrature. Handles single or multiple dimension grids and computes both grid locations and weights. Additionally, acts as a cache system to do transformations, and return marginalized log density.

Any of the input node vectors, when provided, will be processed using nodes <- model\$expandNodeNames(nodes), where nodes may be paramNodes, randomEffectsNodes, and so on. This step allows any of the inputs to include node-name-like syntax that might contain multiple nodes. For example, paramNodes = 'beta[1:10]' can be provided if there are actually 10 scalar parameters, 'beta[1]' through 'beta[10]'. The actual node names in the model will be determined by the exapndNodeNames step.

Available methods include

- buildAGHQ. Builds a adaptive Gauss-Hermite quadrature grid in d dimensions. Calls buildAGHQOne
  to build the one dimensional grid and then expands in each dimension. Some numerical issues occur in Eigen decomposition making the grid weights only accurate up to 35 quadrature
  nodes.
- Options to get internally cached values are getGridSize, getModeIndex for when there are an odd number of quadrature nodes, getLogDensity for the cached values, getAllNodes for the quadrature grids, getNodes for getting a single indexed nodes, getAllNodesTransformed for nodes transformed to the parameter scale, getNodesTransformed for a single transformed node, getAllWeights to get all quadrature weights, getWeights single indexed weight.
- transformGrid(cholNegHess, inner\_mode, method) transforms the grid using either cholesky trasnformations, as default, or spectral that makes use of the Eigen decomposition. For a single dimension transformGrid1D is used.
- As the log density is evaluated externally, it is saved via saveLogDens, which then is summed via quadSum.
- buildGrid builds the grid the initial time and is only run once in code. After, the user must choose to setGridSize to update the grid size.
- check. If TRUE (default), a warning is issued if paramNodes, randomEffectsNodes and/or calcNodes are provided but seek to have missing elements or unnecessary elements based on some default inspection of the model. If unnecessary warnings are emitted, simply set check=FALSE.

- innerOptimControl. A list of control parameters for the inner optimization of Laplace approximation using optim. See 'Details' of optim for further information.
- innerOptimMethod. Optimization method to be used in optim for the inner optimization. See 'Details' of optim. Currently optim in NIMBLE supports: "Nelder-Mead", "BFGS", "CG", and "L-BFGS-B". By default, method "CG" is used when marginalizing over a single (scalar) random effect, and "BFGS" is used for multiple random effects being jointly marginalized over.
- innerOptimStart. Choice of starting values for the inner optimization. This could be "last", "last.best", or a vector of user provided values. "last" means the most recent random effects values left in the model will be used. When finding the MLE, the most recent values will be the result of the most recent inner optimization for Laplace. "last.best" means the random effects values corresponding to the largest Laplace likelihood (from any call to the calcLaplace or calcLogLik method, including during an MLE search) will be used (even if it was not the most recent Laplace likelihood). By default, the initial random effects values will be used for inner optimization.
- outOptimControl. A list of control parameters for maximizing the Laplace log-likelihood using optim. See 'Details' of optim for further information.

# References

Golub, G. H. and Welsch, J. H. (1969). Calculation of Gauss Quadrature Rules. Mathematics of Computation 23 (106): 221-230.

Liu, Q. and Pierce, D. A. (1994). A Note on Gauss-Hermite Quadrature. Biometrika, 81(3) 624-629.

Jackel, P. (2005). A note on multivariate Gauss-Hermite quadrature. London: ABN-Amro. Re.

buildAuxiliaryFilter Placeholder for buildAuxiliaryFilter

#### Description

This function has been moved to the 'nimbleSMC' package.

# Usage

buildAuxiliaryFilter(...)

#### Arguments

... arguments

buildBootstrapFilter Placeholder for buildBootstrapFilter

# Description

This function has been moved to the 'nimbleSMC' package.

# Usage

```
buildBootstrapFilter(...)
```

# Arguments

arguments

buildEnsembleKF Placeholder for buildEnsembleKF

# Description

This function has been moved to the 'nimbleSMC' package.

### Usage

```
buildEnsembleKF(...)
```

# Arguments

... arguments

buildIteratedFilter2 Placeholder for buildIteratedFilter2

# Description

This function has been moved to the 'nimbleSMC' package.

#### Usage

buildIteratedFilter2(...)

#### Arguments

... arguments

buildLaplace

# Description

Build a Laplace or AGHQ approximation algorithm for a given NIMBLE model.

# Usage

```
buildLaplace(
 model,
 paramNodes,
  randomEffectsNodes,
  calcNodes,
  calcNodesOther,
  control = list()
)
buildAGHQ(
 model,
 nQuad = 1,
 paramNodes,
 randomEffectsNodes,
  calcNodes,
  calcNodesOther,
 control = list()
)
```

# Arguments

model	a NIMBLE model object, such as returned by nimbleModel. The model must have automatic derivatives (AD) turned on, e.g. by using buildDerivs=TRUE in nimbleModel.
paramNodes	a character vector of names of parameter nodes in the model; defaults are pro- vided by setupMargNodes. Alternatively, paramNodes can be a list in the format returned by setupMargNodes, in which case randomEffectsNodes, calcNodes, and calcNodesOther are not needed (and will be ignored).
randomEffectsNo	des
	a character vector of names of continuous unobserved (latent) nodes to marginal- ize (integrate) over using Laplace/AGHQ approximation; defaults are provided by setupMargNodes.
calcNodes	a character vector of names of nodes for calculating the integrand for Laplace/AGHQ approximation; defaults are provided by setupMargNodes. There may be deterministic nodes between paramNodes and calcNodes. These will be included in calculations automatically and thus do not need to be included in calcNodes (but there is no problem if they are).

calcNodesOther	a character vector of names of nodes for calculating terms in the log-likelihood that do not depend on any randomEffectsNodes, and thus are not part of the marginalization, but should be included for purposes of finding the MLE. This defaults to stochastic nodes that depend on paramNodes but are not part of and do not depend on randomEffectsNodes. There may be deterministic nodes between paramNodes and calcNodesOther. These will be included in calculations automatically and thus do not need to be included in calcNodesOther (but there is no problem if they are).
control	a named list for providing additional settings used in Laplace/AGHQ approxi- mation. See control section below. Most of these can be updated later with the 'updateSettings' method.
nQuad	number of quadrature points for AGHQ (in one dimension). Laplace approximation is AGHQ with 'nQuad=1'. Only odd numbers of nodes really make sense. Often only one or a few nodes can achieve high accuracy. A maximum

#### buildLaplace and buildAGHQ

buildLaplace creates an object that can run Laplace approximation for a given model or part of a model. buildAGHQ creates an object that can run adaptive Gauss-Hermite quadrature (AGHQ, sometimes called "adaptive Gaussian quadrature") for a given model or part of a model. Laplace approximation is AGHQ with one quadrature point, hence 'buildLaplace' simply calls 'buildAGHQ' with 'nQuad=1'. These methods approximate the integration over continuous random effects in a hierarchical model to calculate the (marginal) likelihood.

nodes will be (number of dimensions)^nQuad.

of 35 nodes is supported. Note that for multivariate quadratures, the number of

buildAGHQ and buildLaplace will by default (unless changed manually via 'control\$split') determine from the model which random effects can be integrated over (marginalized) independently. For example, in a GLMM with a grouping factor and an independent random effect intercept for each group, the random effects can be marginalized as a set of univariate approximations rather than one multivariate approximation. On the other hand, correlated or nested random effects would require multivariate marginalization.

Maximum likelihood estimation is available for Laplace approximation ('nQuad=1') with univariate or multivariate integrations. With 'nQuad > 1', maximum likelihood estimation is available only if all integrations are univariate (e.g., a set of univariate random effects). If there are multivariate integrations, these can be calculated at chosen input parameters but not maximized over parameters. For example, one can find the MLE based on Laplace approximation and then increase 'nQuad' (using the 'updateSettings' method below) to check on accuracy of the marginal log likelihood at the MLE.

Beware that quadrature will use 'nQuad^k' quadrature points, where 'k' is the dimension of each integration. Therefore quadrature for 'k' greater that 2 or 3 can be slow. As just noted, 'buildAGHQ' will determine independent dimensions of quadrature, so it is fine to have a set of univariate random effects, as these will each have k=1. Multivariate quadrature (k>1) is only necessary for nested, correlated, or otherwise dependent random effects.

The recommended way to find the maximum likelihood estimate and associated outputs is by calling runLaplace or runAGHQ. The input should be the compiled Laplace or AGHQ algorithm object. This would be produced by running compileNimble with input that is the result of buildLaplace or buildAGHQ.

For more granular control, see below for methods findMLE and summary. See function summaryLaplace for an easier way to call the summary method and obtain results that include node names. These steps are all done within runLaplace and runAGHQ.

The NIMBLE User Manual at r-nimble.org also contains an example of Laplace approximation.

#### How input nodes are processed

buildLaplace and buildAGHQ make good tries at deciding what to do with the input model and any (optional) of the node arguments. However, random effects (over which approximate integration will be done) can be written in models in multiple equivalent ways, and customized use cases may call for integrating over chosen parts of a model. Hence, one can take full charge of how different parts of the model will be used.

Any of the input node vectors, when provided, will be processed using nodes <- model\$expandNodeNames(nodes), where nodes may be paramNodes, randomEffectsNodes, and so on. This step allows any of the inputs to include node-name-like syntax that might contain multiple nodes. For example, paramNodes = 'beta[1:10]' can be provided if there are actually 10 scalar parameters, 'beta[1]' through 'beta[10]'. The actual node names in the model will be determined by the exapndNodeNames step.

In many (but not all) cases, one only needs to provide a NIMBLE model object and then the function will construct reasonable defaults necessary for Laplace approximation to marginalize over all continuous latent states (aka random effects) in a model. The default values for the four groups of nodes are obtained by calling setupMargNodes, whose arguments match those here (except for a few arguments which are taken from control list elements here).

setupMargNodes tries to give sensible defaults from any combination of paramNodes, randomEffectsNodes, calcNodes, and calcNodesOther that are provided. For example, if you provide only randomEffectsNodes (perhaps you want to marginalize over only some of the random effects in your model), setupMargNodes will try to determine appropriate choices for the others.

setupMargNodes also determines which integration dimensions are conditionally independent, i.e., which can be done separately from each other. For example, when possible, 10 univariate random effects will be split into 10 univariate integration problems rather than one 10-dimensional integration problem.

The defaults make general assumptions such as that randomEffectsNodes have paramNodes as parents. However, The steps for determining defaults are not simple, and it is possible that they will be refined in the future. It is also possible that they simply don't give what you want for a particular model. One example where they will not give desired results can occur when random effects have no prior parameters, such as 'N(0,1)' nodes that will be multiplied by a scale factor (e.g. sigma) and added to other explanatory terms in a model. Such nodes look like top-level parameters in terms of model structure, so you must provide a randomEffectsNodes argument to indicate which they are.

It can be helpful to call setupMargNodes directly to see exactly how nodes will be arranged for Laplace approximation. For example, you may want to verify the choice of randomEffectsNodes or get the order of parameters it has established to use for making sense of the MLE and results from the summary method. One can also call setupMargNodes, customize the returned list, and then provide that to buildLaplace as paramNodes. In that case, setupMargNodes will not be called (again) by buildLaplace.

If setupMargNodes is emitting an unnecessary warning, simply use control=list(check=FALSE).

#### buildLaplace

#### Managing parameter transformations that may be used internally

If any paramNodes (parameters) or randomEffectsNodes (random effects / latent states) have constraints on the range of valid values (because of the distribution they follow), they will be used on a transformed scale determined by parameterTransform. This means the Laplace approximation itself will be done on the transformed scale for random effects and finding the MLE will be done on the transformed scale for parameters. For parameters, prior distributions are not included in calculations, but they are used to determine valid parameter ranges and hence to set up any transformations. For example, if sigma is a standard deviation, you can declare it with a prior such as sigma ~ dhalfflat() to indicate that it must be greater than 0.

For default determination of when transformations are needed, all parameters must have a prior distribution simply to indicate the range of valid values. For a param p that has no constraint, a simple choice is  $p \sim dflat()$ .

#### Understanding inner and outer optimizations

Note that there are two numerical optimizations when finding maximum likelihood estimates with a Laplace or (1D) AGHQ algorithm: (1) maximizing the joint log-likelihood of random effects and data given a parameter value to construct the approximation to the marginal log-likelihood at the given parameter value; (2) maximizing the approximation to the marginal log-likelihood over the parameters. In what follows, the prefix 'inner' refers to optimization (1) and 'outer' refers to optimization (2). Currently both optimizations default to using method "nlminb". However, one can use other optimizers or simply run optimization (2) manually from R; see the example below. In some problems, choice of inner and/or outer optimizer can make a big difference for obtaining accurate results, especially for standard errors. Hence it is worth experimenting if one is in doubt.

#### control list arguments

The control list allows additional settings to be made using named elements of the list. Most (or all) of these can be updated later using the 'updateSettings' method. Supported elements include:

- split. If TRUE (default), randomEffectsNodes will be split into conditionally independent sets if possible. This facilitates more efficient Laplace or AGHQ approximation because each conditionally independent set can be marginalized independently. If FALSE, randomEffectsNodes will be handled as one multivariate block, with one multivariate approximation. If split is a numeric vector, randomEffectsNodes will be split by calling split(randomEffectsNodes, control\$split). The last option allows arbitrary control over how randomEffectsNodes are blocked.
- check. If TRUE (default), a warning is issued if paramNodes, randomEffectsNodes and/or calcNodes are provided but seem to have missing or unnecessary elements based on some default inspections of the model. If unnecessary warnings are emitted, simply set check=FALSE.
- innerOptimControl. A list (either an R list or a 'optimControlNimbleList') of control parameters for the inner optimization of Laplace approximation using nimOptim. See 'Details' of nimOptim for further information. Default is 'nimOptimDefaultControl()'.
- innerOptimMethod. Optimization method to be used in nimOptim for the inner optimization. See 'Details' of nimOptim. Currently nimOptim in NIMBLE supports: "Nelder-Mead"", "BFGS", "CG", "L-BFGS-B", "nlminb", "bobyqa", and user-provided optimizers. By default, method "nlminb" is used for both univariate and multivariate cases. For "nlminb", "bobyqa",

or user-provided optimizers, only a subset of elements of the innerOptimControlList are supported. (Note that control over the outer optimization method is available as an argument to 'findMLE'). Choice of optimizers can be important and so can be worth exploring.

- innerOptimStart. Method for determining starting values for the inner optimization. Options are:
  - "last.best" (default): use optimized random effects values corresponding to the best outer optimization (i.e. the largest marginal log likelihood value) so far for each conditionally independent part of the approximation;
  - "last": use the result of the last inner optimization;
  - "zero": use all zeros;
  - "constant": always use the same values, determined by innerOptimStartValues;
  - "random": randomly draw new starting values from the model (i.e., from the prior);
  - "model": use values for random effects stored in the model, which are determined from the first call.

Note that "model" and "zero" are shorthand for "constant" with particular choices of innerOptimStartValues. Note that "last" and "last.best" require a choice for the very first values, which will come from innerOptimStartValues. The default is innerOptimStart="zero" and may change in the future.

- innerOptimStartValues. Values for some of innerOptimStart approaches. If a scalar is provided, that value is used for all elements of random effects for each conditionally independent set. If a vector is provided, it must be the length of \*all\* random effects. If these are named (by node names), the names will be used to split them correctly among each conditionally independent set of random effects. If they are not named, it is not always obvious what the order should be because it may depend on the conditionally independent sets of random effects. It should match the order of names returned as part of 'summaryLaplace'.
- innerOptimWarning. If FALSE (default), do not emit warnings from the inner optimization. Optimization methods may sometimes emit a warning such as for bad parameter values encountered during the optimization search. Often, a method can recover and still find the optimum. In the approximations here, sometimes the inner optimization search can fail entirely, yet the outer optimization see this as one failed parameter value and can recover. Hence, it is often desirable to silence warnings from the inner optimizer, and this is done by default. Set innerOptimWarning=TRUE to see all warnings.
- useInnerCache. If TRUE (default), use caching system for efficiency of inner optimizations. The caching system records one set of previous parameters and uses the corresponding results if those parameters are used again (e.g., in a gradient call). This should generally not be modified.
- outerOptimMethod. Optimization method to be used in nimOptim for the outer optimization. See 'Details' of nimOptim. Currently nimOptim in NIMBLE supports: "Nelder-Mead"", "BFGS", "CG", "L-BFGS-B", "nlminb", "bobyqa", and user-provided optimizers. By default, method "nlminb" is used for both univariate and multivariate cases, although some problems may benefit from other choices. For "nlminb", "bobyqa", or user-provided optimizers, only a subset of elements of the innerOptimControlList are supported. (Note that control over the outer optimization method is available as an argument to 'findMLE'). Choice of optimizers can be important and so can be worth exploring.
- outerOptimControl. A list of control parameters for maximizing the Laplace log-likelihood using nimOptim. See 'Details' of nimOptim for further information.

- computeMethod. There are three approaches available for internal details of how the approximations, and specifically derivatives involved in their calculation, are handled. These are labeled simply 1, 2, and 3, and the default is 2. The relative performance of the methods will depend on the specific model. Users wanting to explore efficiency can try switching from method 2 (default) to methods 1 or 3 and comparing performance. The first Laplace approximation with each method will be (much) slower than subsequent Laplace approximations. Further details are not provided at this time.
- gridType (relevant only nQuad>1). For multivariate AGHQ, a grid must be constructed based on the Hessian at the inner mode. Options include "cholesky" (default) and "spectral" (i.e., eigenvectors and eigenvalues) for the corresponding matrix decompositions on which the grid can be based.
- # end itemize

#### Available methods

The object returned by buildLaplace or buildAGHQ is a nimbleFunction object with numerous methods (functions). Here these are described in three tiers of user relevance.

# Most useful methods

The most relevant methods to a user are:

 calcLogLik(p, trans=FALSE). Calculate the approximation to the marginal log-likelihood function at parameter value p, which (if trans is FALSE) should match the order of paramNodes. For any non-scalar nodes in paramNodes, the order within the node is column-major. The order of names can be obtained from method getNodeNamesVec(TRUE). Return value is the scalar (approximate, marginal) log likelihood.

If trans is TRUE, then p is the vector of parameters on the transformed scale, if any, described above. In this case, the parameters on the original scale (as the model was written) will be determined by calling the method pInverseTransform(p). Note that the length of the parameter vector on the transformed scale might not be the same as on the original scale (because some constraints of non-scalar parameters result in fewer free transformed parameters than original parameters).

- calcLaplace(p, trans). This is the same as calcLogLik but requires that the approximation be Laplace (i.e nQuad is 1), and results in an error otherwise.
- findMLE(pStart, hessian). Find the maximum likelihood estimates of parameters using the approximated marginal likelihood. This can be used if nQuad is 1 (Laplace case) or if nQuad>1 and all marginalizations involve only univariate random effects. Arguments are pStart: initial parameter values (defaults to parameter values currently in the model); and hessian: whether to calculate and return the Hessian matrix (defaults to TRUE, which is required for subsequent use of summary method). Second derivatives in the Hessian are determined by finite differences of the gradients obtained by automatic differentiation (AD). Return value is a nimbleList of type optimResultNimbleList, similar to what is returned by R's optim. See help(nimOptim). Note that parameters (par) are returned for the natural parameters, i.e. how they are defined in the model. But the hessian, if requested, is computed for the parameters as transformed for optimization if necessary. Hence one must be careful interpreting 'hessian' if any parameters have constraints, and the safest next step is to use the summary method or summaryLaplace function.

• summary(MLEoutput, originalScale, randomEffectsStdError, jointCovariance). Summarize the maximum likelihood estimation results, given object MLEoutput that was returned by findMLE. The summary can include a covariance matrix for the parameters, the random effects, or both), and these can be returned on the original parameter scale or on the (potentially) transformed scale(s) used in estimation. It is often preferred instead to call function (not method) 'summaryLaplace' because this will attach parameter and random effects names (i.e., node names) to the results.

In more detail, summary accepts the following optional arguments:

- originalScale. Logical. If TRUE, the function returns results on the original scale(s) of
  parameters and random effects; otherwise, it returns results on the transformed scale(s).
  If there are no constraints, the two scales are identical. Defaults to TRUE.
- randomEffectsStdError. Logical. If TRUE, standard errors of random effects will be calculated. Defaults to TRUE.
- jointCovariance. Logical. If TRUE, the joint variance-covariance matrix of the parameters and the random effects will be returned. If FALSE, the variance-covariance matrix of the parameters will be returned. Defaults to FALSE.

The object returned by summary is an AGHQuad\_summary nimbleList with elements:

- params. A nimbleList that contains estimates and standard errors of parameters (on the original or transformed scale, as chosen by originalScale).
- randomEffects. A nimbleList that contains estimates of random effects and, if requested (randomEffectsStdError=TRUE) their standard errors, on original or transformed scale. Standard errors are calculated following the generalized delta method of Kass and Steffey (1989).
- vcov. If requested (i.e. jointCovariance=TRUE), the joint variance-covariance matrix of the parameters and random effects, on original or transformed scale. If jointCovariance=FALSE, the covariance matrix of the parameters, on original or transformed scale.
- scale. "original" or "transformed", the scale on which results were requested.

# Methods for more advanced uses

Additional methods to access or control more details of the Laplace/AGHQ approximation include:

- updateSettings. This provides a single function through which many of the settings described above (mostly for the control list) can be later changed. Options that can be changed include: innerOptimMethod, innerOptimStart, innerOptimStartValues, useInnerCache, nQuad, gridType, innerOptimControl, outerOptimMethod, outerOptimControl, and computeMethod. For innerOptimStart, method "zero" cannot be specified but can be achieved by choosing method "constant" with innerOptimStartValues=0. Only provided options will be modified. The exceptions are innerOptimControl, outerOptimControl, which are replaced only when replace\_innerOptimControl=TRUE or replace\_outerOptimControl=TRUE, respectively.
- getNodeNamesVec(returnParams). Return a vector (>1) of names of parameters/random effects nodes, according to returnParams = TRUE/FALSE. Use this if there is more than one node.
- getNodeNameSingle(returnParams). Return the name of a single parameter/random effect node, according to returnParams = TRUE/FALSE. Use this if there is only one node.

#### buildLaplace

- checkInnerConvergence(message). Checks whether all internal optimizers converged. Returns a zero if everything converged and one otherwise. If message = TRUE, it will print more details about convergence for each conditionally independent set.
- gr\_logLik(p, trans). Gradient of the (approximated) marginal log-likelihood at parameter value p. Argument trans is similar to that in calcLaplace. If there are multiple parameters, the vector p is given in the order of parameter names returned by getNodeNamesVec(returnParams=TRUE).
- gr\_Laplace(p, trans). This is the same as gr\_logLik.
- otherLogLik(p). Calculate the calcNodesOther nodes, which returns the log-likelihood of the parts of the model that are not included in the Laplace or AGHQ approximation.
- gr\_otherLogLik(p). Gradient (vector of derivatives with respect to each parameter) of otherLogLik(p). Results should match gr\_otherLogLik\_internal(p) but may be more efficient after the first call.

#### Internal or development methods

Some methods are included for calculating the (approximate) marginal log posterior density by including the prior distribution of the parameters. This is useful for finding the maximum a posteriori probability (MAP) estimate. Currently these are provided for point calculations without estimation methods.

- calcPrior\_p(p). Log density of prior distribution.
- calcPrior\_pTransformed(pTransform). Log density of prior distribution on transformed scale, includes the Jacobian.
- calcPostLogDens(p). Marginal log posterior density in terms of the parameter p.
- calcPostLogDens\_pTransformed (pTransform). Marginal log posterior density in terms of the transformed parameter, which includes the Jacobian transformation.
- gr\_postLogDens\_pTransformed(pTransform). Graident of marginal log posterior density on the transformed scale. Other available options that are used in the derivative for more flexible include logDetJacobian(pTransform) and gr\_logDeJacobian(pTransform), as well as gr\_prior(p).

Finally, methods that are primarily for internal use by other methods include:

- gr\_logLik\_pTransformed. Gradient of the Laplace approximation (calcLogLik\_pTransformed(pTransform)) at transformed (unconstrained) parameter value pTransform.
- pInverseTransform(pTransform). Back-transform the transformed parameter value pTransform to original scale.
- derivs\_pInverseTransform(pTransform, order). Derivatives of the back-transformation (i.e. inverse of parameter transformation) with respect to transformed parameters at pTransform. Derivative order is given by order (any of 0, 1, and/or 2).
- reInverseTransform(reTrans). Back-transform the transformed random effects value reTrans to original scale.
- derivs\_reInverseTransform(reTrans, order). Derivatives of the back-transformation (i.e. inverse of random effects transformation) with respect to transformed random effects at reTrans. Derivative order is given by order (any of 0, 1, and/or 2).

- optimRandomEffects(pTransform). Calculate the optimized random effects given transformed parameter value pTransform. The optimized random effects are the mode of the conditional distribution of random effects given data at parameters pTransform, i.e. the calculation of calcNodes.
- inverse\_negHess(p, reTransform). Calculate the inverse of the negative Hessian matrix of the joint (parameters and random effects) log-likelihood with respect to transformed random effects, evaluated at parameter value p and transformed random effects reTransform.
- hess\_logLik\_wrt\_p\_wrt\_re(p, reTransform). Calculate the Hessian matrix of the joint log-likelihood with respect to parameters and transformed random effects, evaluated at parameter value p and transformed random effects reTransform.
- one\_time\_fixes(). Users never need to run this. Is is called when necessary internally to fix
  dimensionality issues if there is only one parameter in the model.
- calcLogLik\_pTransformed(pTransform). Laplace approximation at transformed (unconstrained) parameter value pTransform. To make maximizing the Laplace likelihood unconstrained, an automated transformation via parameterTransform is performed on any parameters with constraints indicated by their priors (even though the prior probabilities are not used).
- gr\_otherLogLik\_internal(p). Gradient (vector of derivatives with respect to each parameter) of otherLogLik(p). This is obtained using automatic differentiation (AD) with single-taping. First call will always be slower than later calls.
- cache\_outer\_logLik(logLikVal). Save the marginal log likelihood value to the inner Laplace mariginlization functions to track the outer maximum internally.
- reset\_outer\_inner\_logLik(). Reset the internal saved maximum marginal log likelihood.
- get\_inner\_cholesky(atOuterMode = integer(0, default = 0)). Returns the cholesky of the negative Hessian with respect to the random effects. If atOuterMode = 1 then returns the value at the overall best marginal likelihood value, otherwise atOuterMode = 0 returns the last.
- get\_inner\_mode(atOuterMode = integer(0, default = 0)). Returns the mode of the random effects for either the last call to the innner quadrature functions (atOuterMode = 0), or the last best value for the marginal log likelihood, atOuterMode = 1.

#### Author(s)

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#### References

Kass, R. and Steffey, D. (1989). Approximate Bayesian inference in conditionally independent hierarchical models (parametric empirical Bayes models). *Journal of the American Statistical Association*, 84(407), 717-726.

Liu, Q. and Pierce, D. A. (1994). A Note on Gauss-Hermite Quadrature. *Biometrika*, 81(3) 624-629.

Jackel, P. (2005). A note on multivariate Gauss-Hermite quadrature. London: ABN-Amro. Re.

Skaug, H. and Fournier, D. (2006). Automatic approximation of the marginal likelihood in non-Gaussian hierarchical models. *Computational Statistics & Data Analysis*, 56, 699-709.

# buildLiuWestFilter

#### Examples

```
pumpCode <- nimbleCode({</pre>
  for (i in 1:N){
    theta[i] ~ dgamma(alpha, beta)
    lambda[i] <- theta[i] * t[i]</pre>
    x[i] ~ dpois(lambda[i])
  }
  alpha ~ dexp(1.0)
  beta ~ dgamma(0.1, 1.0)
})
pumpConsts <- list(N = 10, t = c(94.3, 15.7, 62.9, 126, 5.24, 31.4, 1.05, 1.05, 2.1, 10.5))
pumpData <- list(x = c(5, 1, 5, 14, 3, 19, 1, 1, 4, 22))</pre>
pumpInits <- list(alpha = 0.1, beta = 0.1, theta = rep(0.1, pumpConsts$N))</pre>
pump <- nimbleModel(code = pumpCode, name = "pump", constants = pumpConsts,</pre>
                     data = pumpData, inits = pumpInits, buildDerivs = TRUE)
# Build Laplace approximation
pumpLaplace <- buildLaplace(pump)</pre>
## Not run:
# Compile the model
Cpump <- compileNimble(pump)</pre>
CpumpLaplace <- compileNimble(pumpLaplace, project = pump)</pre>
# Calculate MLEs of parameters
MLEres <- CpumpLaplace$findMLE()</pre>
# Calculate estimates and standard errors for parameters and random effects on original scale
allres <- CpumpLaplace$summary(MLEres, randomEffectsStdError = TRUE)</pre>
# Change the settings and also illustrate runLaplace
CpumpLaplace$updateSettings(innerOptimControl = list(maxit = 1000),
                              replace_innerOptimControl)
newres <- runLaplace(CpumpLaplace)</pre>
# Illustrate use of the component log likelihood and gradient functions to
# run an optimizer manually from R.
# Use nlminb to find MLEs
MLEres.manual <- nlminb(c(0.1, 0.1),</pre>
                         function(x) -CpumpLaplace$calcLogLik(x),
                         function(x) -CpumpLaplace$gr_Laplace(x))
## End(Not run)
```

buildLiuWestFilter *Placeholder for buildLiuWestFilter* 

# Description

This function has been moved to the 'nimbleSMC' package.

#### Usage

buildLiuWestFilter(...)

#### Arguments

... arguments

buildMacro

EXPERIMENTAL: Turn a function into a model macro

#### Description

A model macro expands one line of code in a nimbleModel into one or more new lines. This supports compact programming by defining re-usable modules. buildMacro takes as input a function that constructs new lines of model code from the original line of code. It returns a function suitable for internal use by nimbleModel that arranges arguments for input function. Macros are an experimental feature and are available only after setting nimbleOptions(enableMacros = TRUE).

#### Usage

buildMacro(fun, use3pieces = TRUE, unpackArgs = TRUE)

#### Arguments

fun	A function written to construct new lines of model code (see below).
use3pieces	logical indicating whether the arguments from the input line be split into pieces for the LHS (left-hand side), RHS (right-hand side, possibly further split depending on unpackArgs), and stoch (TRUE if the line uses a ~ and FALSE otherwise). (default = TRUE)
unpackArgs	logical indicating whether arguments be passed as a list (FALSE) or as separate arguments (TRUE). (default = TRUE)

#### **Details**

The arguments use3pieces and unpackArgs indicate how fun expects to have arguments arranged from an input line of code (processed by nimbleModel).

Consider the defaults use3pieces = TRUE and unpackArgs = TRUE, for a macro called macro1. In this case, the line of model code x ~ macro1(arg1 = z[1:10], arg2 = "hello") will be passed to fun as fun(stoch = TRUE, LHS = x, arg1 = z[1:10], arg2 = "hello").

If use3pieces = TRUE but unpackArgs = FALSE, then the RHS will be passed as is, without unpacking its arguments into separate arguments to fun. In this case, x ~ macro1(arg1 = z[1:10], arg2 = "hello") will be passed to fun as fun(stoch = TRUE, LHS = x, RHS = macro1(arg1 = z[1:10], arg2 = "hello")).

If use3pieces = FALSE and unpackArgs = FALSE, the entire line of code is passed as a single object. In this case,  $x \sim macro1(arg1 = z[1:10], arg2 = "hello")$  will be passed to fun as fun( $x \sim macro1(arg1 = z[1:10], arg2 = macro1(arg1 = z[1:10])$ 

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#### buildMacro

macro1(arg1 = z[1:10], arg2 = "hello")). It is also possible in this case to pass a macro without using a ~ or <-. For example, the line macro1(arg1 = z[1:10], arg2 = "hello") will be passed to fun as fun(macro1(arg1 = z[1:10], arg2 = "hello")).

If use3pieces = FALSE and unpackArgs = TRUE, it won't make sense to anticipate a declaration using ~ or <-. Instead, arguments from an arbitrary call will be passed as separate arguments. For example, the line macro1(arg1 = z[1:10], arg2 = "hello") will be passed to fun as fun(arg1 = z[1:10], arg2 = "hello").

In addition, the final two arguments of fun must be called modelInfo and .env respectively.

During macro processing, nimbleModel passes a named list to the modelInfo argument of fun containing, among other things, elements called constants and dimensions. Macro developers can modify these two elements (for example, to add a new constant needed for a macro) and these changes will be reflected in the final model object. Note that currently it is not possible for a macro to modify the data. Furthermore, if your macro add a new element to the constants that nimbleModel then moves to the data, this new data will not be retained in the final model object and thus will not be usable.

nimbleModel passes the R environment from which nimbleModel was called to the .env argument.

The fun function must return a named list with two elements: code, the replacement code, and modelInfo, the modelInfo list described above. modelInfo must be in the output even if the macro does not modify it.

It is extremely useful to be familiar with processing R code as an object to write fun correctly. Functions such as substitute and as.name (e.g. as.name('~')), quote, parse and deparse are particularly handy.

Multiple lines of new code should be contained in {}. Extra curly braces are not a problem. See example 2.

Macro expansion is done recursively: One macro can return code that invokes another macro.

#### Value

A list of class model\_macro with one element called process, which contains the macro function suitable for use by nimbleModel.

#### Examples

```
nimbleOptions(enableMacros = TRUE)
nimbleOptions(enableMacroComments = FALSE)
nimbleOptions(verbose = FALSE)
## Example 1: Say one is tired of writing "for" loops.
## This macro will generate a "for" loop with dnorm declarations
all_dnorm <- buildMacro(
    function(stoch, LHS, RHSvar, start, end, sd = 1, modelInfo, .env) {
        newCode <- substitute(
            for(i in START:END) {
                LHS[i] ~ dnorm(RHSvar[i], SD)
            },
            list(START = start,
                END = end,
            LHS = LHS,</pre>
```

```
RHSvar = RHSvar,
                  SD = sd)
        list(code = newCode)
    },
    use3pieces = TRUE,
    unpackArgs = TRUE
)
model1 <- nimbleModel(</pre>
    nimbleCode(
    {
        ## Create a "for" loop of dnorm declarations by invoking the macro
        x \sim all_dnorm(mu, start = 1, end = 10)
    }
    ))
## show code from expansion of macro
model1$getCode()
## The result should be:
## {
##
       for (i in 1:10) {
##
           x[i] ~ dnorm(mu[i], 1)
##
       }
## }
## Example 2: Say one is tired of writing priors.
## This macro will generate a set of priors in one statement
flat_normal_priors <- buildMacro(</pre>
    function(..., modelInfo, .env) {
        allVars <- list(...)</pre>
        priorDeclarations <- lapply(allVars,</pre>
                                      function(x)
                                          substitute(VAR ~ dnorm(0, sd = 1000),
                                                      list(VAR = x)))
        newCode <- quote({})</pre>
        newCode[2:(length(allVars)+1)] <- priorDeclarations</pre>
        list(code = newCode)
    },
    use3pieces = FALSE,
    unpackArgs = TRUE
)
model2 <- nimbleModel(</pre>
    nimbleCode(
    {
        flat_normal_priors(mu, beta, gamma)
    }
    ))
## show code from expansion of macro
model2$getCode()
## The result should be:
## {
```

```
##
      mu \sim dnorm(0, sd = 1000)
##
      beta ~ dnorm(0, sd = 1000)
##
      gamma ~ dnorm(0, sd = 1000)
## }
## Example 3: Macro that modifies constants
new_constant <- buildMacro(</pre>
   function(stoch, LHS, RHS, modelInfo, .env) {
     # number of elements
     n <- as.numeric(length(modelInfo$constants[[deparse(LHS)]]))</pre>
     code <- substitute({</pre>
       for (i in 1:N){
         L[i] ~ dnorm(mu[i], 1)
       }
     }, list(L = LHS, N = n))
     # Add a new constant mu
     modelInfo$constants$mu <- rnorm(n, 0, 1)</pre>
     list(code = code, modelInfo = modelInfo)
   },
   use3pieces = TRUE,
   unpackArgs = TRUE
)
const <- list(y = rnorm(10))</pre>
code <- nimbleCode({</pre>
y ~ new_constant()
})
mod <- nimbleModel(code = code, constants=const)</pre>
mod$getCode()
mod$getConstants() # new constant is here
```

```
buildMCEM
```

Builds an MCEM algorithm for a given NIMBLE model

# Description

Takes a NIMBLE model (with some missing data, aka random effects or latent state nodes) and builds a Monte Carlo Expectation Maximization (MCEM) algorithm for maximum likelihood estimation. The user can specify which latent nodes are to be integrated out in the E-Step, or default choices will be made based on model structure. All other stochastic non-data nodes will be maximized over. The E-step is done with a sample from a nimble MCMC algorithm. The M-step is done by a call to optim.

#### Usage

buildMCEM(
 model,

```
paramNodes,
latentNodes,
calcNodes,
calcNodesOther,
control = list(),
...
```

)

# Arguments

model	a NIMBLE model object, either compiled or uncompiled.
paramNodes	a character vector of names of parameter nodes in the model; defaults are pro- vided by setupMargNodes. Alternatively, paramNodes can be a list in the for- mat returned by setupMargNodes, in which case latentNodes, calcNodes, and calcNodesOther are not needed (and will be ignored).
latentNodes	a character vector of names of unobserved (latent) nodes to marginalize (sum or integrate) over; defaults are provided by setupMargNodes (as the randomEffectsNodes in its return list).
calcNodes	a character vector of names of nodes for calculating components of the full-data likelihood that involve latentNodes; defaults are provided by setupMargNodes. There may be deterministic nodes between paramNodes and calcNodes. These will be included in calculations automatically and thus do not need to be in- cluded in calcNodes (but there is no problem if they are).
calcNodesOther	a character vector of names of nodes for calculating terms in the log-likelihood that do not depend on any latentNodes, and thus are not part of the marginal- ization, but should be included for purposes of finding the MLE. This defaults to stochastic nodes that depend on paramNodes but are not part of and do not de- pend on latentNodes. There may be deterministic nodes between paramNodes and calcNodesOther. These will be included in calculations automatically and thus do not need to be included in calcNodesOther (but there is no problem if they are).
control	a named list for providing additional settings used in MCEM. See control sec- tion below.
	provided only as a means of checking if a user is using the deprecated interface to 'buildMCEM' in nimble versions $< 1.2.0$ .

# Details

buildMCEM is a nimbleFunction that creates an MCEM algorithm for a model and choices (perhaps default) of nodes in different roles in the model. The MCEM can then be compiled for fast execution with a compiled model.

Note that buildMCEM was re-written for nimble version 1.2.0 and is not backward-compatible with previous versions. The new version is considered to be in beta testing.

Denote data by Y, latent states (or missing data) by X, and parameters by T. MCEM works by the following steps, starting from some T:

1. Draw a sample of size M from P(X | Y, T) using MCMC.

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- 2. Update T to be the maximizer of  $E[\log P(X, Y | T)]$  where the expectation is approximated as a Monte Carlo average over the sample from step(1)
- 3. Repeat until converged.

The default version of MCEM is the ascent-based MCEM of Caffo et al. (2015). This attempts to update M when necessary to ensure that step 2 really moves uphill given that it is maximizing a Monte Carlo approximation and could accidently move downhill on the real surface of interest due to Monte Carlo error. The main tuning parameters include alpha, beta, gamma, Mfactor, C, and tol (tolerance).

If the model supports derivatives via nimble's automatic differentiation (AD) (and buildDerivs=TRUE in nimbleModel), the maximization step can use gradients from AD. You must manually set useDerivs=FALSE in the control list if derivatives aren't supported or if you don't want to use them.

In the ascent-based method, after maximization in step 2, the Monte Carlo standard error of the uphill movement is estimated. If the standardized uphill step is bigger than 0 with Type I error rate alpha, the iteration is accepted and the algorithm continues. Otherwise, it is not certain that step 2 really moved uphill due to Monte Carlo error, so the MCMC sample size M is incremented by a fixed factor (e.g. 0.33 or 0.5, called Mfactor in the control list), the additional samples are added by continuing step 1, and step 2 is tried again. If the Monte Carlo noise still overwhelms the magnitude of uphill movement, the sample size is increased again, and so on. alpha should be between 0 and 0.5. A larger value than usually used for inference is recommended so that there is an easy threshold to determine uphill movement, which avoids increasing M prematurely. M will never be increased above maxM.

Convergence is determined in a similar way. After a definite move uphill, we determine if the uphill increment is less than tol, with Type I error rate gamma. (But if M hits a maximum value, the convergence criterion changes. See below.)

beta is used to help set M to a minimal level based on previous iterations. This is a desired Type II error rate, assuming an uphill move and standard error based on the previous iteration. Set adjustM=FALSE in the control list if you don't want this behavior.

There are some additional controls on convergence for practical purposes. Set C in the control list to be the number of times the convergence criterion mut be satisfied in order to actually stop. E.g setting C=2 means there will always be a restart after the first convergence.

One problem that can occur with ascent-based MCEM is that the final iteration can be very slow if M must become very large to satisfy the convergence criterion. Indeed, if the algorithm starts near the MLE, this can occur. Set maxM in the control list to set the MCMC sample size that should never be exceeded.

If M==maxM, a softer convergence criterion is used. This second convergence criterion is to stop if we can't be sure we moved uphill using Type I error rate delta. This is a soft criterion because for small delta, Type II errors will be common (e.g. if we really did move uphill but can't be sure from the Monte Carlo sample), allowing the algorithm to terminate. One can continue the algorithm from where it stopped, so it is helpful to not have it get stuck when having a very hard time with the first (stricter) convergence criterion.

All of alpha, beta, delta, and gamma are utilized based on asymptotic arguments but in practice must be chosen heuristically. In other words, their theoretical basis does not exactly yield practical advice on good choices for efficiency and accuracy, so some trial and error will be needed.

It can also be helpful to set a minimum and maximum of allowed iterations (of steps 1 and 2 above). Setting minIter>1 in the control list can sometimes help avoid a false convergence on the

first iteration by forcing at least one more iteration. Setting maxIter provides a failsafe on a stuck run.

If you don't want the ascent-based method at all and simply want to run a set of iterations, set ascent=FALSE in the control list. This will use the second (softer) convergence criterion.

Parameters to be maximized will by default be handled in an unconstrained parameter space, transformed if necessary by a parameterTransform object. In that case, the default optim method will be "BFGS" and can can be changed by setting optimMehod in the control list. Set useTransform=FALSE in the control list if you don't want the parameters transformed. In that case the default optimMethod will be "L-BFGS-B" if there are any actual constraints, and you can provide a list of boxConstraints in the control list. (Constraints may be determined by priors written in the model for parameters, even though their priors play no other role in MLE. E.g. sigma ~ halfflat() indicates sigma > 0).

Most of the control list elements can be overridden when calling the findMLE method. The findMLE argument continue=TRUE results in attempting to continue the algorithm where the previous call finished, including whatever settings were in use.

See setupMargNodes (which is called with the given arguments for paramNodes, calcNodes, and calcNodesOther; and with allowDiscreteLatent=TRUE, randomEffectsNodes=latentNodes, and check=check) for more about how the different groups of nodes are determined. In general, you can provide none, one, or more of the different kinds of nodes and setupMargNodes will try to determine the others in a sensible way. However, note that this cannot work for all ways of writing a model. One key example is that if random (latent) nodes are written as top-level nodes (e.g. following N(0,1)), they appear structurally to be parameters and you must tell buildMCEM that they are latentNodes. The various "Nodes" arguments will all be passed through model\$expandNodeNames, allowing for example simply "x" to be provided when there are many nodes within "x".

Estimating the Monte Carlo standard error of the uphill step is not trivial because the sample was obtained by MCMC and so likely is autocorrelated. This is done by calling whatever function in R's global environment is called "MCEM\_mcse", which is required to take two arguments: samples (which will be a vector of the differences in log(P(Y, X | T)) between the new and old values of T, across the sample of X) and m, the sample size. It must return an estimate of the standard error of the mean of the sample. NIMBLE provides a default version (exported from the package namespace), which calls mcmcse::mcse with method "obm". Simply provide a different function with this name in your R session to override NIMBLE's default.

# **Control list details**

The control list accepts the following named elements:

- initM initial MCMC sample size, M. Default=1000.
- Mfactor Factor by which to increase MCMC sample size when step 2 results in noise overwhelming the uphill movement. The new M will be 1+Mfactor)\*M (rounded up). Mfactor is 1/k of Caffo et al. (2015). Default=1/3.
- maxM Maximum allowed value of M (see above). Default=initM\*20.
- burnin Number of burn-in iterations for the MCMC in step 1. Note that the initial states of one MCMC will be the last states from the previous MCMC, so they will often be good initial values after multiple iterations. Default=500.
- thin Thinning interval for the MCMC in step 1. Default=1.

- alpha Type I error rate for determining when step 2 has moved uphill. See above. Default=0.25.
- beta Used for determining a minimal value of \$M\$ based on previous iteration, if adjustM is TRUE. beta is a desired Type II error rate for determining uphill moves. Default=0.25.
- delta Type I error rate for the soft convergence approach (second approach above). Default=0.25.
- gamma Type I error rate for determining when step 2 has moved less than tol uphill, in which case ascent-based convergence is achieved (first approach above). Default=0.05.
- buffer A small amount added to lower box constraints and substracted from upper box constraints for all parameters, relevant only if useTransform=FALSE and some parameters do have boxConstraints set or have bounds that can be determined from the model. Default=1e-6.
- tol Ascent-based convergence tolerance. Default=0.001.
- ascent Logical to determine whether to use the ascent-based method of Caffo et al. De-fault=TRUE.
- C Number of convergences required to actually stop the algorithm. Default = 1.
- maxIter Maximum number of MCEM iterations to run.
- minIter Minimum number of MCEM iterations to run.
- adjustM Logical indicating whether to see if M needs to be increased based on statistical power argument in each iteration (using beta). Default=TRUE.
- verbose Logical indicating whether verbose output is desired. Default=TRUE.
- MCMCprogressBar Logical indicating whether MCMC progress bars should be shown for every iteration of step 1. This argument is passed to configureMCMC, or to config if provided. Default=TRUE.
- derivsDelta If AD derivatives are not used, then the method vcov must use finite difference derivatives to implement the method of Louis (1982). The finite differences will be delta or delta/2 for various steps. This is the same for all dimensions. Default=0.0001.
- mcmcControl This is passed to configureMCMC, or config if provided, as the control argument. i.e. control=mcmcControl.
- boxContrainst List of box constraints for the nodes that will be maximized over, only relevant if useTransform=FALSE and forceNoConstraints=FALSE (and ignored otherwise). Each constraint is a list in which the first element is a character vector of node names to which the constraint applies and the second element is a vector giving the lower and upper limits. Limits of -Inf or Inf are allowed. Any nodes that are not given constraints will have their constraints automatically determined by NIMBLE. See above. Default=list().
- forceNoConstraints Logical indicating whether to force ignoring constraints even if they might be necessary. Default=FALSE.
- useTransform Logical indicating whether to use a parameter transformation (see parameterTransform) to create an unbounded parameter space for the paramNodes. This allows unconstrained maximization algorithms to be used. Default=TRUE.
- check Logical passed as the check argument to setupMargNodes. Default=TRUE.
- useDerivs Logical indicating whether to use AD. If TRUE, the model must have been build with 'buildDerivs=TRUE'. It is not automatically determined from the model whether derivatives are supported. Default=TRUE.

• config Function to create the MCMC configuration used for step 1. The MCMC configuration is created by calling

```
config(model, nodes = latentNodes, monitors = latentNodes,
thin = thinDefault, control = mcmcControl, print = FALSE)
```

The default for config (if it is missing) is configureMCMC, which is nimble's general default MCMC configuration function.

#### Methods in the returned algorithm

The object returned by buildMCEM is a nimbleFunction object with the following methods

- findMLE is the main method of interest, launching the MCEM algorithm. It takes the following arguments:
  - pStart. Vector of initial parameter values. If omitted, the values currently in the model object are used.
  - returnTrans. Logical indicating whether to return parameters in the transformed space, if a parameter transformation is in use. Default=FALSE.
  - continue. Logical indicating whether to continue the MCEM from where the last call stopped. In addition, if TRUE, any other control setting provided in the last call will be used again. If FALSE, all control settings are reset to the values provided when buildMCEM was called. Any control settings provided in the same call as continue=TRUE will over-ride these behaviors and be used in the continued run.
  - All run-time control settings available in the control list for buildMCEM (except for buffer, boxConstraints, forceNoConstraints, useTransform, and useDerivs) are accepted as individual arguments to over-ride the values provided in the control list.

findMLE returns on object of class optimResultNimbleList with the results of the final optimization of step 2. The par element of this list is the vector of maximum likelihood (MLE) parameters.

- vcov computes the approximate variance-covariance matrix of the MLE using the method of Louis (1982). It takes the following arguments:
  - params. Vector of parameters at which to compute the Hessian matrix used to obtain the vcov result. Typically this will be MLE\$par, if MLE is the output of findMLE.
  - trans. Logical indicating whether params is on the transformed prameter scale, if a
    parameter transformation is in use. Typically this should be the same as the returnTrans
    argument to findMLE. Default=FALSE.
  - returnTrans. Logical indicting whether the vcov result should be for the transformed parameter space. Default matches trans.
  - M. Number of MCMC samples to obtain if resetSamples=TRUE. Default is the final value of M from the last call to findMLE. It can be helpful to increase M to obtain a more accurate vcov result (i.e. with less Monte Carlo noise).
  - resetSamples. Logical indicating whether to generate a new MCMC sample from P(X | Y, T), where T is params. If FALSE, the last sample from findMLE will be used. If MLE convergence was reasonable, this sample can be used. However, if the last MCEM step made a big move in parameter space (e.g. if convergence was not achieved), the last MCMC sample may not be accurate for obtaining vcov. Default=FALSE.

- atMLE. Logical indicating whether you believe the params represents the MLE. If TRUE, one part of the computation will be skipped because it is expected to be 0 at the MLE. If there are parts of the model that are not connected to the latent nodes, i.e. of calcNodesOther is not empty, then atMLE will be ignored and set to FALSE. Default=FALSE. It is not really worth using TRUE unless you are confident and the time saving is meaningful, which is not very likely. In other words, this argument is provided for technical completeness.

vcov returns a matrix that is the inverse of the negative Hessian of the log likelihood surface, i.e. the usual asymptotic approximation of the parameter variance-covariance matrix.

- doMCMC. This method runs the MCMC to sample from P(X | Y, T). One does not need to call this, as it is called via the MCEM algorithm in findMLE. This method is provided for users who want to use the MCMC for latent states directly. Samples should be retrieved by as.matrix(MCEM\$mvSamples), where MCEM is the (compiled or uncompiled) MCEM algorithm object. This method takes the following arguments:
  - M. MCMC sample size.
  - thin. MCMC thinning interval.
  - reset. Logical indicating whether to reset the MCMC (passed to the MCMC run method as reset).
- transform and inverseTransform. Convert a parameter vector to an unconstrained parameter space and vice-versa, if useTransform=TRUE in the call to buildDerivs.
- resetControls. Reset all control arguments to the values provided in the call to buildMCEM. The user does not normally need to call this.

#### Author(s)

Perry de Valpine, Clifford Anderson-Bergman and Nicholas Michaud

#### References

Caffo, Brian S., Wolfgang Jank, and Galin L. Jones (2005). Ascent-based Monte Carlo expectationmaximization. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 67(2), 235-251.

Louis, Thomas A (1982). Finding the Observed Information Matrix When Using the EM Algorithm. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)*, 44(2), 226-233.

#### Examples

```
## Not run:
pumpCode <- nimbleCode({
  for (i in 1:N){
     theta[i] ~ dgamma(alpha,beta);
     lambda[i] <- theta[i]*t[i];
     x[i] ~ dpois(lambda[i])
  }
  alpha ~ dexp(1.0);
  beta ~ dgamma(0.1,1.0);
})
pumpConsts <- list(N = 10,</pre>
```

buildMCMC

*Create an MCMC object from a NIMBLE model, or an MCMC configuration object* 

#### Description

First required argument, which may be of class MCMCconf (an MCMC configuration object), or inherit from class modelBaseClass (a NIMBLE model object). Returns an uncompiled executable MCMC object. See details.

# Usage

```
buildMCMC(conf, print, ...)
```

#### Arguments

conf	Either an MCMC configuration object of class MCMCconf or a NIMBLE model object. An MCMC configuration object would be returned from configureMCMC and contains information on the model, samplers, monitors, and thinning intervals to be used. Alternatively, conf may a NIMBLE model object, in which case default configuration from calling configureMCMC(model,1) will be used.
print	A logical argument, specifying whether to print details of the MCMC samplers and monitors.
	Additional arguments to be passed to configureMCMC if conf is a NIMBLE model object (see help(configureMCMC)).

### buildMCMC

#### Details

Calling buildMCMC(conf) will produce an uncompiled MCMC object. The object contains several methods, including the main run function for running the MCMC, a getTimes function for determining the computation time spent in each sampler (see 'getTimes' section below), and functions related to WAIC (getWAIC, getWAICdetails, calculateWAIC (see help(waic)).

The uncompiled run function will have arguments:

niter: The number of iterations to run the MCMC.

nburnin: Number of initial, pre-thinning, MCMC iterations to discard (default = 0).

thin: The thinning interval for the monitors that were specified in the MCMC configuration. If this argument is provided at MCMC runtime, it will take precedence over the thin interval that was specified in the MCMC configuration. If omitted, the thin interval from the MCMC configuration will be used.

thin2: The thinning interval for the second set of monitors (monitors2) that were specified in the MCMC configuration. If this argument is provided at MCMC runtime, it will take precedence over the thin2 interval that was specified in the MCMC configuration. If omitted, the thin2 interval from the MCMC configuration will be used.

reset: Boolean specifying whether to reset the internal MCMC sampling algorithms to their initial state (in terms of self-adapting tuning parameters), and begin recording posterior sample chains anew. Specifying reset = FALSE allows the MCMC algorithm to continue running from where it left off, appending additional posterior samples to the already existing sample chains. Generally, reset = FALSE should only be used when the MCMC has already been run (default = TRUE).

resetMV: Boolean specifying whether to begin recording posterior sample chains anew. This argument is only considered when using reset = FALSE. Specifying reset = FALSE, resetMV = TRUE allows the MCMC algorithm to continue running from where it left off, but without appending the new posterior samples to the already existing samples, i.e. all previously obtained samples will be erased. This option can help reduce memory usage during burn-in (default = FALSE).

resetWAIC: Boolean specifying whether to reset the WAIC summary statistics to their initial states and thereby begin the WAIC calculation anew (default = TRUE). Specifying resetWAIC = FALSE allows the WAIC calculation to continue running from where it left off.

initializeModel: Boolean specifying whether to run the initializeModel routine on the underlying model object, prior to beginning MCMC sampling (default = TRUE).

chain: Integer specifying the MCMC chain number. The chain number is passed to each MCMC sampler's before\_chain and after\_chain methods. The value for this argument is specified automatically from invocation via runMCMC, and genernally need not be supplied when calling mcmc\$run (default = 1). time: Boolean specifying whether to record runtimes of the individual internal MCMC samplers. When time = TRUE, a vector of runtimes (measured in seconds) can be extracted from the MCMC using the method mcmc\$getTimes() (default = FALSE).

progressBar: Boolean specifying whether to display a progress bar during MCMC execution (default = TRUE). The progress bar can be permanently disabled by setting the system option nimbleOptions(MCMCprogressBar = FALSE).

Samples corresponding to the monitors and monitors2 from the MCMCconf are stored into the interval variables mvSamples and mvSamples2, respectively. These may be accessed and converted into R matrix or list objects via: as.matrix(mcmc\$mvSamples) as.list(mcmc\$mvSamples) as.matrix(mcmc\$mvSamples2) as.list(mcmc\$mvSamples2)

The uncompiled MCMC function may be compiled to a compiled MCMC object, taking care to compile in the same project as the R model object, using: Cmcmc <- compileNimble(Rmcmc, project = Rmodel)

The compiled object will function identically to the uncompiled object except acting on the compiled model object.

#### **Timing the MCMC samplers**

If you want to obtain the computation time spent in each sampler, you can set time=TRUE as a run-time argument to run() and then use the method getTimes() to obtain the times.

### **Calculating WAIC**

Please see help(waic) for more information.

#### Author(s)

Daniel Turek

### References

Watanabe, S. (2010). Asymptotic equivalence of Bayes cross validation and widely applicable information criterion in singular learning theory. *Journal of Machine Learning Research* 11: 3571-3594.

Gelman, A., Hwang, J. and Vehtari, A. (2014). Understanding predictive information criteria for Bayesian models. *Statistics and Computing* 24(6): 997-1016.

Ariyo, O., Quintero, A., Munoz, J., Verbeke, G. and Lesaffre, E. (2019). Bayesian model selection in linear mixed models for longitudinal data. *Journal of Applied Statistics* 47: 890-913.

#### See Also

configureMCMC runMCMC nimbleMCMC

### Examples

```
## Not run:
code <- nimbleCode({
    mu ~ dnorm(0, 1)
    x ~ dnorm(mu, 1)
    y ~ dnorm(x, 1)
})
Rmodel <- nimbleModel(code, data = list(y = 0))
conf <- configureMCMC(Rmodel, monitors = c('mu', 'x'), enableWAIC = TRUE)
Rmcmc <- buildMCMC(conf)
Cmodel <- compileNimble(Rmodel)
Cmcmc <- compileNimble(Rmcmc, project=Rmodel)
## Running the MCMC with `run`
Cmcmc$run(10000)
samples <- as.matrix(Cmcmc$mvSamples)</pre>
```

### calculateWAIC

```
samplesAsList <- as.list(Cmcmc$mvSamples)
head(samples)
## Getting WAIC
waicInfo <- Cmcmc$getWAIC()
waicInfo$WAIC
waicInfo$pWAIC
## Timing the samplers (must set `time = TRUE` when running the MCMC)
Cmcmc$run(1000, time = TRUE)
Cmcmc$getTimes()
## End(Not run)
```

calculateWAIC Calculating WAIC using an offline algorithm

#### Description

In addition to the core online algorithm, NIMBLE implements an offline WAIC algorithm that can be computed on the results of an MCMC. In contrast to NIMBLE's built-in online WAIC, offline WAIC can compute only conditional WAIC and does not allow for grouping data nodes.

#### Usage

calculateWAIC(mcmc, model, nburnin = 0, thin = 1)

### Arguments

mcmc	An MCMC object (compiled or uncompiled) or matrix or dataframe of MCMC samples as the first argument of calculateWAIC.
model	A model (compiled or uncompiled) as the second argument of calculateWAIC. Only required if mcmc is a matrix/dataframe of samples.
nburnin	The number of pre-thinning MCMC samples to remove from the beginning of the posterior samples for offline WAIC calculation via calculateWAIC (default = 0). These samples are discarded in addition to any burn-in specified when running the MCMC.
thin	Thinning factor interval to apply to the samples for offline WAIC calculation using calculateWAIC (default = 1, corresponding to no thinning).

## Details

The ability to calculate WAIC post hoc after all MCMC sampling has been done has certain advantages (e.g., allowing a user to calculate WAIC from MCMC chains run separately) in addition to providing compatibility with versions of NIMBLE before 0.12.0. This functionality includes the ability to call the calculateWAIC function on an MCMC object or matrix of samples after running an MCMC and without setting up the MCMC initially to use WAIC. Important: The necessary variables to compute WAIC (all stochastic parent nodes of the data nodes) must have been monitored when setting up the MCMC.

Also note that while the model argument can be either a compiled or uncompiled model, the model must have been compiled prior to calling calculateWAIC.

See help(waic) for details on using NIMBLE's recommended online algorithm for WAIC.

#### Offline WAIC (WAIC computed after MCMC sampling)

As an alternative to online WAIC, NIMBLE also provides a function, calculateWAIC, that can be called on an MCMC object or a matrix of samples, after running an MCMC. This function does not require that one set enableWAIC = TRUE nor WAIC = TRUE when calling runMCMC. The function checks that the necessary variables were monitored in the MCMC and returns an error if they were not. This function behaves identically to the calculateWAIC method of an MCMC object. Note that to use this function when using nimbleMCMC one would need to build the model outside of nimbleMCMC.

The calculateWAIC function requires either an MCMC object or a matrix (or dataframe) of posterior samples plus a model object. In addition, one can provide optional burnin and thin arguments.

In addition, for compatibility with older versions of NIMBLE (prior to v0.12.0), one can also use the calculateWAIC method of the MCMC object to calculate WAIC after all sampling has been completed.

The calculateWAIC() method accepts a single argument, nburnin, equivalent to the nburnin argument of the calculateWAIC function described above.

The calculateWAIC method can only be used if the enableWAIC argument to configureMCMC or to buildMCMC is set to TRUE, or if the NIMBLE option enableWAIC is set to TRUE. If a user attempts to call calculateWAIC without having set enableWAIC = TRUE (either in the call to configureMCMC, or buildMCMC, or as a NIMBLE option), an error will occur.

The calculateWAIC function and method calculate the WAIC based on Equations 5, 12, and 13 in Gelman et al. (2014) (i.e., using pWAIC2).

Note that there is not a unique value of WAIC for a model. The calculateWAIC function and method only provide the conditional WAIC, namely the version of WAIC where all parameters directly involved in the likelihood are treated as *theta* for the purposes of Equation 5 from Gelman et al. (2014). As a result, the user must set the MCMC monitors (via the monitors argument) to include all stochastic nodes that are parents of any data nodes; by default the MCMC monitors are only the top-level nodes of the model. For more detail on the use of different predictive distributions, see Section 2.5 from Gelman et al. (2014) or Ariyo et al. (2019). Also note that WAIC relies on a partition of the observations, i.e., 'pointwise' prediction. In calculateWAIC the sum over log pointwise predictive density values treats each data node as contributing a single value to the sum. When a data node is multivariate, that data node contributes a single value to the sum based on the joint density of the elements in the node. Note that if one wants the WAIC calculation via calculateWAIC to be based on the joint predictive density for each group of observations (e.g., grouping the observations from each person or unit in a longitudinal data context), one would need to use a multivariate distribution for the observations in each group (potentially by writing a user-defined distribution).

For more control over and flexibility in how WAIC is calculated, see help(waic).

#### calculateWAIC

#### Author(s)

Joshua Hug and Christopher Paciorek

#### References

Watanabe, S. (2010). Asymptotic equivalence of Bayes cross validation and widely applicable information criterion in singular learning theory. *Journal of Machine Learning Research* 11: 3571-3594.

Gelman, A., Hwang, J. and Vehtari, A. (2014). Understanding predictive information criteria for Bayesian models. *Statistics and Computing* 24(6): 997-1016.

Ariyo, O., Quintero, A., Munoz, J., Verbeke, G. and Lesaffre, E. (2019). Bayesian model selection in linear mixed models for longitudinal data. *Journal of Applied Statistics* 47: 890-913.

Vehtari, A., Gelman, A. and Gabry, J. (2017). Practical Bayesian model evaluation using leave-oneout cross-validation and WAIC. *Statistics and Computing* 27: 1413-1432.

Hug, J.E. and Paciorek, C.J. (2021). A numerically stable online implementation and exploration of WAIC through variations of the predictive density, using NIMBLE. *arXiv e-print* <arXiv:2106.13359>.

#### See Also

waic configureMCMC buildMCMC runMCMC nimbleMCMC

#### Examples

```
code <- nimbleCode({</pre>
  for(j in 1:J) {
    for(i in 1:n)
      y[j, i] ~ dnorm(mu[j], sd = sigma)
    mu[j] ~ dnorm(mu0, sd = tau)
  3
  tau ~ dunif(0, 10)
  sigma ~ dunif(0, 10)
})
J <- 5
n <- 10
y <- matrix(rnorm(J*n), J, n)</pre>
Rmodel <- nimbleModel(code, constants = list(J = J, n = n), data = list(y = y),</pre>
                       inits = list(tau = 1, sigma = 1))
## Make sure the needed variables are monitored.
## Only conditional WAIC without data grouping is available via this approach.
conf <- configureMCMC(Rmodel, monitors = c('mu', 'sigma'))</pre>
## Not run:
Cmodel <- compileNimble(Rmodel)</pre>
Rmcmc <- buildMCMC(conf)</pre>
Cmcmc <- compileNimble(Rmcmc, project = Rmodel)</pre>
output <- runMCMC(Cmcmc, niter = 1000)</pre>
calculateWAIC(Cmcmc)
                               # Can run on the MCMC object
calculateWAIC(output, Rmodel) # Can run on the samples directly
```

## Apply additional burnin (additional to any burnin already done in the MCMC.

```
calculateWAIC(Cmcmc, burnin = 500)
## End(Not run)
```

CAR-Normal

The CAR-Normal Distribution

# Description

Density function and random generation for the improper (intrinsic) Gaussian conditional autoregressive (CAR) distribution.

# Usage

```
dcar_normal(
 х,
  adj,
 weights = adj/adj,
 num,
  tau,
  c = CAR_calcNumIslands(adj, num),
  zero_mean = 0,
  log = FALSE
)
rcar_normal(
 n = 1,
 adj,
 weights = adj/adj,
 num,
  tau,
 c = CAR_calcNumIslands(adj, num),
 zero_mean = 0
)
```

# Arguments

х	vector of values.
adj	vector of indices of the adjacent locations (neighbors) of each spatial location. This is a sparse representation of the full adjacency matrix.
weights	vector of symmetric unnormalized weights associated with each pair of adjacent locations, of the same length as adj. If omitted, all weights are taken to be one.
num	vector giving the number of neighboring locations of each spatial location, with length equal to the total number of locations.
tau	scalar precision of the Gaussian CAR prior.

## CAR-Normal

с	integer number of constraints to impose on the improper density function. If omitted, c is calculated as the number of disjoint groups of spatial locations in the adjacency structure, which implicitly assumes a first-order CAR process for each group. Note that c should be equal to the number of eigenvalues of the precision matrix that are zero. For example, if the neighborhood structure is based on a second-order Markov random field in one dimension then the matrix has two zero eigenvalues and in two dimensions it has three zero eigenvalues. See Rue and Held (2005) and the NIMBLE User Manual for more information.
zero_mean	integer specifying whether to set the mean of all locations to zero during MCMC sampling of a node specified with this distribution in BUGS code (default $\emptyset$ ). This argument is used only in BUGS model code when specifying models in NIMBLE. If $\emptyset$ , the overall process mean is included implicitly in the value of each location in a BUGS model; if 1, then during MCMC sampling, the mean of all locations is set to zero at each MCMC iteration, and a separate intercept term should be included in the BUGS model. Note that centering during MCMC as implemented in NIMBLE follows the ad hoc approach of <b>WinBUGS</b> and does not sample under the constraint that the mean is zero as discussed on p. 36 of Rue and Held (2005). See 'Details'.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.

### Details

When specifying a CAR distribution in BUGS model code, the zero\_mean parameter should be specified as either 0 or 1 (rather than TRUE or FALSE).

Note that because the distribution is improper, rcar\_normal does not generate a sample from the distribution. However, as discussed in Rue and Held (2005), it is possible to generate a sample from the distribution under constraints imposed based on the eigenvalues of the precision matrix that are zero.

# Value

dcar\_normal gives the density, while rcar\_normal returns the current process values, since this distribution is improper.

#### Author(s)

Daniel Turek

## References

Banerjee, S., Carlin, B.P., and Gelfand, A.E. (2015). *Hierarchical Modeling and Analysis for Spatial Data*, 2nd ed. Chapman and Hall/CRC.

Rue, H. and L. Held (2005). Gaussian Markov Random Fields, Chapman and Hall/CRC.

# See Also

CAR-Proper, Distributions for other standard distributions

# Examples

```
x <- c(1, 3, 3, 4)
num <- c(1, 2, 2, 1)
adj <- c(2, 1,3, 2,4, 3)
weights <- c(1, 1, 1, 1, 1, 1)
lp <- dcar_normal(x, adj, weights, num, tau = 1)</pre>
```

CAR-Proper

### The CAR-Proper Distribution

# Description

Density function and random generation for the proper Gaussian conditional autoregressive (CAR) distribution.

### Usage

```
dcar_proper(
 х,
 mu,
 C = CAR_calcC(adj, num),
 adj,
 num,
 M = CAR_calcM(num),
  tau,
 gamma,
 evs = CAR_calcEVs3(C, adj, num),
 log = FALSE
)
rcar_proper(
 n = 1,
 mu,
 C = CAR_calcC(adj, num),
 adj,
 num,
 M = CAR_calcM(num),
 tau,
 gamma,
 evs = CAR_calcEVs3(C, adj, num)
)
```

### Arguments

Х	vector of values.
mu	vector of the same length as x, specifying the mean for each spatial location.

С	vector of the same length as adj, giving the weights associated with each pair of neighboring locations. See 'Details'.
adj	vector of indices of the adjacent locations (neighbors) of each spatial location. This is a sparse representation of the full adjacency matrix.
num	vector giving the number of neighboring locations of each spatial location, with length equal to the number of locations.
М	vector giving the diagonal elements of the conditional variance matrix, with length equal to the number of locations. See 'Details'.
tau	scalar precision of the Gaussian CAR prior.
gamma	scalar representing the overall degree of spatial dependence. See 'Details'.
evs	vector of eigenvalues of the adjacency matrix implied by C, adj, and num. This parameter should not be provided; it will always be calculated using the adjacency information.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.

# Details

If both C and M are omitted, then all weights are taken as one, and corresponding values of C and M are generated.

The C and M parameters must jointly satisfy a symmetry constraint: that  $M^{(-1)}$  C is symmetric, where M is a diagonal matrix and C is the full weight matrix that is sparsely represented by the parameter vector C.

For a proper CAR model, the value of gamma must lie within the inverse minimum and maximum eigenvalues of  $M^{(-0.5)} \times C \times M^{(0.5)}$ , where M is a diagonal matrix and C is the full weight matrix. These bounds can be calculated using the deterministic functions carMinBound(C, adj, num, M) and carMaxBound(C, adj, num, M), or simultaneously using carBounds(C, adj, num, M). In the case where C and M are omitted (all weights equal to one), the bounds on gamma are necessarily (-1, 1).

## Value

dcar\_proper gives the density, and rcar\_proper generates random deviates.

### Author(s)

Daniel Turek

# References

Banerjee, S., Carlin, B.P., and Gelfand, A.E. (2015). *Hierarchical Modeling and Analysis for Spatial Data*, 2nd ed. Chapman and Hall/CRC.

# See Also

CAR-Normal, Distributions for other standard distributions

### Examples

```
x <- c(1, 3, 3, 4)
mu < -rep(3, 4)
adj <- c(2, 1,3, 2,4, 3)
num <- c(1, 2, 2, 1)
## omitting C and M uses all weights = 1
dcar_proper(x, mu, adj = adj, num = num, tau = 1, gamma = 0.95)
## equivalent to above: specifying all weights = 1,
## then using as.carCM to generate C and M arguments
weights <- rep(1, 6)
CM <- as.carCM(adj, weights, num)</pre>
C <- CM$C
M <- CM$M
dcar_proper(x, mu, C, adj, num, M, tau = 1, gamma = 0.95)
## now using non-unit weights
weights <- c(2, 2, 3, 3, 4, 4)
CM2 <- as.carCM(adj, weights, num)
C2 <- CM2$C
M2 <- CM2$M
dcar_proper(x, mu, C2, adj, num, M2, tau = 1, gamma = 0.95)
```

carBounds	Calculate	bounds	for	the	autocorrelation	parameter	of	the
	dcar_prop	per <i>distril</i>	outior	ı				

# Description

Calculate the lower and upper bounds for the gamma parameter of the dcar\_proper distribution

# Usage

carBounds(C, adj, num, M)

### Arguments

С	vector of the same length as adj, giving the normalized weights associated with each pair of neighboring locations.
adj	vector of indices of the adjacent locations (neighbors) of each spatial location. This is a sparse representation of the full adjacency matrix.
num	vector giving the number of neighboring locations of each spatial location, with length equal to the number of locations.
М	vector giving the diagonal elements of the conditional variance matrix, with length equal to the number of locations.

## carMaxBound

# Details

Bounds for gamma are the inverse of the minimum and maximum eigenvalues of:  $M^{(-0.5)}CM^{(0.5)}$ . The lower and upper bounds are returned in a numeric vector.

### Value

A numeric vector containing the bounds (minimum and maximum allowable values) for the gamma parameter of the dcar\_proper distribution.

#### Author(s)

Daniel Turek

### See Also

CAR-Proper, carMinBound, carMaxBound

carMaxBound	Calculate the upper bound for the autocorrelation parameter of the
	dcar_proper <i>distribution</i>

# Description

Calculate the upper bound for the gamma parameter of the dcar\_proper distribution

### Usage

```
carMaxBound(C, adj, num, M)
```

#### Arguments

С	vector of the same length as adj, giving the normalized weights associated with each pair of neighboring locations.
adj	vector of indices of the adjacent locations (neighbors) of each spatial location. This is a sparse representation of the full adjacency matrix.
num	vector giving the number of neighboring locations of each spatial location, with length equal to the number of locations.
М	vector giving the diagonal elements of the conditional variance matrix, with length equal to the number of locations.

# Details

Bounds for gamma are the inverse of the minimum and maximum eigenvalues of  $M^{(-0.5)}CM^{(0.5)}$ .

#### Value

The upper bound (maximum allowable value) for the gamma parameter of the dcar\_proper distribution.

#### Author(s)

Daniel Turek

# See Also

CAR-Proper, carMinBound, carBounds

carMinBound	Calculate the lower bound for the autocorrelation parameter of the
	dcar_proper <i>distribution</i>

# Description

Calculate the lower bound for the gamma parameter of the dcar\_proper distribution

### Usage

carMinBound(C, adj, num, M)

# Arguments

С	vector of the same length as adj, giving the normalized weights associated with each pair of neighboring locations.
adj	vector of indices of the adjacent locations (neighbors) of each spatial location. This is a sparse representation of the full adjacency matrix.
num	vector giving the number of neighboring locations of each spatial location, with length equal to the number of locations.
М	vector giving the diagonal elements of the conditional variance matrix, with length equal to the number of locations.

# Details

Bounds for gamma are the inverse of the minimum and maximum eigenvalues of:  $M^{(-0.5)}CM^{(0.5)}$ .

### Value

The lower bound (minimum allowable value) for the gamma parameter of the dcar\_proper distribution.

# Author(s)

Daniel Turek

# See Also

CAR-Proper, carMaxBound, carBounds

CAR\_calcNumIslands Calculate number of islands based on a CAR adjacency matrix.

# Description

Calculate number of islands (distinct connected groups) based on a CAR adjacency matrix.

# Usage

```
CAR_calcNumIslands(adj, num)
```

# Arguments

adj	vector of indices of the adjacent locations (neighbors) of each spatial location.
	This is a sparse representation of the full adjacency matrix.
num	vector giving the number of neighbors of each spatial location, with length equal
	to the total number of locations.

# Author(s)

Daniel Turek

### See Also

CAR-Normal

Categorical	The Categorical Distribution

# Description

Density and random generation for the categorical distribution

# Usage

dcat(x, prob, log = FALSE)

rcat(n = 1, prob)

# Arguments

Х	non-negative integer-value numeric value.
prob	vector of probabilities, internally normalized to sum to one.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.

### Details

See the BUGS manual for mathematical details.

#### Value

dcat gives the density and rcat generates random deviates.

#### Author(s)

Christopher Paciorek

#### See Also

Distributions for other standard distributions

# Examples

probs <- c(1/4, 1/10, 1 - 1/4 - 1/10)
x <- rcat(n = 30, probs)
dcat(x, probs)</pre>

checkInterrupt	Check for interrupt (e.g.	Ctrl-C) during nimbleFunction execution.
	Part of the NIMBLE lange	lage.

### Description

Check for interrupt (e.g. Ctrl-C) during nimbleFunction execution. Part of the NIMBLE language.

### Usage

```
checkInterrupt()
```

# Details

During execution of nimbleFunctions that take a long time, it is nice to occassionally check if the user has entered an interrupt and bail out of execution if so. This function does that. During uncompiled nimbleFunction execution, it does nothing. During compiled execution, it calls  $R_checkUserInterrupt()$  of the R headers.

### Author(s)

Perry de Valpine

ChineseRestaurantProcess

The Chinese Restaurant Process Distribution

## Description

Density and random generation for the Chinese Restaurant Process distribution.

### Usage

dCRP(x, conc = 1, size, log = 0)
rCRP(n, conc = 1, size)

## Arguments

х	vector of values.
conc	scalar concentration parameter.
size	integer-valued length of x (required).
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only $n = 1$ is handled currently).

### Details

The Chinese restaurant process distribution is a distribution on the space of partitions of the positive integers. The distribution with concentration parameter  $\alpha$  equal to conc has probability function

$$f(x_i \mid x_1, \dots, x_{i-1}) = \frac{1}{i-1+\alpha} \sum_{j=1}^{i-1} \delta_{x_j} + \frac{\alpha}{i-1+\alpha} \delta_{x^{new}},$$

where  $x^{new}$  is a new integer not in  $x_1, \ldots, x_{i-1}$ .

If conc is not specified, it assumes the default value of 1. The conc parameter has to be larger than zero. Otherwise, NaN are returned.

# Value

dCRP gives the density, and rCRP gives random generation.

#### Author(s)

Claudia Wehrhahn

#### References

Blackwell, D., and MacQueen, J. B. (1973). Ferguson distributions via Pólya urn schemes. *The Annals of Statistics*, 1: 353-355.

Aldous, D. J. (1985). Exchangeability and related topics. In École d'Été de Probabilités de Saint-Flour XIII - 1983 (pp. 1-198). Springer, Berlin, Heidelberg.

Pitman, J. (1996). Some developments of the Blackwell-MacQueen urn scheme. *IMS Lecture Notes-Monograph Series*, 30: 245-267.

### Examples

```
x <- rCRP(n=1, conc = 1, size=10)
dCRP(x, conc = 1, size=10)</pre>
```

clearCompiled Clear compiled objects from a project and unload shared library

#### Description

Clear all compiled objects from a project and unload the shared library produced by the C++ compiler. Has no effect on Windows.

### Usage

clearCompiled(obj)

### Arguments

#### obj

A compiled nimbleFunction or nimble model

# Details

This will clear all compiled objects associated with your NIMBLE project. For example, if cModel is a compiled model, clearCompiled(cModel) will clear both the model and all associated nimbleFunctions such as compiled MCMCs that use that model.

Use of this function can be dangerous. There is some risk that if you have copies of the R objects that interfaced to compiled C++ objects that have been removed, and you attempt to use those R objects after clearing their compiled counterparts, you will crash R. We have tried to minimize that risk, but we can't guarantee safe behavior.

CmodelBaseClass-class Class CmodelBaseClass

### Description

Classes used internally in NIMBLE and not expected to be called directly by users.

CnimbleFunctionBase-class

Class CnimbleFunctionBase

### Description

Classes used internally in NIMBLE and not expected to be called directly by users.

codeBlockClass-class Class codeBlockClass

# Description

Classes used internally in NIMBLE and not expected to be called directly by users.

compileNimble compile	NIMBLE models and nimbleFunctions
-----------------------	-----------------------------------

## Description

compile a collection of models and nimbleFunctions: generate C++, compile the C++, load the result, and return an interface object

# Usage

```
compileNimble(
   ...,
   project,
   dirName = NULL,
   projectName = "",
   control = list(),
   resetFunctions = FALSE,
   showCompilerOutput = getNimbleOption("showCompilerOutput")
)
```

## Arguments

	An arbitrary set of NIMBLE models and nimbleFunctions, or lists of them. If given as named parameters, those names may be used in the return list.
project	Optional NIMBLE model or nimbleFunction already associated with a project, which the current units for compilation should join. If not provided, a new project will be created and the current compilation units will be associated with it.

	dirName	Optional directory name in which to generate the C++ code. If not provided, a temporary directory will be generated using R's tempdir function.
	projectName	Optional character name for labeling the project if it is new
	control	A list mostly for internal use. See details.
	resetFunctions	Logical value stating whether nimbleFunctions associated with an existing project should all be reset for compilation purposes. See details.
showCompilerOutput		
		Logical value indicating whether details of $C_{++}$ compilation should be printed

Logical value indicating whether details of C++ compilation should be printed.

### Details

This is the main function for calling the NIMBLE compiler. A set of compiler calls and output will be seen. Compiling in NIMBLE does 4 things: 1. It generates C++ code files for all the model and nimbleFunction components. 2. It calls the system's C++ compiler. 3. It loads the compiled object(s) into R using dyn.load. And 4. it generates R objects for using the compiled model and nimbleFunctions.

When the units for compilation provided in ... include multiple models and/or nimbleFunctions, models are compiled first, in the order in which they are provided. Groups of nimbleFunctions that were specialized from the same nimbleFunction generator (the result of a call to nimbleFunction, which then takes setup arguments and returns a specialized nimbleFunction) are then compiled as a group, in the order of first appearance.

The behavior of adding new compilation units to an existing project is limited. For example, one can compile a model in one call to compileNimble and then compile a nimbleFunction that uses the model (i.e. was given the model as a setup argument) in a second call to compileNimble, with the model provided as the project argument. Either the uncompiled or compiled model can be provided. However, compiling a second nimbleFunction and adding it to the same project will only work in limited circumstances. Basically, the limitations occur because it attempts to re-use already compiled pieces, but if these do not have all the necessary information for the new compilation, it gives up. An attempt has been made to give up in a controlled manner and provide somewhat informative messages.

When compilation is not allowed or doesn't work, try using resetFunctions = TRUE, which will force recompilation of all nimbleFunctions in the new call. Previously compiled nimbleFunctions will be unaffected, and their R interface objects should continue to work. The only cost is additional compilation time for the current compilation call. If that doesn't work, try re-creating the model and/or the nimbleFunctions from their generators. An alternative possible fix is to compile multiple units in one call, rather than sequentially in multiple calls.

The control list can contain the following named elements, each with TRUE or FALSE: debug, which sets a debug mode for the compiler for development purposes; debugCpp, which inserts an output message before every line of C++ code for debugging purposes; compileR, which determines whether the R-only steps of compilation should be executed; writeCpp, which determines whether the C++ files should be generated; compileCpp, which determines whether the C++ should be compiled; loadSO, which determines whether the DLL or shared object should be loaded and interfaced; and returnAsList, which determines whether calls to the compiled nimbleFunction should return only the returned value of the call (returnAsList = FALSE) or whether a list including the input arguments, possibly modified, should be returned in a list with the returned value of the call at the end (returnAsList = TRUE). The control list is mostly for developer use, although returnAsArgs

#### configureMCMC

may be useful to a user. An example of developer use is that one can have the compiler write the C++ files but not compile them, then modify them by hand, then have the C++ compiler do the subsequent steps without over-writing the files.

See the NIMBLE User Manual Manual for examples

### Value

If there is only one compilation unit (one model or nimbleFunction), an R interface object is returned. This object can be used like the uncompiled model or nimbleFunction, but execution will call the corresponding compiled objects or functions. If there are multiple compilation units, they will be returned as a list of interface objects, in the order provided. If names were included in the arguments, or in a list if any elements of . . . are lists, those names will be used for the corresponding element of the returned list. Otherwise an attempt will be made to generate names from the argument code. For example compileNimble(A = fun1, B = fun2, project = myModel) will return a list with named elements A and B, while compileNimble(fun1, fun2, project = myModel) will return a list with named elements fun1 and fun2.

#### Author(s)

Perry de Valpine

configureMCMC

Build the MCMC conf object for construction of an MCMC object

### Description

Creates a default MCMC configuration for a given model.

### Usage

```
configureMCMC(
 model,
  nodes.
  control = list(),
 monitors,
  thin = 1,
 monitors2 = character(),
  thin2 = 1,
  useConjugacy = getNimbleOption("MCMCuseConjugacy"),
  onlyRW = FALSE,
  onlySlice = FALSE,
 multivariateNodesAsScalars = getNimbleOption("MCMCmultivariateNodesAsScalars"),
  enableWAIC = getNimbleOption("MCMCenableWAIC"),
  controlWAIC = list(),
  print = getNimbleOption("verbose"),
  autoBlock = FALSE,
 oldConf,
  . . .
)
```

# Arguments

model	A NIMBLE model object, created from nimbleModel	
nodes	An optional character vector, specifying the nodes and/or variables for which samplers should be created. Nodes may be specified in their indexed form, $y[1, 3]$ . Alternatively, nodes specified without indexing will be expanded fully, e.g., x will be expanded to x[1], x[2], etc. If missing, the default value is all non-data stochastic nodes. If NULL, then no samplers are added.	
control	An optional list of control arguments to sampler functions. If a control list is provided, the elements will be provided to all sampler functions which uti- lize the named elements given. For example, the standard Metropolis-Hastings random walk sampler (sampler_RW) utilizes control list elements adaptive, adaptInterval, and scale. (Internally it also uses targetNode, but this should not generally be provided as a control list element). The default values for con- trol list arguments for samplers (if not otherwise provided as an argument to configureMCMC() ) are in the setup code of the sampling algorithms.	
monitors	A character vector of node names or variable names, to record during MCMC sampling. This set of monitors will be recorded with thinning interval thin, and the samples will be stored into the mvSamples object. The default value is all top-level stochastic nodes of the model – those having no stochastic parent nodes.	
thin	The thinning interval for monitors. Default value is one.	
monitors2	A character vector of node names or variable names, to record during MCMC sampling. This set of monitors will be recorded with thinning interval thin2, and the samples will be stored into the mvSamples2 object. The default value is an empty character vector, i.e. no values will be recorded.	
thin2	The thinning interval for monitors2. Default value is one.	
useConjugacy	A logical argument, with default value TRUE. If specified as FALSE, then no conjugate samplers will be used, even when a node is determined to be in a conjugate relationship.	
onlyRW	A logical argument, with default value FALSE. If specified as TRUE, then Metropolis-Hastings random walk samplers (sampler_RW) will be assigned for all non-terminal continuous-valued nodes nodes. Discrete-valued nodes are assigned a slice sampler (sampler_slice), and terminal nodes are assigned a posterior_predictive sampler (sampler_posterior_predictive).	
onlySlice	A logical argument, with default value FALSE. If specified as TRUE, then a slice sampler is assigned for all non-terminal nodes. Terminal nodes are still assigned a posterior_predictive sampler.	
multivariateNodesAsScalars		
	A logical argument, with default value FALSE. If specified as TRUE, then non- terminal multivariate stochastic nodes will have scalar samplers assigned to each of the scalar components of the multivariate node. The default value of FALSE results in a single block sampler assigned to the entire multivariate node. Note, multivariate nodes appearing in conjugate relationships will be assigned the cor- responding conjugate sampler (provided useConjugacy == TRUE), regardless of the value of this argument.	

enableWAIC	A logical argument, specifying whether to enable WAIC calculations for the re- sulting MCMC algorithm. Defaults to the value of nimbleOptions('MCMCenableWAIC'), which in turn defaults to FALSE. Setting nimbleOptions('enableWAIC' = TRUE) will ensure that WAIC is enabled for all calls to configureMCMC and buildMCMC.
controlWAIC	A named list of inputs that control the behavior of the WAIC calculation. See help(waic).
print	A logical argument, specifying whether to print the ordered list of default sam- plers.
autoBlock	A logical argument specifying whether to use an automated blocking procedure to determine blocks of model nodes for joint sampling. If TRUE, an MCMC configuration object will be created and returned corresponding to the results of the automated parameter blocking. Default value is FALSE.
oldConf	An optional MCMCconf object to modify rather than creating a new MCMC- conf from scratch
	Additional named control list elements for default samplers, or additional arguments to be passed to the autoBlock function when autoBlock = TRUE

## Details

See MCMCconf for details on how to manipulate the MCMCconf object

### Author(s)

Daniel Turek

# See Also

buildMCMC runMCMC nimbleMCMC

configureRJ

Configure Reversible Jump for Variable Selection

# Description

Modifies an MCMC configuration object to perform a reversible jump MCMC sampling for variable selection, using a univariate normal proposal distribution. Users can control the mean and scale of the proposal. This function supports two different types of model specification: with and without indicator variables.

### Usage

```
configureRJ(
   conf,
   targetNodes,
   indicatorNodes = NULL,
   priorProb = NULL,
   control = list(mean = NULL, scale = NULL, fixedValue = NULL)
)
```

#### Arguments

conf	An MCMCconf object.
targetNodes	A character vector, specifying the nodes and/or variables for which variable se- lection is to be performed. Nodes may be specified in their indexed form, ' $y[1, 3]$ '. Alternatively, nodes specified without indexing will be expanded, e.g., 'x' will be expanded to ' $x[1]$ ', ' $x[2]$ ', etc.
indicatorNodes	An optional character vector, specifying the indicator nodes and/or variables paired with targetNodes. Nodes may be specified in their indexed form, 'y[1, 3]'. Alternatively, nodes specified without indexing will be expanded, e.g., 'x' will be expanded to 'x[1]', 'x[2]', etc. Nodes must be provided consistently with targetNodes. See details.
priorProb	An optional value or vector of prior probabilities for each node to be in the model. See details.
control	An optional list of control arguments:
	<ul> <li>mean. The mean of the normal proposal distribution (default = 0).</li> <li>scale. The standard deviation of the normal proposal distribution (default = 1).</li> <li>fixedValue. Value for the variable when it is out of the model, which can be used only when priorProb is provided (default = 0). If specified when indicatorNodes is passed, a warning is given and fixedValue is ignored.</li> </ul>

# Details

This function modifies the samplers in MCMC configuration object for each of the nodes provided in the targetNodes argument. To these elements two samplers are assigned: a reversible jump sampler to transition the variable in/out of the model, and a modified version of the original sampler, which performs updates only when the target node is already in the model.

configureRJ can handle two different ways of writing a NIMBLE model, either with or without indicator variables. When using indicator variables, the indicatorNodes argument must be provided. Without indicator variables, the priorProb argument must be provided. In the latter case, the user can provide a non-zero value for fixedValue if desired.

Note that this functionality is intended for variable selection in regression-style models but may be useful for other situations as well. At the moment, setting a variance component to zero and thereby removing a set of random effects that are explicitly part of a model will not work because MCMC sampling in that case would need to propose values for multiple parameters (the random effects), whereas the current functionality only proposes adding/removing a single model node.

#### Value

NULL configureRJ modifies the input MCMC configuration object in place.

#### Author(s)

Sally Paganin, Perry de Valpine, Daniel Turek

#### configureRJ

### References

Peter J. Green. (1995). Reversible jump Markov chain Monte Carlo computation and Bayesian model determination. *Biometrika*, 82(4), 711-732.

#### See Also

samplers configureMCMC

# Examples

## Not run:

## Linear regression with intercept and two covariates, using indicator variables

```
code <- nimbleCode({</pre>
  beta0 ~ dnorm(0, sd = 100)
  beta1 ~ dnorm(0, sd = 100)
  beta2 ~ dnorm(0, sd = 100)
  sigma ~ dunif(0, 100)
  z1 ~ dbern(psi)  ## indicator variable associated with beta1
z2 ~ dbern(psi)  ## indicator variable associated with beta2
  psi ~ dunif(0, 1) ## hyperprior on inclusion probability
  for(i in 1:N) {
    Ypred[i] <- beta0 + beta1 * z1 * x1[i] + beta2 * z2 * x2[i]</pre>
    Y[i] ~ dnorm(Ypred[i], sd = sigma)
  }
})
## simulate some data
set.seed(1)
N <- 100
x1 <- runif(N, -1, 1)
x2 <- runif(N, -1, 1) ## this covariate is not included
Y \le rnorm(N, 1 + 2.5 * x1, sd = 1)
## build the model
rIndicatorModel <- nimbleModel(code, constants = list(N = N),</pre>
                                 data = list(Y = Y, x1 = x1, x2 = x2),
                               inits = list(beta0 = 0, beta1 = 0, beta2 = 0, sigma = sd(Y),
                                 z1 = 1, z2 = 1, psi = 0.5)
indicatorModelConf <- configureMCMC(rIndicatorModel)</pre>
## Add reversible jump
configureRJ(conf = indicatorModelConf,
                                                ## model configuration
             targetNodes = c("beta1", "beta2"), ## coefficients for selection
             indicatorNodes = c("z1", "z2"), ## indicators paired with coefficients
             control = list(mean = 0, scale = 2))
indicatorModelConf$addMonitors("beta1", "beta2", "z1", "z2")
rIndicatorMCMC <- buildMCMC(indicatorModelConf)</pre>
```

```
cIndicatorModel <- compileNimble(rIndicatorModel)</pre>
cIndicatorMCMC <- compileNimble(rIndicatorMCMC, project = rIndicatorModel)</pre>
set.seed(1)
samples <- runMCMC(cIndicatorMCMC, 10000, nburnin = 6000)</pre>
## posterior probability to be included in the mode
mean(samples[ , "z1"])
mean(samples[ , "z2"])
## posterior means when in the model
mean(samples[ , "beta1"][samples[ , "z1"] != 0])
mean(samples[ , "beta2"][samples[ , "z2"] != 0])
## Linear regression with intercept and two covariates, without indicator variables
code <- nimbleCode({</pre>
 beta0 ~ dnorm(0, sd = 100)
 beta1 ~ dnorm(0, sd = 100)
 beta2 ~ dnorm(0, sd = 100)
 sigma ~ dunif(0, 100)
 for(i in 1:N) {
   Ypred[i] <- beta0 + beta1 * x1[i] + beta2 * x2[i]</pre>
    Y[i] ~ dnorm(Ypred[i], sd = sigma)
 }
})
rNoIndicatorModel <- nimbleModel(code, constants = list(N = N),</pre>
                                  data = list(Y = Y, x1 = x1, x2 = x2),
                              inits= list(beta0 = 0, beta1 = 0, beta2 = 0, sigma = sd(Y)))
noIndicatorModelConf <- configureMCMC(rNoIndicatorModel)</pre>
## Add reversible jump
configureRJ(conf = noIndicatorModelConf,
                                             ## model configuration
            targetNodes = c("beta1", "beta2"), ## coefficients for selection
                                                 ## prior probability of inclusion
            priorProb = 0.5,
            control = list(mean = 0, scale = 2))
## add monitors
noIndicatorModelConf$addMonitors("beta1", "beta2")
rNoIndicatorMCMC <- buildMCMC(noIndicatorModelConf)</pre>
cNoIndicatorModel <- compileNimble(rNoIndicatorModel)</pre>
cNoIndicatorMCMC <- compileNimble(rNoIndicatorMCMC, project = rNoIndicatorModel)</pre>
set.seed(1)
samples <- runMCMC(cNoIndicatorMCMC, 10000, nburnin = 6000)</pre>
## posterior probability to be included in the mode
mean(samples[ , "beta1"] != 0)
mean(samples[ , "beta2"] != 0)
```

## Constraint

```
## posterior means when in the model
mean(samples[, "beta1"][samples[, "beta1"] != 0])
mean(samples[, "beta2"][samples[, "beta2"] != 0])
## End(Not run)
```

Constraint

Constraint calculations in NIMBLE

# Description

Calculations to handle censoring

### Usage

dconstraint(x, cond, log = FALSE)

rconstraint(n = 1, cond)

# Arguments

х	value indicating whether cond is TRUE or FALSE
cond	logical value
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

# Details

Used for working with constraints in BUGS code. See the NIMBLE manual for additional details.

### Value

dconstraint gives the density and rconstraint generates random deviates, but these are unusual as the density is 1 if x matches cond and 0 otherwise and the deviates are simply the value of cond

## Author(s)

Christopher Paciorek

### See Also

Distributions for other standard distributions

decide

### Examples

```
constr <- 3 > 2 && 4 > 0
x <- rconstraint(1, constr)
dconstraint(x, constr)
dconstraint(0, 3 > 4)
dconstraint(1, 3 > 4)
rconstraint(1, 3 > 4)
```

decide

Makes the Metropolis-Hastings acceptance decision, based upon the input (log) Metropolis-Hastings ratio

## Description

This function returns a logical TRUE/FALSE value, indicating whether the proposed transition should be accepted (TRUE) or rejected (FALSE).

## Usage

```
decide(logMetropolisRatio)
```

#### Arguments

logMetropolisRatio

The log of the Metropolis-Hastings ratio, which is calculated from model probabilities and forward/reverse transition probabilities. Calculated as the ratio of the model probability under the proposal to that under the current values multiplied by the ratio of the reverse transition probability to the forward transition probability.

### Details

The Metropolis-Hastings accept/reject decisions is made as follows. If logMetropolisRatio is greater than 0, accept (return TRUE). Otherwise draw a uniform random number between 0 and 1 and accept if it is less that exp(logMetropolisRatio. The proposed transition will be rejected (return FALSE). If logMetropolisRatio is NA, NaN, or -Inf, a reject (FALSE) decision will be returned.

### Author(s)

Daniel Turek

decideAndJump	Creates a nimbleFunction for executing the Metropolis-Hastings jumping decision, and updating values in the model, or in a carbon
	copy modelValues object, accordingly.

### Description

This nimbleFunction generator must be specialized to three required arguments: a model, a model-Values, and a character vector of node names.

#### Usage

decideAndJump(model, mvSaved, target, UNUSED)

### Arguments

model	An uncompiled or compiled NIMBLE model object.
mvSaved	A modelValues object containing identical variables and logProb variables as the model. Can be created by modelValues(model).
target	A character vector providing the target node.
UNUSED	Unused placeholder argument.

## Details

Calling decideAndJump(model, mvSaved, target) will generate a specialized nimbleFunction with four required numeric arguments:

modelLP1: The model log-probability associated with the newly proposed value(s)

modelLP0: The model log-probability associated with the original value(s)

propLP1: The log-probability associated with the proposal forward-transition

propLP0: The log-probability associated with the proposal reverse-tranisiton

Executing this function has the following effects: - Calculate the (log) Metropolis-Hastings ratio, as logMHR = modelLP1 - modelLP0 - propLP1 + propLP0 – Make the proposal acceptance decision based upon the (log) Metropolis-Hastings ratio – If the proposal is accepted, the values and associated logProbs of all calcNodes are copied from the model object into the mvSaved object – If the proposal is rejected, the values and associated logProbs of all calcNodes are copied logProbs of all calcNodes are copied from the model object methods are copied from the mvSaved object method

# Author(s)

Daniel Turek

declare

#### Description

Explicitly declare a variable in run-time code of a nimbleFunction, for cases when its dimensions cannot be inferred before it is used. Works in R and NIMBLE.

#### Usage

declare(name, def)

#### Arguments

name	Name of a variable to declare, without quotes
def	NIMBLE type declaration, of the form TYPE(nDim, sizes), where TYPE is integer, double, or logical, nDim is the number of dimensions, and sizes is an optional vector of sizes concatenated with c. If nDim is omitted, it defaults to 0, indicating a scalar. If sizes are provided, they should not be changed subsequently in the function, including by assignment. Omitting nDim results in a scalar. For logical, only scalar is currently supported.

## Details

In a run-time function of a nimbleFunction (either the run function or a function provided in methods when calling nimbleFunction), the dimensionality and numeric type of a variable is inferred when possible from the statement first assigning into it. E.g.  $A \le B + C$  infers that A has numeric types, dimensions and sizes taken from B + C. However, if the first appearance of A is e.g.  $A[i] \le 5$ , A must have been explicitly declared. In this case, declare(A, double(1)) would make A a 1-dimensional (i.e. vector) double.

When sizes are not set, they can be set by a call to setSize or by assignment to the whole object. Sizes are not automatically extended if assignment is made to elements beyond the current sizes. In compiled nimbleFunctions doing so can cause a segfault and crash the R session.

This part of the NIMBLE language is needed for compilation, but it also runs in R. When run in R, is works by the side effect of creating or modifying name in the calling environment.

#### Author(s)

NIMBLE development team

#### Examples

```
declare(A, logical())  ## scalar logical, the only kind allowed
declare(B, integer(2, c(10, 10))) ## 10 x 10 integer matrix
declare(C, double(3))  ## 3-dimensional double array with no sizes set.
```

deregisterDistributions

Remove user-supplied distributions from use in NIMBLE BUGS models

# Description

Deregister distributional information originally supplied by the user for use in BUGS model code

# Usage

```
deregisterDistributions(
   distributionsNames,
   userEnv = parent.frame(),
   warn = TRUE
)
```

### Arguments

distributionsNames

	a character vector giving the names of the distributions to be deregistered.
userEnv	environment in which to look for the nimbleFunctions that provide the distribu- tion; this will generally not need to be set by the user as it will default to the environment from which this function was called.
warn	logical indicating whether to warn if trying to deregister a distribution that is not registered (default = TRUE).

# Author(s)

Christopher Paciorek

Dirichlet

The Dirichlet Distribution

# Description

Density and random generation for the Dirichlet distribution

### Usage

ddirch(x, alpha, log = FALSE)

rdirch(n = 1, alpha)

# Arguments

х	vector of values.
alpha	vector of parameters of same length as x
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

# Details

See Gelman et al., Appendix A or the BUGS manual for mathematical details.

# Value

ddirch gives the density and rdirch generates random deviates.

### Author(s)

**Christopher Paciorek** 

### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

### See Also

Distributions for other standard distributions

# Examples

alpha <- c(1, 10, 30) x <- rdirch(1, alpha) ddirch(x, alpha)

distributionInfo Get information about a distribution

# Description

Give information about each BUGS distribution

### distributionInfo

### Usage

```
getDistributionInfo(dist)
isUserDefined(dist)
pqDefined(dist)
getType(
   dist,
   params = NULL,
   valueOnly = is.null(params) && !includeParams,
   includeParams = !is.null(params)
)
```

getParamNames(dist, includeValue = TRUE)

### Arguments

dist	a character vector of length one, giving the name of the distribution (as used in BUGS code), e.g. 'dnorm'
params	an optional character vector of names of parameters for which dimensions are desired (possibly including \'value\' and alternate parameters)
valueOnly	a logical indicating whether to only return the dimension of the value of the node
includeParams	a logical indicating whether to return dimensions of parameters. If TRUE and \'params\' is NULL then dimensions of all parameters, including the dimension of the value of the node, are returned
includeValue	a logical indicating whether to return the string 'value', which is the name of the node value

#### Details

NIMBLE provides various functions to give information about a BUGS distribution. In some cases, functions of the same name and similar functionality operate on the node(s) of a model as well (see help(modelBaseClass)).

getDistributionInfo returns an internal data structure (a reference class object) providing various information about the distribution. The output is not very user-friendly, but does contain all of the information that NIMBLE has about the distribution.

isDiscrete tests if a BUGS distribution is a discrete distribution.

isUserDefined tests if a BUGS distribution is a user-defined distribution.

pqAvail tests if a BUGS distribution provides distribution ('p') and quantile ('q') functions.

getDimension provides the dimension of the value and/or parameters of a BUGS distribution. The return value is a numeric vector with an element for each parameter/value requested.

getType provides the type (numeric, logical, integer) of the value and/or parameters of a BUGS distribution. The return value is a character vector with an element for each parameter/value requested. At present, all quantities are stored as numeric (double) values, so this function is of little practical use but could be exploited in the future.

getParamNames provides the value and/or parameter names of a BUGS distribution.

### Author(s)

Christopher Paciorek

### Examples

```
distInfo <- getDistributionInfo('dnorm')</pre>
distInfo
distInfo$range
isDiscrete('dbin')
isUserDefined('dbin')
pqDefined('dgamma')
pqDefined('dmnorm')
getDimension('dnorm')
getDimension('dnorm', includeParams = TRUE)
getDimension('dnorm', c('var', 'sd'))
getDimension('dcat', includeParams = TRUE)
getDimension('dwish', includeParams = TRUE)
getType('dnorm')
getType('dnorm', includeParams = TRUE)
getType('dnorm', c('var', 'sd'))
getType('dcat', includeParams = TRUE)
getType('dwish', includeParams = TRUE)
getParamNames('dnorm', includeValue = FALSE)
getParamNames('dmnorm')
```

Double-Exponential The Double Exponential (Laplace) Distribution

#### Description

Density, distribution function, quantile function and random generation for the double exponential distribution, allowing non-zero location, mu, and non-unit scale, sigma, or non-unit rate, tau

## Usage

```
ddexp(x, location = 0, scale = 1, rate = 1/scale, log = FALSE)
rdexp(n, location = 0, scale = 1, rate = 1/scale)
```

```
pdexp(
  q,
  location = 0,
  scale = 1,
  rate = 1/scale,
 lower.tail = TRUE,
 log.p = FALSE
)
qdexp(
  p,
  location = 0,
  scale = 1,
  rate = 1/scale,
 lower.tail = TRUE,
  log.p = FALSE
)
```

### Arguments

х	vector of values.
location	vector of location values.
scale	vector of scale values.
rate	vector of inverse scale values.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.
q	vector of quantiles.
lower.tail	logical; if TRUE (default) probabilities are $P[X \le x]$ ; otherwise, $P[X > x]$ .
log.p	logical; if TRUE, probabilities p are given by user as log(p).
р	vector of probabilities.

# Details

See Gelman et al., Appendix A or the BUGS manual for mathematical details.

# Value

ddexp gives the density, pdexp gives the distribution function, qdexp gives the quantile function, and rdexp generates random deviates.

# Author(s)

Christopher Paciorek

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

### See Also

Distributions for other standard distributions

#### Examples

```
x <- rdexp(50, location = 2, scale = 1)
ddexp(x, 2, 1)</pre>
```

eigenNimbleList eigenNimbleList definition

#### Description

nimbleList definition for the type of nimbleList returned by nimEigen.

### Usage

eigenNimbleList

## Format

An object of class list of length 1.

#### Author(s)

NIMBLE development team

### See Also

nimEigen

Exponential

The Exponential Distribution

#### Description

Density, distribution function, quantile function and random generation for the exponential distribution with rate (i.e., mean of 1/rate) or scale parameterizations.

### Usage

```
dexp_nimble(x, rate = 1/scale, scale = 1, log = FALSE)
rexp_nimble(n = 1, rate = 1/scale, scale = 1)
pexp_nimble(q, rate = 1/scale, scale = 1, lower.tail = TRUE, log.p = FALSE)
qexp_nimble(p, rate = 1/scale, scale = 1, lower.tail = TRUE, log.p = FALSE)
```

# Exponential

#### Arguments

x	vector of values.
rate	vector of rate values.
scale	vector of scale values.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.
q	vector of quantiles.
lower.tail	logical; if TRUE (default) probabilities are $P[X \le x]$ ; otherwise, $P[X > x]$ .
log.p	logical; if TRUE, probabilities p are given by user as log(p).
р	vector of probabilities.

# Details

NIMBLE's exponential distribution functions use Rmath's functions under the hood, but are parameterized to take both rate and scale and to use 'rate' as the core parameterization in C, unlike Rmath, which uses 'scale'. See Gelman et al., Appendix A or the BUGS manual for mathematical details.

### Value

dexp\_nimble gives the density, pexp\_nimble gives the distribution function, qexp\_nimble gives the quantile function, and rexp\_nimble generates random deviates.

# Author(s)

Christopher Paciorek

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

# See Also

Distributions for other standard distributions

# Examples

```
x <- rexp_nimble(50, scale = 3)
dexp_nimble(x, scale = 3)</pre>
```

extractControlElement Extract named elements from MCMC sampler control list

# Description

Extract named elements from MCMC sampler control list

# Usage

```
extractControlElement(controlList, elementName, defaultValue, error)
```

# Arguments

controlList	control list object, which is passed as an argument to all MCMC sampler setup functions.
elementName	character string, giving the name of the element to be extracted from the control list.
defaultValue	default value of the control list element, giving the value to be used when the elementName does not exactly match the name of an element in the controlList.
error	character string, giving the error message to be printed if no defaultValue is provided and elementName does not match the name of an element in the controlList.

# Value

The element of controlList whose name matches elementName. If no controlList name matches elementName, then defaultValue is returned.

### Author(s)

Daniel Turek

flat

The Improper Uniform Distribution

# Description

Improper flat distribution for use as a prior distribution in BUGS models

## getBound

# Usage

dflat(x, log = FALSE)
rflat(n = 1)
dhalfflat(x, log = FALSE)
rhalfflat(n = 1)

### Arguments

х	vector of values.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.

# Value

dflat gives the pseudo-density value of 1, while rflat and rhalfflat return NaN, since one cannot simulate from an improper distribution. Similarly, dhalfflat gives a pseudo-density value of 1 when x is non-negative.

## Author(s)

Christopher Paciorek

# See Also

Distributions for other standard distributions

# Examples

dflat(1)

 ${\tt getBound}$ 

Get value of bound of a stochastic node in a model

### Description

Get the value of the lower or upper bound for a single stochastic node in a model.

## Usage

getBound(model, node, bound, nodeFunctionIndex)

#### Arguments

model	A NIMBLE model object	
node	The name of a stochastic node in the model	
bound	Either 'lower' or 'upper' indicating the desired bound for the node	
nodeFunctionIndex		
	For internal NIMBLE use only	

## Details

Standard usage is as a method of a model, in the form model\$getBound(node, bound), but the usage as a simple function with the model as the first argument as above is also allowed.

For nodes that do not involve truncation of the distribution this will return the lower or upper bound of the distribution, which may be a constant or for a limited number of distributions a parameter or functional of a parameter (at the moment in NIMBLE, the only case where a bound is a parameter is for the uniform distribution. For nodes that are truncated, this will return the desired bound, which may be a functional of other quantities in the model or may be a constant.

getBUGSexampleDir Get the directory path to one of the classic BUGS examples installed with NIMBLE package

#### Description

NIMBLE comes with some of the classic BUGS examples. getBUGSexampleDir looks up the location of an example from its name.

#### Usage

```
getBUGSexampleDir(example)
```

#### Arguments

example The name of the classic BUGS example.

## Value

Character string of the fully pathed directory of the BUGS example.

### Author(s)

Christopher Paciorek

### See Also

readBUGSmodel for usage in creating a model from a classic BUGS example

getConditionallyIndependentSets

Get a list of conditionally independent sets of nodes in a nimble model

# Description

A conditionally independent set of nodes is such that the joint probability (density) of nodes in the set will not change even if any non-given node outside the set is changed. Default given nodes are data nodes and parameter nodes (aka "top-level" nodes, i.e. nodes with no parent nodes), but this can be controlled.

## Usage

```
getConditionallyIndependentSets(
  model,
  nodes,
  givenNodes,
  omit = integer(),
  explore = c("both", "down", "up"),
  unknownAsGiven = TRUE,
  returnType = "names",
  returnScalarComponents = FALSE,
  endAsGiven = FALSE
)
```

## Arguments

model	A nimble model object (uncompiled or compiled), such as returned by nimbleModel
nodes	A vector of stochastic node names (or their graph IDs) to split into conditionally independent sets, conditioned on the givenNodes. If unknownAsGiven=FALSE, the nodes are the starting nodes from which conditionally independent sets of nodes should be found, possibly including additional nodes not included in the nodes argument. If nodes is omitted, the default will be all latent nodes (defined as stochastic nodes that are not data and have at least one stochastic parent node, possibly with determinstic nodes in-between) that are a parent of a givenNode (either provided or default). Note that this will omit latent states that have no hyperparameters. An example is the first latent state in some state-space (time-series) models, which is sometimes declared with known prior.
givenNodes	A vector of node names or their graph IDs that should be considered as fixed (given) and hence can be conditioned on. If omitted, the default will be all data nodes and all parameter nodes, the latter defined as nodes with no stochastic parent nodes (skipping over deterministic parent nodes). See endAsGiven for a variant on defaults.
omit	A vector of node names or their graph IDs that should be omitted and should block further graph exploration.

explore	The method of graph exploration, which may corresond to what the nodes ar- gument represents. For "down", graph exploration starts only down (towards descendants) from nodes. For "up", graph exploration starts only up (towards ancestors) from nodes. For "both" (the default and normal setting), both direc- tions are explored.	
unknownAsGiven	Logical for whether a model node not in nodes or givenNodes should be treated as given (default = TRUE). Otherwise (and by default) such a node may be grouped into a conditionally independent set, resulting in more output nodes than input nodes.	
returnType	Either "names" for returned nodes to be node names or "ids" for returned nodes to be graph IDs.	
returnScalarComponents		
	If FALSE (default), multivariate nodes are returned as full names (e.g. $x[1:3]$ ). If TRUE, they are returned as scalar elements (e.g. $x[1], x[2], x[3]$ ).	
endAsGiven	If TRUE, end nodes (defined as nodes with stochastic parents but no stochastic children, skipping through deterministic nodes) are included in the default for givenNodes.	

## Details

This function returns sets of conditionally independent nodes. Multiple input nodes might be in the same set or different sets.

The nodes input and the returned sets include only stochastic nodes because conditional independence is a property of random variables. Deterministic nodes are considered in determining the sets. givenNodes may contain stochastic or deterministic nodes.

## Value

List of nodes that are in conditionally independent sets. With each set, nodes are returned in topologically sorted order. The sets themselves are returned in topologically sorted order of their first nodes.

Other nodes (not in nodes) may be included in the output if unknownAsGiven=FALSE.

### Author(s)

Perry de Valpine

getDefinition Get nimbleFunction definition

# Description

Returns a list containing the nimbleFunction definition components (setup function, run function, and other member methods) for the supplied nimbleFunction generator or specialized instance.

## getMacroParameters

# Usage

getDefinition(nf)

# Arguments

nf

A nimbleFunction generator, or a compiled or un-compiled specialized nimble-Function.

# Author(s)

Daniel Turek

getMacroParameters EXPERIMENTAL: Get list of parameter names generated by model macros

# Description

Get a list of all parameter names (or certain categories of parameters) generated by model macros in the model code.

# Usage

```
getMacroParameters(
  model,
  includeLHS = TRUE,
  includeRHS = TRUE,
  includeDeterm = TRUE,
  includeStoch = TRUE,
  includeIndexPars = FALSE
)
```

## Arguments

model	A NIMBLE model object	
includeLHS	Include generated parameters on the left-hand side (LHS) of assignments (<- or ~) in the output	
includeRHS	Include generated parameters on the left-hand side (RHS) of assignments (<- or ~) in the output	
includeDeterm	Include deterministic generated parameters in the output	
includeStoch	Include stochastic generated parameters in the output	
includeIndexPars		
	Include index parameters generated for use in for loops in the output	

### Details

Some model macros will generate new parameters to be included in the output code. NIMBLE automatically detects these new parameters and records them in the model object. This function allows easy access to this stored list, or subsets of it (see arguments).

## Value

A named list of generated parameters, with the element names corresponding to the original source macro.

## Examples

```
nimbleOptions(enableMacros = TRUE)
nimbleOptions(enableMacroComments = FALSE)
nimbleOptions(verbose = FALSE)
testMacro <- list(process = function(code, modelInfo, .env){</pre>
  code <- quote({</pre>
    for (i_ in 1:n){
      mu[i_] <- alpha + beta</pre>
      y[i_] ~ dnorm(0, sigma)
    }
    alpha ~ dnorm(0, 1)
  })
  list(code = code, modelInfo=modelInfo)
})
 class(testMacro) <- "model_macro"</pre>
code <- nimbleCode({</pre>
  y[1:n] ~ testMacro()
})
const <- list(y = rnorm(10), n = 10)</pre>
mod <- nimbleModel(code, constants=const)</pre>
mod$getMacroParameters()
# should be list(testMacro = list(c("mu", "alpha", "beta", "sigma")))
mod$getMacroParameters(includeRHS = FALSE)
# should be list(testMacro = list(c("mu", "alpha")))
```

getNimbleOption Get NIMBLE Option

### Description

Allow the user to get the value of a global \_option\_ that affects the way in which NIMBLE operates

# getParam

# Usage

getNimbleOption(x)

# Arguments

x a character string holding an option name

## Value

The value of the option.

## Author(s)

Christopher Paciorek

# Examples

getNimbleOption('verifyConjugatePosteriors')

getParam

Get value of a parameter of a stochastic node in a model

## Description

Get the value of a parameter for any single stochastic node in a model.

## Usage

```
getParam(model, node, param, nodeFunctionIndex, warn = TRUE)
```

# Arguments

model	A NIMBLE model object
node	The name of a stochastic node in the model
param	The name of a parameter for the node
nodeFunctionIn	dex
	For internal NIMBLE use only
warn	For internal NIMBLE use only

## Details

Standard usage is as a method of a model, in the form model\$getParam(node, param), but the usage as a simple function with the model as the first argument as above is also allowed.

For example, suppose node 'x[1:5]' follows a multivariate normal distribution (dmnorm) in a model declared by BUGS code. model\$getParam('x[1:5]', 'mean') would return the current value of the mean parameter (which may be determined from other nodes). The parameter requested does not have to be part of the parameterization used to declare the node. Rather, it can be any parameter known to the distribution. For example, one can request the scale or rate parameter of a gamma distribution, regardless of which one was used to declare the node.

getSamplesDPmeasure Get posterior samples for a Dirichlet process measure

## Description

This function obtains posterior samples from a Dirichlet process distributed random measure of a model specified using the dCRP distribution.

#### Usage

```
getSamplesDPmeasure(
    MCMC,
    epsilon = 1e-04,
    setSeed = FALSE,
    progressBar = getNimbleOption("MCMCprogressBar")
)
```

### Arguments

MCMC	an MCMC class object, either compiled or uncompiled.
epsilon	used for determining the truncation level of the representation of the random measure.
setSeed	Logical or numeric argument. If a single numeric value is provided, R's random number seed will be set to this value. In the case of a logical value, if TRUE, then R's random number seed will be set to 1. Note that specifying the argument setSeed = 0 does not prevent setting the RNG seed, but rather sets the random number generation seed to 0. Default value is FALSE.
progressBar	Logical specifying whether to display a progress bar during execution (default = TRUE). The progress bar can be permanently disabled by setting the system option nimbleOptions(MCMCprogressBar = FALSE)

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#### Details

This function provides samples from a random measure having a Dirichlet process prior. Realizations are almost surely discrete and represented by a (finite) stick-breaking representation (Sethuraman, 1994), whose atoms (or point masses) are independent and identically distributed. This sampler can only be used with models containing a dCRP distribution.

The MCMC argument is an object of class MCMC provided by buildMCMC, or its compiled version. The MCMC should already have been run, as getSamplesDPmeasure uses the posterior samples to generate samples of the random measure. Note that the monitors associated with that MCMC must include the cluster membership variable (which has the dCRP distribution), the cluster parameter variables, all variables directly determining the dCRP concentration parameter, and any stochastic parent variables of the cluster parameter variables. See help(configureMCMC) or help(addMonitors) for information on specifying monitors for an MCMC.

The epsilon argument is optional and used to determine the truncation level of the random measure. epsilon is the tail probability of the random measure, which together with posterior samples of the concentration parameter, determines the truncation level. The default value is 1e-4.

The output is a list of matrices. Each matrix represents a sample from the random measure. In order to reduce the output's dimensionality, the weights of identical atoms are added up. The stick-breaking weights are named weights and the atoms are named based on the cluster variables in the model.

For more details about sampling the random measure and determining its truncation level, see Section 3 in Gelfand, A.E. and Kottas, A. 2002.

#### Author(s)

Claudia Wehrhahn and Christopher Paciorek

#### References

Sethuraman, J. (1994). A constructive definition of Dirichlet priors. *Statistica Sinica*, 639-650.

Gelfand, A.E. and Kottas, A. (2002). A computational approach for full nonparametric Bayesian inference under Dirichlet process mixture models. *Journal of Computational and Graphical Statistics*, 11(2), 289-305.

#### See Also

buildMCMC, configureMCMC,

#### Examples

```
## Not run:
    conf <- configureMCMC(model)
    mcmc <- buildMCMC(conf)
    cmodel <- compileNimble(model)
    cmcmc <- compileNimble(mcmc, project = model)
    runMCMC(cmcmc, niter = 1000)
    outputG <- getSamplesDPmeasure(cmcmc)</pre>
```

## End(Not run)

getsize

# Description

Returns the number of rows of NIMBLE modelValues object. Works in R and NIMBLE.

## Usage

```
getsize(container)
```

## Arguments

container modelValues object

# Details

See the User Manual or help(modelValuesBaseClass) for information about modelValues objects

#### Author(s)

Clifford Anderson-Bergman

#### Examples

```
mvConf <- modelValuesConf(vars = 'a', types = 'double', sizes = list(a = 1) )
mv <- modelValues(mvConf)
resize(mv, 10)
getsize(mv)</pre>
```

identityMatrix Create an Identity matrix (Deprecated)

#### Description

Returns a d-by-d identity matrix (square matrix of 0's, with 1's on the main diagnol).

## Usage

```
identityMatrix(d)
```

#### Arguments

d

The size of the identity matrix to return, will return a d-by-d matrix

### initializeModel

## Details

This function can be used in NIMBLE run code. It is deprecated because now one can use diag(d) instead.

### Value

A d-by-d identity matrix

#### Author(s)

Daniel Turek

#### Examples

Id <- identityMatrix(d = 3)</pre>

initializeModel	Performs initialization of nimble model node values and log probabil- ities
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### Description

Performs initialization of nimble model node values and log probabilities

#### Usage

```
initializeModel(model, silent = FALSE)
```

## Arguments

model	A setup argument, which specializes an instance of this nimble function to a
	particular model.
silent	logical indicating whether to suppress logging information

# Details

This nimbleFunction may be used at the beginning of nimble algorithms to perform model initialization. The intended usage is to specialize an instance of this nimbleFunction in the setup function of an algorithm, then execute that specialied function at the beginning of the algorithm run function. The specialized function takes no arguments.

Executing this function ensures that all right-hand-side only nodes have been assigned real values, that all stochastic nodes have a real value, or otherwise have their simulate() method called, that all deterministic nodes have their simulate() method called, and that all log-probabilities have been calculated with the current model values. An error results if model initialization encounters a problem, for example a missing right-hand-side only node value.

Interval

#### Author(s)

Daniel Turek

## Examples

Interval

Interval calculations

## Description

Calculations to handle censoring

#### Usage

dinterval(x, t, c, log = FALSE)

rinterval(n = 1, t, c)

#### Arguments

х	vector of interval indices.
t	vector of values.
С	vector of one or more values delineating the intervals.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.

# Details

Used for working with censoring in BUGS code. Taking c to define the endpoints of two or more intervals (with implicit endpoints of plus/minus infinity), x (or the return value of rinterval) gives the non-negative integer valued index of the interval in which t falls. See the NIMBLE manual for additional details.

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## Inverse-Gamma

## Value

dinterval gives the density and rinterval generates random deviates, but these are unusual as the density is 1 if x indicates the interval in which t falls and 0 otherwise and the deviates are simply the interval(s) in which t falls.

### Author(s)

Christopher Paciorek

## See Also

Distributions for other standard distributions

### Examples

```
endpoints <- c(-3, 0, 3)
vals <- c(-4, -1, 1, 5)
x <- rinterval(4, vals, endpoints)
dinterval(x, vals, endpoints)
dinterval(c(1, 5, 2, 3), vals, endpoints)</pre>
```

Inverse-Gamma The Inverse Gamma Distribution

## Description

Density, distribution function, quantile function and random generation for the inverse gamma distribution with rate or scale (mean = scale / (shape - 1)) parameterizations.

## Usage

```
dinvgamma(x, shape, scale = 1, rate = 1/scale, log = FALSE)
rinvgamma(n = 1, shape, scale = 1, rate = 1/scale)
pinvgamma(
    q,
    shape,
    scale = 1,
    rate = 1/scale,
    lower.tail = TRUE,
    log.p = FALSE
)
qinvgamma(
    p,
    shape,
    scale = 1,
```

```
rate = 1/scale,
lower.tail = TRUE,
log.p = FALSE
)
```

## Arguments

x	vector of values.
shape	vector of shape values, must be positive.
scale	vector of scale values, must be positive.
rate	vector of rate values, must be positive.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.
q	vector of quantiles.
lower.tail	logical; if TRUE (default) probabilities are $P[X \le x]$ ; otherwise, $P[X > x]$ .
log.p	logical; if TRUE, probabilities p are given by user as log(p).
р	vector of probabilities.

## Details

The inverse gamma distribution with parameters shape  $= \alpha$  and scale  $= \sigma$  has density

$$f(x) = \frac{s^a}{\Gamma(\alpha)} x^{-(\alpha+1)} e^{-\sigma/x}$$

for  $x \ge 0$ ,  $\alpha > 0$  and  $\sigma > 0$ . (Here  $\Gamma(\alpha)$  is the function implemented by R's gamma() and defined in its help.

The mean and variance are  $E(X) = \frac{\sigma}{\alpha} - 1$  and  $Var(X) = \frac{\sigma^2}{(\alpha-1)^2(\alpha-2)}$ , with the mean defined only for  $\alpha > 1$  and the variance only for  $\alpha > 2$ .

See Gelman et al., Appendix A or the BUGS manual for mathematical details.

## Value

dinvgamma gives the density, pinvgamma gives the distribution function, qinvgamma gives the quantile function, and rinvgamma generates random deviates.

## Author(s)

**Christopher Paciorek** 

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

### See Also

Distributions for other standard distributions

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## Inverse-Wishart

### Examples

```
x <- rinvgamma(50, shape = 1, scale = 3)
dinvgamma(x, shape = 1, scale = 3)
```

Inverse-Wishart The Inverse Wishart Distribution

## Description

Density and random generation for the Inverse Wishart distribution, using the Cholesky factor of either the scale matrix or the rate matrix.

### Usage

dinvwish\_chol(x, cholesky, df, scale\_param = TRUE, log = FALSE)
rinvwish\_chol(n = 1, cholesky, df, scale\_param = TRUE)

## Arguments

х	vector of values.
cholesky	upper-triangular Cholesky factor of either the scale matrix (when scale_param is TRUE) or rate matrix (otherwise).
df	degrees of freedom.
scale_param	logical; if TRUE the Cholesky factor is that of the scale matrix; otherwise, of the rate matrix.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

### Details

See Gelman et al., Appendix A for mathematical details. The rate matrix as used here is defined as the inverse of the scale matrix,  $S^{-1}$ , given in Gelman et al.

# Value

dinvwish\_chol gives the density and rinvwish\_chol generates random deviates.

## Author(s)

**Christopher Paciorek** 

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

# See Also

Distributions for other standard distributions

## Examples

```
df <- 40
ch <- chol(matrix(c(1, .7, .7, 1), 2))
x <- rwish_chol(1, ch, df = df)
dwish_chol(x, ch, df = df)</pre>
```

is.nf

#### check if a nimbleFunction

## Description

Checks an object to determine if it is a nimbleFunction (i.e., a function created by nimbleFunction using setup code).

#### Usage

is.nf(f, inputIsName = FALSE, where = -1)

# Arguments

f	object to be tested
inputIsName	logical indicating whether the function is provided as the character name of the function or the function object itself
where	Optional argument needed due to R package namespace issues but which should not need to be provided by a user.

# See Also

nimbleFunction for how to create a nimbleFunction

is.nl

# Description

Checks an object to determine if it is a nimbleList (i.e., a list created by nlDef\$new()).

# Usage

is.nl(l)

## Arguments

1

object to be tested

# See Also

nimbleList for how to create a nimbleList

LKJ

The LKJ Distribution for the Cholesky Factor of a Correlation Matrix

# Description

Density and random generation for the LKJ distribution for the Cholesky factor of a correlation matrix.

# Usage

dlkj\_corr\_cholesky(x, eta, p, log = FALSE)

```
rlkj_corr_cholesky(n = 1, eta, p)
```

### Arguments

х	upper-triangular Cholesky factor of a correlation matrix.
eta	shape parameter.
р	size of the correlation matrix (number of rows and columns); required because random generation function has no information about dimension of matrix to generate without this argument.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

See Stan Development Team for mathematical details.

# Value

dlkj\_corr\_cholesky gives the density and rlkj\_corr\_cholesky generates random deviates.

## Author(s)

Christopher Paciorek

# References

Stan Development Team. Stan Reference Functions, version 2.27.

## See Also

Distributions for other standard distributions

#### Examples

```
eta <- 3
x <- rlkj_corr_cholesky(1, eta, 5)
dlkj_corr_cholesky(x, eta, 5)</pre>
```

makeBoundInfo	Make an object of information about a model-bound pairing for get-
	Bound. Used internally

## Description

Creates a simple getBound\_info object, which has a list with a boundID and a type. Unlike makeParamInfo this is more bare-bones, but keeping it for parallelism with getParam.

## Usage

makeBoundInfo(model, nodes, bound)

#### Arguments

model	A model such as returned by nimbleModel.
nodes	A character string naming a stochastic nodes, such as 'mu'.
bound	A character string naming a bound of the distribution, either 'lower' or 'upper'.

# Details

This is used internally by getBound. It is not intended for direct use by a user or even a nimble-Function programmer. makeModelDerivsInfo Information on model structure used for derivatives

#### Description

Inspect structure of a nimble model to determine nodes needed as "update" and/or "constant" entries in usage of nimDerivs. This will typically be used in the setup code of a nimbleFunction.

#### Usage

makeModelDerivsInfo(model, wrtNodes, calcNodes, dataAsConstantNodes = TRUE)

#### Arguments

model	a nimble model object, such as returned from nimbleModel.
wrtNodes	a character vector of node names in the model with respect to which derivatives will be taken through a call to nimDerivs (same as derivs).
calcNodes	a character vector of node names in the model that will be used in model\$calculate(calcNodes) while derivatives are being recorded.
dataAsConstantNodes	
	logical indicating whether data nodes in the model should automatically be
	treated as "constant" entries (TRUE) or "update" entries (FALSE). Defaults to
	TRUE.

#### Details

In the compilable parts of a nimbleFunction (i.e. run or other method code, not setup code), a call like nimDerivs(foo(x), ...) records derivatives of foo(x). If foo contains any calls to model\$calculate(calcNodes), it may be necessary to provide auxiliary information about the model in further arguments to nimDerivs, specifically the model, updateNodes and constantNodes arguments. 'makeModelDerivsInfo' is a utility to set up that information for typical use cases. It returns a list with elements updateNodes and constantNodes to be passed as arguments of the same name to nimDerivs (along with passing the model as the model argument).

The reason auxiliary information is needed is that recording of derivatives uses a different model than for regular calculations. Together, updateNodes and constantNodes should contain all nodes whose values are needed for the model calculations being recorded and that are not part of wrtNodes. These may include parents of nodes that are in calcNodes but are not themselves in calcNodes, as well as the values of stochastic nodes in calcNodes, which are needed to calculate the corresponding log probabilities. updateNodes will have their values updated from the regular model every time that recorded derivative calculations are used. constantNodes will not be updated every time, which means their values will be permanently fixed either the first time the call to 'nimDerivs' is invoked or on any subsequent call that has reset=TRUE. Use of constantNodes can be slightly more efficient, but one must be careful to be aware that values will not be updated unless reset=TRUE. See the automatic differentiation section of the User Manual for more information.

In the above explanation, care must be taken to understand what should be included in wrtNodes. In a typical use case, some arguments to foo are put into the model using values(model, nodes) <-some\_foo\_arguments. Next there is typically a call to model\$calculate(calcNodes). Here the nodes are considered "with-respect-to" nodes because derivative tracking will follow the arguments of foo, including when they are put into a model and hence used in model\$calculate. Therefore these nodes should be the wrtNodes for makeModelDerivsInfo.

#### Value

A list with elements updateNodes and constantNodes. These shouls be provided as the samenamed arguments to nimDerivs (same as derivs).

When using double-taping of derivatives (i.e. foo contains another call to nimDerivs), both calls to nimDerivs should include the model, updateNodes, and constantNodes arguments.

makeParamInfo	Make an object of information about a model-parameter pairing for
	getParam. Used internally

## Description

Creates a simple getParam\_info object, which has a list with a paramID and a type

# Usage

```
makeParamInfo(model, nodes, param, vector = FALSE)
```

### Arguments

model	A model such as returned by nimbleModel.
nodes	A character string naming one one or more stochastic nodes, such as "mu", "c('mu', 'beta[2]')", or "eta[1:3, 2]". getParam only works for one node at a time, but if it is indexed (nodes[i]), then makeParamInfo sets up the information for the entire vector nodes. The processing pathway is used by the NIMBLE compiler.
param	A character string naming a parameter of the distribution followed by node, such as "mean", "rate", "lambda", or whatever parameter names are relevant for the distribution of the node.
vector	A logical indicating whether nodes should definitely be treated as a vector in compiled code, even if it has length $= 1$ . For type consistency, the compiler needs this option. If nodes has length $> 1$ , this argument is ignored.

#### Details

This is used internally by getParam. It is not intended for direct use by a user or even a nimble-Function programmer.

#### Description

Objects of this class configure an MCMC algorithm, specific to a particular model. Objects are normally created by calling configureMCMC. Given an MCMCconf object, the actual MCMC function can be built by calling buildMCMC(conf). See documentation below for method initialize() for details of creating an MCMCconf object.

#### Methods

addDefaultSampler( nodes = character(), control = list(), useConjugacy = getNimbleOption("MCMCuseConjuga For internal use. Adds default MCMC samplers to the specified nodes.

addMonitors(..., ind = 1, print = TRUE) Adds variables to the list of monitors.

Arguments:

...: One or more character vectors of indexed nodes, or variables, which are to be monitored. These are added onto the current monitors list.

print: A logical argument specifying whether to print all current monitors (default TRUE). Details:

See the initialize() function

addMonitors2(..., print = TRUE) Adds variables to the list of monitors2.

Arguments:

...: One or more character vectors of indexed nodes, or variables, which are to be monitored. These are added onto the current monitors2 list.

print: A logical argument specifying whether to print all current monitors (default TRUE). Details:

See the initialize() function

addOneSampler(thisSamplerName, samplerFunction, targetOne, thisControlList, allowData, print) For internal use only

addSampler( target = character(), type = "RW", control = list(), print = NULL, name, targetByNode = FALSE, n Adds a sampler to the list of samplers contained in the MCMCconf object.

Arguments:

target: The target node or nodes to be sampled. This may be specified as a character vector of model node and/or variable names. For univariate samplers, only a single target node should be provided (unless 'targetByNode' is TRUE). For multivariate samplers, one instance of the multivariate sampler will be assigned to all nodes specified. Nodes are specified in combination with the 'targetByNode' and 'multivariateNodesAsScalars' arguments.

type: When 'default' is FALSE, specifies the type of sampler to add, specified as either a character string or a nimbleFunction object. If the character argument type='newSamplerType', then either newSamplerType or sampler\_newSamplerType must correspond to a nimbleFunction (i.e. a function returned by nimbleFunction, not a specialized nimbleFunction). Alternatively, the type argument may be provided as a nimbleFunction itself rather than its name. In that case, the 'name' argument may also be supplied to provide a meaningful name for this sampler. The default value is 'RW' which specifies scalar adaptive Metropolis-Hastings sampling with a normal proposal distribution. This default will result in an error if 'target' specifies more than one target node (unless 'targetByNode' is TRUE). This argument is not used when the 'default' argument is TRUE.

control: An optional list of control arguments to sampler functions. These will override those specified in the control list argument to configureMCMC. If a control list is provided, the elements will be provided to all sampler functions which utilize the named elements given. For example, the standard Metropolis-Hastings random walk sampler (sampler\_RW) utilizes control list elements 'adaptive', 'adaptInterval', 'scale'. The default values for control list arguments for samplers (if not otherwise provided as an argument to configureMCMC or addSampler) are contained in the setup code of each sampling algorithm.

print: Logical argument, specifying whether to print the details of newly added sampler(s).

name: Optional character string name for the sampler, which is used by the printSamplers method. If 'name' is not provided, the 'type' argument is used to generate the sampler name.

targetByNode: Logical argument, with default FALSE. This arguments controls whether separate instances of the specified sampler 'type' should be assigned to each node contained in 'target'. When FALSE, a single instance of sampler 'type' is assigned to operate on 'target'. When TRUE, potentially multiple instances of sampler 'type' will be added to the MCMC configuration, operating on the distinct nodes which compose 'target'. For example, if 'target' is a vector of distinct node names, then a separate sampler will be assigned to each node in this vector. If 'target' is a model variable which itself is comprised of multiple distinct nodes, then a separate sampler is assigned to each node composing the 'target' variable. Additional control of the handling of multivariate nodes is provided using the 'multivariateNodesAsScalars' argument.

multivariateNodesAsScalars: Logical argument, with default value FALSE. This argument is used in two ways. Functionally, both uses result in separate instances of samplers being added to the scalar components which compose multivariate nodes. See details below.

silent: Logical argument, specifying whether to print warning messages when assigning samplers.

default: Logical argument, with default value FALSE. When FALSE, the 'type' argument dictates what sampling algorithm is assigned to the specified nodes. When TRUE, default samplers will be assigned to the specified nodes following the same logic as the configureMCMC method, and also using the 'useConjugacy', 'onlyRW', 'onlySlice' and 'multivariateNodesAsScalars' arguments.

useConjugacy: Logical argument, with default value TRUE. If specified as FALSE, then no conjugate samplers will be used, even when a node is determined to be in a conjugate relationship. This argument is only used when the 'default' argument is TRUE.

onlyRW: Logical argument, with default value FALSE. If specified as TRUE, then Metropolis-Hastings random walk samplers will be assigned for all non-terminal continuous-valued nodes nodes. Discrete-valued nodes are assigned a slice sampler, and terminal nodes are assigned a posterior\_predictive sampler. This argument is only used when the 'default' argument is TRUE.

onlySlice: Logical argument, with default value FALSE. If specified as TRUE, then a slice sampler is assigned for all non-terminal nodes. Terminal nodes are still assigned a posterior\_predictive sampler. This argument is only used when the 'default' argument is TRUE.

allowData: Logical argument, with default value FALSE. When FALSE, samplers will not be assigned to operate on data nodes, even if data nodes are included in 'target'. When TRUE,

samplers will be assigned to 'target' without regard to whether nodes are designated as data. ...: Additional named arguments passed through ... will be used as additional control list elements.

Details:

Samplers are added to the end of the list of samplers for this MCMCconf object, and do not replace any existing samplers. Samplers are removed using the removeSamplers method.

Invisibly returns a list of the current sampler configurations, which are samplerConf reference class objects.

'multivariateNodesAsScalars' has two usages. The first usage occurs when 'targetByNode' is TRUE and therefore separate instances of sampler 'type' are assigned to each node which compose 'target'. In this first usage, this argument controls how multivariate nodes (those included in the 'target') are handled. If FALSE, any multivariate nodes in 'target' have a single instance of sampler 'type' assigned. If TRUE, any multivariate nodes appearing in 'target' are themselves decomposed into their scalar elements, and a separate instance of sampler 'type' is assigned to operate on each scalar element.

The second usage of 'multivariateNodesAsScalars' occurs when 'default' is TRUE, and therefore samplers are assigned according to the default logic of configureMCMC, which is further controlled by the arguments 'useConjugacy', 'onlyRW', 'onlySlice' and 'multivariateNodesAsScalars'. In this second usage, if 'multivariateNodesAsScalars' is TRUE, then multivariate nodes will be decomposed into their scalar components, and separate samplers assigned to each scalar element. Note, however, that multivariate nodes appearing in conjugate relationships will still be assigned the corresponding conjugate sampler (provided 'useConjugacy' is TRUE), regardless of the value of this argument. If 'multivariateNodesAsScalars' is FALSE, then a single multivarate sampler will be assigned to update each multivariate node. The default value of this argument can be controlled using the nimble option 'MCMCmultivariateNodesAsScalars'.

getMonitors() Returns a character vector of the current monitors

Details:

See the initialize() function

getMonitors2() Returns a character vector of the current monitors2

Details:

See the initialize() function

getSamplerDefinition(ind, print = FALSE) Returns the nimbleFunction definition of an MCMC sampler.

Arguments:

ind: A numeric vector or character vector. A numeric vector may be used to specify the index of the sampler definition to return, or a character vector may be used to indicate a target node for which the sampler acting on this nodes will be printed. For example, getSamplerDefinition('x[2]') will return the definition of the sampler whose target is model node 'x[2]'. If more than one sampler function is specified, only the first is returned.

Returns a list object, containing the setup function, run function, and additional member methods for the specified nimbleFunction sampler.

getSamplerExecutionOrder() Returns a numeric vector, specifying the ordering of sampler function execution.

The indices of execution specified in this numeric vector correspond to the enumeration of samplers printed by printSamplers(), or returned by getSamplers().

getSamplers(ind) Returns a list of samplerConf objects.

Arguments:

ind: A numeric vector or character vector. A numeric vector may be used to specify the indices of the samplerConf objects to return, or a character vector may be used to indicate a set of target nodes and/or variables, for which all samplers acting on these nodes will be returned. For example, getSamplers('x') will return all samplerConf objects whose target is model node 'x', or whose targets are contained (entirely or in part) in the model variable 'x'. If omitted, then all samplerConf objects in this MCMC configuration object are returned.

initialize( model, nodes, control = list(), monitors, thin = 1, monitors2 = character(), thin2 = 1, useConj Creates a MCMC configuration for a given model. The resulting object is suitable as an argument to buildMCMC.

Arguments:

model: A NIMBLE model object, created from nimbleModel(...)

nodes: An optional character vector, specifying the nodes for which samplers should be created. Nodes may be specified in their indexed form, 'y[1, 3]', or nodes specified without indexing will be expanded fully, e.g., 'x' will be expanded to 'x[1]', 'x[2]', etc. If missing, the default value is all non-data stochastic nodes. If NULL, then no samplers are added.

control: An optional list of control arguments to sampler functions. If a control list is provided, the elements will be provided to all sampler functions which utilize the named elements given. For example, the standard Metropolis-Hastings random walk sampler (sampler\_RW) utilizes control list elements 'adaptive', 'adaptInterval', 'scale'. The default values for control list arguments for samplers (if not otherwise provided as an argument to configureMCMC() or addSampler()) are contained in the setup code of each sampling algorithm.

monitors: A character vector of node names or variable names, to record during MCMC sampling. This set of monitors will be recorded with thinning interval 'thin', and the samples will be stored into the 'mvSamples' object. The default value is all top-level stochastic nodes of the model – those having no stochastic parent nodes.

monitors2: A character vector of node names or variable names, to record during MCMC sampling. This set of monitors will be recorded with thinning interval 'thin2', and the samples will be stored into the 'mvSamples2' object. The default value is an empty character vector, i.e. no values will be recorded.

thin: The thinning interval for 'monitors'. Default value is one.

thin2: The thinning interval for 'monitors2'. Default value is one.

useConjugacy: A logical argument, with default value TRUE. If specified as FALSE, then no conjugate samplers will be used, even when a node is determined to be in a conjugate relationship.

onlyRW: A logical argument, with default value FALSE. If specified as TRUE, then Metropolis-Hastings random walk samplers will be assigned for all non-terminal continuous-valued nodes nodes. Discrete-valued nodes are assigned a slice sampler, and terminal nodes are assigned a posterior\_predictive sampler.

onlySlice: A logical argument, with default value FALSE. If specified as TRUE, then a slice sampler is assigned for all non-terminal nodes. Terminal nodes are still assigned a posterior\_predictive sampler.

multivariateNodesAsScalars: A logical argument, with default value FALSE. If specified as TRUE, then non-terminal multivariate stochastic nodes will have scalar samplers assigned to each of the scalar components of the multivariate node. The default value of FALSE results

in a single block sampler assigned to the entire multivariate node. Note, multivariate nodes appearing in conjugate relationships will be assigned the corresponding conjugate sampler (provided useConjugacy == TRUE), regardless of the value of this argument.

enableWAIC: A logical argument, specifying whether to enable WAIC calculations for the resulting MCMC algorithm. Defaults to the value of nimbleOptions('MCMCenableWAIC'), which in turn defaults to FALSE. Setting nimbleOptions('MCMCenableWAIC' = TRUE) will ensure that WAIC is enabled for all calls to 'configureMCMC' and 'buildMCMC'.

controlWAIC A named list of inputs that control the behavior of the WAIC calculation, passed as the 'control' input to 'buildWAIC'. See 'help(waic)'.

print: A logical argument specifying whether to print the montiors and samplers. Default is TRUE.

...: Additional named control list elements for default samplers, or additional arguments to be passed to the autoBlock function when autoBlock = TRUE.

printMonitors() Prints all current monitors and monitors2

Details:

See the initialize() function

Arguments:

...: Character node or variable names, or numeric indices. Numeric indices may be used to specify the indices of the samplers to print, or character strings may be used to indicate a set of target nodes and/or variables, for which all samplers acting on these nodes will be printed. For example, printSamplers('x') will print all samplers whose target is model node 'x', or whose targets are contained (entirely or in part) in the model variable 'x'. If omitted, then all samplers are printed.

ind: A numeric vector or character vector. A numeric vector may be used to specify the indices of the samplers to print, or a character vector may be used to indicate a set of target nodes and/or variables, for which all samplers acting on these nodes will be printed. For example, printSamplers('x') will print all samplers whose target is model node 'x', or whose targets are contained (entirely or in part) in the model variable 'x'. If omitted, then all samplers are printed.

type: a character vector containing sampler type names. Only samplers with one of these specified types, as printed by this printSamplers method, will be displayed. Standard regular expression mathing using is also applied.

displayConjugateDependencies: A logical argument, specifying whether to display the dependency lists of conjugate samplers (default FALSE).

displayNonScalars: A logical argument, specifying whether to display the values of non-scalar control list elements (default FALSE).

executionOrder: A logical argument, specifying whether to print the sampler functions in the (possibly modified) order of execution (default FALSE).

byType: A logical argument, specifying whether the nodes being sampled should be printed, sorted and organized according to the type of sampler (the sampling algorithm) which is acting on the nodes (default FALSE).

removeSampler(...) Alias for removeSamplers method

removeSamplers(..., ind, print = FALSE) Removes one or more samplers from an MCMCconf object. This function also has the side effect of resetting the sampler execution ordering so as to iterate over the remaining set of samplers, sequentially, executing each sampler once. Arguments:

...: Character node names or numeric indices. Character node names specify the node names for samplers to remove, or numeric indices can provide the indices of samplers to remove.

ind: A numeric vector or character vector specifying the samplers to remove. A numeric vector may specify the indices of the samplers to be removed. Alternatively, a character vector may be used to specify a set of model nodes and/or variables, and all samplers whose 'target' is among these nodes will be removed. If omitted, then all samplers are removed.

print: A logical argument specifying whether to print the current list of samplers once the removal has been done (default FALSE).

replaceSampler(...) Alias for replaceSamplers method

replaceSamplers(...) Replaces one or more samplers from an MCMCconf object with newly specified sampler(s). Operation and arguments are identical to the 'addSampler' method, with the additional side effect of first removing any existing samplers which operate on the specified node(s).

This function also has the side effect of resetting the sampler execution ordering so as to iterate over the remaining set of samplers, sequentially, executing each sampler once.

See 'addSamplers' for a description of the arguments.

This function also has the side effect of resetting the sampler execution ordering so as to iterate over the newly specified set of samplers, sequentially, executing each sampler once.

resetMonitors() Resets the current monitors and monitors2 lists to nothing.

Details:

See the initialize() function

setMonitors(..., ind = 1, print = TRUE) Sets new variables to the list of monitors.

Arguments:

...: One or more character vectors of indexed nodes, or variables, which are to be monitored. These replace the current monitors list.

print: A logical argument specifying whether to print all current monitors (default TRUE). Details:

See the initialize() function

setMonitors2(..., print = TRUE) Sets new variables to the list of monitors2.

Arguments:

...: One or more character vectors of indexed nodes, or variables, which are to be monitored. These replace the current monitors2 list.

print: A logical argument specifying whether to print all current monitors (default TRUE). Details:

See the initialize() function

setSampler(...) Alias for setSamplers method

setSamplerExecutionOrder(order, print = FALSE) Sets the ordering in which sampler functions will execute.

This allows some samplers to be "turned off", or others to execute multiple times in a single MCMC iteration. The ordering in which samplers execute can also be interleaved.

#### Arguments:

order: A numeric vector, specifying the ordering in which the sampler functions will execute. The indices of execution specified in this numeric vector correspond to the enumeration of samplers printed by printSamplers(), or returned by getSamplers(). If this argument is omitted, the sampler execution ordering is reset so as to sequentially execute each sampler once.

print: A logical argument specifying whether to print the current list of samplers in the modified order of execution (default FALSE).

setSamplers(..., ind, print = FALSE) Sets the ordering of the list of MCMC samplers.

This function also has the side effect of resetting the sampler execution ordering so as to iterate over the specified set of samplers, sequentially, executing each sampler once.

Arguments:

...: Chracter strings or numeric indices. Character names may be used to specify the node names for samplers to retain. Numeric indices may be used to specify the indices for the new list of MCMC samplers, in terms of the current ordered list of samplers.

ind: A numeric vector or character vector. A numeric vector may be used to specify the indicies for the new list of MCMC samplers, in terms of the current ordered list of samplers. For example, if the MCMCconf object currently has 3 samplers, then the ordering may be reversed by calling MCMCconf\$setSamplers(3:1), or all samplers may be removed by calling MCMCconf\$setSamplers(0)).

Alternatively, a character vector may be used to specify a set of model nodes and/or variables, and the sampler list will modified to only those samplers acting on these target nodes.

As another alternative, a list of samplerConf objects may be used as the argument, in which case this ordered list of samplerConf objects will define the samplers in this MCMC configuration object, completely over-writing the current list of samplers. No checking is done to ensure the validity of the contents of these samplerConf objects; only that all elements of the list argument are, in fact, samplerConf objects.

print: A logical argument specifying whether to print the new list of samplers (default FALSE).

setThin(thin, print = TRUE, ind = 1) Sets the value of thin.

Arguments:

thin: The new value for the thinning interval 'thin'.

print: A logical argument specifying whether to print all current monitors (default TRUE). Details:

See the initialize() function

setThin2(thin2, print = TRUE) Sets the value of thin2.

Arguments:

thin2: The new value for the thinning interval 'thin2'.

print: A logical argument specifying whether to print all current monitors (default TRUE). Details:

See the initialize() function

#### Author(s)

Daniel Turek

## See Also

configureMCMC

## Examples

```
code <- nimbleCode({
  mu ~ dnorm(0, 1)
  x ~ dnorm(mu, 1)
})
Rmodel <- nimbleModel(code)
conf <- configureMCMC(Rmodel)
conf$setSamplers(1)
conf$setSampler(target = 'x', type = 'slice', control = list(adaptInterval = 100))
conf$addSampler(target = 'x', type = 'slice', control = list(adaptInterval = 100))
conf$addMonitors('mu')
conf$addMonitors2('x')
conf$setThin(5)
conf$setThin2(10)
conf$printMonitors()
conf$printSamplers()</pre>
```

modelBaseClass-class Class modelBaseClass

## Description

This class underlies all NIMBLE model objects: both R model objects created from the return value of nimbleModel(), and compiled model objects. The model object contains a variety of member functions, for providing information about the model structure, setting or querying properties of the model, or accessing various internal components of the model. These member functions of the modelBaseClass are commonly used in the body of the setup function argument to nimbleFunction(), to aid in preparation of node vectors, nimbleFunctionLists, and other runtime inputs. See documentation for nimbleModel for details of creating an R model object.

### Methods

calculate(nodes) See 'help(calculate)'

calculateDiff(nodes) See 'help(calculateDiff)'

- check() Checks for errors in model specification and for missing values that prevent use of calculate/simulate on any nodes
- checkBasics() Checks for size/dimension mismatches and for presence of NAs in model variables (the latter is not an error but a note of this is given to the user)

Arguments:

nodeVector: A character vector specifying one or more node or variable names. If omitted, all stochastic non-data nodes are checked for conjugacy.

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Details: The return value is a named list, with an element corresponding to each conjugate node. The list names are the conjugate node names, and list elements are the control list arguments required by the corresponding MCMC conjugate sampler functions. If no model nodes are conjugate, an empty list is returned.

expandNodeNames( nodes, env = parent.frame(), returnScalarComponents = FALSE, returnType = "names", sort Takes a vector of names of nodes or variables and returns the unique and expanded names in the model, i.e. 'x' expands to 'x[1]', 'x[2]', ...

Arguments:

nodes: a vector of names of nodes (or variables) to be expanded. Alternatively, can be a vector of integer graph IDs, but this use is intended only for advanced users

returnScalarComponents: should multivariate nodes (i.e. dmnorm or dmulti) be broken up into scalar components?

returnType: return type. Options are 'names' (character vector) or 'ids' (graph IDs)

sort: should names be topologically sorted before being returned?

unique: should names be the unique names or should original ordering of nodes (after expansion of any variable names into node names) be preserved

- getBound(node, bound) See 'help(getBound)'
- getCode() Return the code for a model after processing if-then-else statements, expanding macros, and replacing some keywords (e.g. nimStep for step) to avoid R ambiguity.
- getConditionallyIndependentSets( nodes, givenNodes, omit = integer(), explore = c("both", "down", "up"), see "help(getConditionallyIndependentSets)", which this calls with the model as the first argument.

getConstants() Return model constants, including any changes to the constants made by macros.

getDependencies( nodes, omit = character(), self = TRUE, determOnly = FALSE, stochOnly = FALSE, includeDat Returns a character vector of the nodes dependent upon the input argument nodes, sorted topologically according to the model graph. In the genealogical metaphor for a graphical model, this function returns the "children" of the input nodes. In the river network metaphor, it returns downstream nodes. By default, the returned nodes include the input nodes, include both deterministic and stochastic nodes, and stop at stochastic nodes. Additional input arguments provide flexibility in the values returned.

Arguments:

nodes: Character vector of node names, with index blocks allowed, and/or variable names, the dependents of which will be returned.

omit: Character vector of node names, which will be omitted from the nodes returned. In addition, dependent nodes subsequent to these omitted nodes will not be returned. The omitted nodes argument serves to stop the downward search within the hierarchical model structure, and excludes the specified node.

self: Logical argument specifying whether to include the input argument nodes in the return vector of dependent nodes. Default is TRUE.

determOnly: Logical argument specifying whether to return only deterministic nodes. Default is FALSE.

stochOnly: Logical argument specifying whether to return only stochastic nodes. Default is FALSE. If both determOnly and stochOnly are TRUE, no nodes will be returned.

includeData: Logical argument specifying whether to include 'data' nodes (set via nimble-Model or the setData method). Default is TRUE.

dataOnly: Logical argument specifying whether to return only 'data' nodes. Default is FALSE. includePredictive: Logical argument specifying whether to include predictive nodes. Predictive nodes are stochastic nodes that are not data and have no downstream stochastic dependents that are data. In Bayesian settings, these are "posterior predictive" nodes. Used primarily to exclude predictive node calculations when setting up MCMC samplers on model parameters. Default value is controlled by 'nimbleOptions("getDependenciesIncludesPredictiveNodes")', which has a default value of 'TRUE'.

predictiveOnly: Logical argument specifying whether to return only predictive nodes (see "includePredictive"). Default is FALSE.

includeRHSonly: Logical argument specifying whether to include right-hand-side-only nodes (model nodes which never appear on the left-hand-side of  $\sim$  or <- in the model code). These nodes are neither stochastic nor deterministic, but instead function as variable inputs to the model. Default is FALSE.

downstream: Logical argument specifying whether the downward search through the hierarchical model structure should continue beyond the first and subsequent stochastic nodes encountered, hence returning all nodes downstream of the input nodes. Default is FALSE.

returnType: Character argument specifying type of object returned. Options are 'names' (returns character vector) and 'ids' (returns numeric graph IDs for model).

returnScalarComponenets: Logical argument specifying whether multivariate nodes should be returned as full node names (i.e. 'x[1:2]') or as scalar componenets (i.e. 'x[1]' and 'x[2]'). Details: The downward search for dependent nodes propagates through deterministic nodes, but by default will halt at the first level of stochastic nodes encountered. Use getDependenciesList for a list of one-step dependent nodes of each node in the model.

getDependenciesList(returnNames = TRUE, sort = TRUE) Returns a list of all dependent neighbor relationships. Each list element gives the one-step dependencies of one vertex, and the element name is the vertex label (integer ID or character node name)

Arguments:

returnNames: If TRUE (default), list names and element contents are returns as character node names, e.g. 'x[1]'. If FALSE, everything is returned using graph IDs, which are unique integer labels for each node.

sort: If TRUE (default), each list element is returned in topologically sorted order. If FALSE, they are returned in arbitrary order.

Details: This provides a fairly raw representation of the graph (model) structure that may be useful for inspecting what NIMBLE has created from model code.

getDimension( node, params = NULL, valueOnly = is.null(params) && !includeParams, includeParams = !is.nul Determines the dimension of the value and/or parameters of the node

Arguments:

node: A character vector specifying a single node

params: an optional character vector of names of parameters for which dimensions are desired (possibly including 'value' and alternate parameters)

valueOnly: a logical indicating whether to only return the dimension of the value of the node includeParams: a logical indicating whether to return dimensions of parameters. If TRUE and 'params' is NULL then dimensions of all parameters, including the dimension of the value of the node, are returned

Details: The return value is a numeric vector with an element for each parameter/value requested. getDistribution(nodes) Returns the names of the distributions for the requested node or nodes Arguments:

nodes: A character vector specifying one or more node or variable names.

Details: The return value is a character vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent node names, so the length of the output may be longer than that of the input.

getDownstream(...) Identical to getDependencies(..., downstream = TRUE)

Details: See documentation for member method getDependencies.

getLogProb(nodes) See 'help(getLogProb)'

getMacroInits() EXPERIMENTAL: Return initial values generated by macros.

- getMacroParameters( includeLHS = TRUE, includeRHS = TRUE, includeDeterm = TRUE, includeStoch = TRUE, inclu See 'help(getMacroParameters)'
- getNodeNames( determOnly = FALSE, stochOnly = FALSE, includeData = TRUE, dataOnly = FALSE, includeRHSonly =
  Returns a character vector of all node names in the model, in topologically sorted order. A
  variety of logical arguments allow for flexible subsetting of all model nodes.

Arguments:

determOnly: Logical argument specifying whether to return only deterministic nodes. Default is FALSE.

stochOnly: Logical argument specifying whether to return only stochastic nodes. Default is FALSE.

includeData: Logical argument specifying whether to include 'data' nodes (set via the member method setData). Default is TRUE.

dataOnly: Logical argument specifying whether to return only 'data' nodes. Default is FALSE. includeRHSonly: Logical argument specifying whether to include right-hand-side-only nodes (model nodes which never appear on the left-hand-side of ~ or <- in the model code). Default is FALSE.

topOnly: Logical argument specifying whether to return only top-level nodes from the hierarchical model structure.

latentOnly: Logical argument specifying whether to return only latent (mid-level) nodes from the hierarchical model structure.

endOnly: Logical argument specifying whether to return only end nodes from the hierarchical model structure.

includePredictive: Logical argument specifying whether to include predictive nodes (stochastic nodes, which themselves are not data and have no downstream stochastic dependents which are data) from the hierarchical model structure.

predictiveOnly: Logical argument specifying whether to return only predictive nodes (stochastic nodes, which themselves are not data and have no downstream stochastic dependents which are data) from the hierarchical model structure.

returnType: Character argument specific type object returned. Options are 'names' (returns character vector) and 'ids' (returns numeric graph IDs for model)

returnScalar Componenets: Logical argument specifying whether multivariate nodes should return full node name (i.e. 'x[1:2]') or should break down into scalar componenets (i.e. 'x[1]' and 'x[2]')

Details: Multiple logical input arguments may be used simultaneously. For example, 'model\$getNodeNames(endOnly = TRUE, dataOnly = TRUE)' will return all end-level nodes from the model which are designated as 'data'.

getParam(node, param, warn = TRUE) See 'help(getParam)'

getParents( nodes, omit = character(), self = FALSE, determOnly = FALSE, stochOnly = FALSE, includeData = T Returns a character vector of the nodes on which the input nodes depend, sorted topologically according to the model graph, by default recursing and stopping at stochastic parent nodes. In the genealogical metaphor for a graphical model, this function returns the "parents" of the input nodes. In the river network metaphor, it returns upstream nodes. By default, the returned nodes omit the input nodes. Additional input arguments provide flexibility in the values returned.

Arguments:

nodes: Character vector of node names, with index blocks allowed, and/or variable names, the parents of which will be returned.

omit: Character vector of node names, which will be omitted from the nodes returned. In addition, parent nodes beyond these omitted nodes will not be returned. The omitted nodes argument serves to stop the upward search through the hierarchical model structure, and excludes the specified node.

self: Logical argument specifying whether to include the input argument nodes in the return vector of dependent nodes. Default is FALSE.

determOnly: Logical argument specifying whether to return only deterministic nodes. Default is FALSE.

stochOnly: Logical argument specifying whether to return only stochastic nodes. Default is FALSE. If both determOnly and stochOnly are TRUE, no nodes will be returned.

includeData: Logical argument specifying whether to include 'data' nodes (set via nimble-Model or the setData method). Default is TRUE.

dataOnly: Logical argument specifying whether to return only 'data' nodes. Default is FALSE.

includeRHSonly: Logical argument specifying whether to include right-hand-side-only nodes (model nodes which never appear on the left-hand-side of  $\sim$  or <- in the model code). These nodes are neither stochastic nor deterministic, but instead function as variable inputs to the model. Default is FALSE.

upstream: Logical argument specifying whether the upward search through the hierarchical model structure should continue beyond the first and subsequent stochastic nodes encountered, hence returning all nodes upstream of the input nodes. Default is FALSE.

immediateOnly: Logical argument specifying whether only the immediate parent nodes should be returned, even if they are deterministic. If FALSE, getParents recurses and stops at stochastic nodes. Default is FALSE.

returnType: Character argument specifying type of object returned. Options are 'names' (returns character vector) and 'ids' (returns numeric graph IDs for model).

returnScalarComponenets: Logical argument specifying whether multivariate nodes should be returned as full node names (i.e. 'x[1:2]') or as scalar componenets (i.e. 'x[1]' and 'x[2]').

Details: The upward search for dependent nodes propagates through deterministic nodes, but by default will halt at the first level of stochastic nodes encountered. Use getParentsList for a list of one-step parent nodes of each node in the model.

getParentsList(returnNames = TRUE, sort = TRUE) Returns a list of all parent neighbor relationships. Each list element gives the one-step parents of one vertex, and the element name is the vertex label (integer ID or character node name)

Arguments:

returnNames: If TRUE (default), list names and element contents are returns as character node names, e.g. 'x[1]'. If FALSE, everything is returned using graph IDs, which are unique integer labels for each node.

sort: If TRUE (default), each list element is returned in topologically sorted order. If FALSE, they are returned in arbitrary order.

Details: This provides a fairly raw representation of the graph (model) structure that may be useful for inspecting what NIMBLE has created from model code.

Arguments:

logProb: Logical argument specifying whether or not to include the logProb variables. Default is FALSE.

nodes: An optional character vector supplying a subset of nodes for which to extract the variable names and return the unique set of variable names

initializeInfo(stochasticLogProbs = FALSE) Provides more detailed information on which model nodes are not initialized.

Arguments:

stochasticLogProbs: Boolean argument. If TRUE, the log-density value associated with each stochastic model variable is calculated and printed.

isBinary(nodes) Determines whether one or more nodes represent binary random variables

Arguments:

nodes: A character vector specifying one or more node or variable names.

Details: The return value is a character vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent node names, so the length of the output may be longer than that of the input.

isData(nodes) Returns a vector of logical TRUE / FALSE values, corresponding to the 'data' flags of the input node names.

Arguments:

nodes: A character vector of node or variable names.

Details: The variable or node names specified is expanded into a vector of model node names. A logical vector is returned, indicating whether each model node has been flagged as containing 'data'. Multivariate nodes for which any elements are flagged as containing 'data' will be assigned a value of TRUE.

isDeterm(nodes, includeRHSonly = FALSE, nodesAlreadyExpanded = FALSE) Determines whether one or more nodes are deterministic

Arguments:

nodes: A character vector specifying one or more node or variable names.

nodesAlreadyExpanded: Boolean argument indicating whether 'nodes' should be expanded. Generally intended for internal use. Default is 'FALSE'.

Details: The return value is a character vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent node names, so the length of the output may be longer than that of the input.

isDiscrete(nodes) Determines whether one or more nodes represent discrete random variables Arguments: nodes: A character vector specifying one or more node or variable names.

Details: The return value is a character vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent node names, so the length of the output may be longer than that of the input.

isEndNode(nodes) Determines whether one or more nodes are end nodes (nodes with no stochastic dependences)

Arguments:

nodes: A character vector specifying one or more node or variable names.

Details: The return value is logical vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent node names, so the length of the output may be longer than that of the input.

isMultivariate(nodes) Determines whether one or more nodes represent multivariate nodes Arguments:

nodes: A character vector specifying one or more node or variable names.

Details: The return value is a logical vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent node names, so the length of the output may be longer than that of the input.

isStoch(nodes, nodesAlreadyExpanded = FALSE) Determines whether one or more nodes are stochastic

Arguments:

nodes: A character vector specifying one or more node or variable names.

nodesAlreadyExpanded: Boolean argument indicating whether 'nodes' should be expanded. Generally intended for internal use. Default is 'FALSE'.

Details: The return value is a character vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent node names, so the length of the output may be longer than that of the input.

isTruncated(nodes) Determines whether one or more nodes are truncated

Arguments:

nodes: A character vector specifying one or more node or variable names.

Details: The return value is a character vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent nodes names, so the length of the output may be longer than that of the input

isUnivariate(nodes) Determines whether one or more nodes represent univariate random variables

Arguments:

nodes: A character vector specifying one or more node or variable names.

Details: The return value is a character vector with an element for each node indicated in the input. Note that variable names are expanded to their constituent nodes names, so the length of the output may be longer than that of the input

newModel( data = NULL, inits = NULL, modelName = character(), replicate = FALSE, check = getNimbleOption("o Returns a new R model object, with the same model definiton (as defined from the original model code) as the existing model object.

Arguments:

data: A named list specifying data nodes and values, for use in the newly returned model. If not provided, the data argument from the creation of the original R model object will be used. inits: A named list specifying initial values, for use in the newly returned model. If not provided, the inits argument from the creation of the original R model object will be used.

modelName: An optional character string, used to set the internal name of the model object. If provided, this name will propagate throughout the generated C++ code, serving to improve readability.

replicate: Logical specifying whether to replicate all current values and data flags from the current model in the new model. If TRUE, then the data and inits arguments are not used. Default value is FALSE.

check: A logical indicating whether to check the model object for missing or invalid values. Default is given by the NIMBLE option 'checkModel', see help on 'nimbleOptions' for details.

calculate: A logical indicating whether to run 'calculate' on the model; this will calculate all deterministic nodes and logProbability values given the current state of all nodes. Default is TRUE. For large models, one might want to disable this, but note that deterministic nodes, including nodes introduced into the model by NIMBLE, may be NA.

Details: The newly created model object will be identical to the original model in terms of structure and functionality, but entirely distinct in terms of the internal values.

- resetData() Resets the 'data' property of ALL model nodes to FALSE. Subsequent to this call, the model will have no nodes flagged as 'data'.
- setData(..., warnAboutMissingNames = TRUE) Sets the 'data' flag for specified stochastic nodes to TRUE, and also sets the value of these nodes to the value provided. This is the exclusive method for specifying 'data' nodes in a model object. When a 'data' argument is provided to 'nimbleModel()', it uses this method to set the data nodes. This also allows one to set the 'data' flag for nodes appearing only on the right-hand side of model declarations, thereby preventing their values from being overwritten via 'inits'.

Arguments:

...: Arguments may be provided as named elements with numeric values or as character names of model variables. These may be provided in a single list, a single character vector, or as multiple arguments. When a named element with a numeric value is provided, the size and dimension must match the corresponding model variable. This value will be copied to the model variable and any non-NA elements will be marked as data. When a character name is provided, the value of that variable in the model is not changed but any currently non-NA values are marked as data. Examples: setData('x', y = 1:10) will mark both x and y as data and will set the value of y to 1:10. setData(list('x', y = 1:10)) is equivalent. setData(c('x','y')) or setData('x','y') will mark both x and y as data.

Details: If a provided value (or the current value in the model when only a name is specified) contains some NA values, then the model nodes corresponding to these NAs will not have their value set, and will not be designated as 'data'. Only model nodes corresponding to numeric values in the argument list elements will be designated as data. Designating a deterministic model node as 'data' will be ignored. Designating part of a multivariate node as 'data' and part as non-data (NA) is allowed, but 'isData()' will report such a node as being 'data', calculations with the node will generally return NA, and MCMC samplers will not be assigned to such nodes.

setInits(inits) Sets initial values (or more generally, any named list of value elements) into the
model

Arguments:

inits: A named list. The names of list elements must correspond to model variable names. The elements of the list must be of class numeric, with size and dimension each matching the corresponding model variable.

simulate(nodes, includeData = FALSE) See 'help(simulate)'

Arguments:

nodes: A character vector of node or variable names, which is to be topologically sorted. Alternatively can be a numeric vector of graphIDs

returnType: character vector indicating return type. Choices are "names" or "ids"

Details: This function merely reorders its input argument. This may be important prior to calls such as model\$simulate(nodes) or model\$calculate(nodes), to enforce that the operation is performed in topological order.

## Author(s)

Daniel Turek

## See Also

initializeModel

#### Examples

```
code <- nimbleCode({
    mu ~ dnorm(0, 1)
    x[1] ~ dnorm(mu, 1)
    x[2] ~ dnorm(mu, 1)
})
Rmodel <- nimbleModel(code)
modelVars <- Rmodel$getVarNames() ## returns 'mu' and 'x'
modelNodes <- Rmodel$getNodeNames() ## returns 'mu', 'x[1]' and 'x[2]'
Rmodel$resetData()
Rmodel$resetData(list(x = c(1.2, NA))) ## flags only 'x[1]' node as data
Rmodel$isData(c('mu', 'x[1]', 'x[2]')) ## returns c(FALSE, TRUE, FALSE)</pre>
```

modelDefClass-class Class for NIMBLE model definition

#### Description

Class for NIMBLE model definition that is not usually needed directly by a user.

#### Details

See modelBaseClass for information about creating NIMBLE BUGS models.

modelInitialization Information on initial values in a NIMBLE model

#### Description

Having uninitialized nodes in a NIMBLE model can potentially cause some algorithms to fail and can lead to poor performance in others. Here are some general guidelines on how non-initialized variables can affect performance:

- MCMC will auto-initialize but will do so from the prior distribution. This can cause slow convergence, especially in the case of diffuse priors.
- Likewise, particle filtering methods will initialize top-level parameters from their prior distributions, which can lead to errors or poor performance in these methods.

Please see this Section (https://r-nimble.org/html\_manual/cha-mcmc.html#sec:initMCMC) of the NIMBLE user manual for further suggestions.

modelValues

Create a NIMBLE modelValues Object

### Description

Builds modelValues object from a model values configuration object, which can include a NIMBLE model

#### Usage

```
modelValues(conf, m = 1)
```

### Arguments

conf	An object which includes information for building modelValues. Can either be a NIMBLE model (see help(modelBaseClass)) or the object returned from modelValuesConf
m	The number of rows to create in the modelValues object. Can later be changed with resize

## Details

See the User Manual or help(modelValuesBaseClass) for information about manipulating NIM-BLE modelValues object returned by this function

### Author(s)

NIMBLE development team

### Examples

```
#From model object:
code <- nimbleCode({</pre>
 a \sim dnorm(0,1)
for(i in 1:3){
for(j in 1:3)
b[i,j] ~ dnorm(0,1)
}
})
Rmodel <- nimbleModel(code)</pre>
Rmodel_mv <- modelValues(Rmodel, m = 2)</pre>
#Custom modelValues object:
mvConf <- modelValuesConf(vars = c('x', 'y'),</pre>
              types = c('double', 'int'),
              sizes = list(x = 3, y = c(2,2))
custom_mv <- modelValues(mvConf, m = 2)</pre>
custom_mv['y',]
```

### Description

modelValues are NIMBLE containers built to store values from models. They can either be built directly from a model or be custom built via the modelValuesConf function. They consist of rows, where each row can be thought of as a set of values from a model. Like most nimble objects, and unlike most R objects, they are passed by reference instead of by value.

See the User Manual for more details.

## Examples

```
mvConf <- modelValuesConf(vars = c('a', 'b'),</pre>
types = c('double', 'double'),
sizes = list(a = 1, b = c(2,2)))
mv <- modelValues(mvConf)</pre>
as.matrix(mv)
resize(mv, 2)
as.matrix(mv)
mv['a',1] <- 1
mv['a',2] <- 2
mv['b',1] <- matrix(0, nrow = 2, ncol = 2)</pre>
mv['b',2] <- matrix(1, nrow = 2, ncol = 2)</pre>
mv['a',]
as.matrix(mv)
basicModelCode <- nimbleCode({</pre>
a ~ dnorm(0,1)
for(i in 1:4)
b[i] ~ dnorm(0,1)
```

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```
})
basicModel <- nimbleModel(basicModelCode)
basicMV <- modelValues(basicModel, m = 2) # m sets the number of rows
basicMV['b',]</pre>
```

modelValuesConf Create the confs for a custom NIMBLE modelValues object

### Description

Builds an R-based modelValues conf object

## Usage

```
modelValuesConf(
   symTab,
   className,
   vars,
   types,
   sizes,
   modelDef = NA,
   where = globalenv()
)
```

### Arguments

symTab	For internal use only
className	For internal use only
vars	A vector of character strings naming each variable in the modelValues object
types	A vector of character strings describing the type of data for the modelValues object. Options include 'double' (for real-valued variables) and 'int'.
sizes	A list in which the named items of the list match the var arguments and each item is a numeric vector of the dimensions
modelDef	For internal use only
where	For internal use only

## Details

See the User Manual or help(modelValuesBaseClass) and help(modelValues) for information

## Author(s)

Clifford Anderson-Bergman

### Examples

```
#Custom modelValues object:
mvConf <- modelValuesConf(vars = c('x', 'y'),
types = c('double', 'int'),
sizes = list(x = 3, y = c(2,2)))
custom_mv <- modelValues(mvConf, m = 2)
custom_mv['y',]
```

Multinomial

#### The Multinomial Distribution

### Description

Density and random generation for the multinomial distribution

#### Usage

dmulti(x, size = sum(x), prob, log = FALSE)

rmulti(n = 1, size, prob)

#### Arguments

х	vector of values.
size	number of trials.
prob	vector of probabilities, internally normalized to sum to one, of same length as $\boldsymbol{x}$
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

#### Details

See Gelman et al., Appendix A or the BUGS manual for mathematical details.

### Value

dmulti gives the density and rmulti generates random deviates.

## Author(s)

Christopher Paciorek

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

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#### Multivariate-t

#### See Also

Distributions for other standard distributions

#### Examples

```
size <- 30
probs <- c(1/4, 1/10, 1 - 1/4 - 1/10)
x <- rmulti(1, size, probs)
dmulti(x, size, probs)</pre>
```

Multivariate-t The Multivariate t Distribution

#### Description

Density and random generation for the multivariate t distribution, using the Cholesky factor of either the precision matrix (i.e., inverse scale matrix) or the scale matrix.

### Usage

```
dmvt_chol(x, mu, cholesky, df, prec_param = TRUE, log = FALSE)
rmvt_chol(n = 1, mu, cholesky, df, prec_param = TRUE)
```

## Arguments

x	vector of values.
mu	vector of values giving the location of the distribution.
cholesky	upper-triangular Cholesky factor of either the precision matrix (i.e., inverse scale matrix) (when prec_param is TRUE) or scale matrix (otherwise).
df	degrees of freedom.
prec_param	logical; if TRUE the Cholesky factor is that of the precision matrix; otherwise, of the scale matrix.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

### Details

See Gelman et al., Appendix A or the BUGS manual for mathematical details. The 'precision' matrix as used here is defined as the inverse of the scale matrix,  $\Sigma^{-1}$ , given in Gelman et al.

#### Value

dmvt\_chol gives the density and rmvt\_chol generates random deviates.

#### Author(s)

Peter Sujan

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

### See Also

Distributions for other standard distributions

#### Examples

```
mu <- c(-10, 0, 10)
scalemat <- matrix(c(1, .9, .3, .9, 1, -0.1, .3, -0.1, 1), 3)
ch <- chol(scalemat)
x <- rmvt_chol(1, mu, ch, df = 1, prec_param = FALSE)
dmvt_chol(x, mu, ch, df = 1, prec_param = FALSE)</pre>
```

MultivariateNormal The Multivariate Normal Distribution

## Description

Density and random generation for the multivariate normal distribution, using the Cholesky factor of either the precision matrix or the covariance matrix.

## Usage

```
dmnorm_chol(x, mean, cholesky, prec_param = TRUE, log = FALSE)
rmnorm_chol(n = 1, mean, cholesky, prec_param = TRUE)
```

#### Arguments

х	vector of values.
mean	vector of values giving the mean of the distribution.
cholesky	upper-triangular Cholesky factor of either the precision matrix (when prec_param is TRUE) or covariance matrix (otherwise).
prec_param	logical; if TRUE the Cholesky factor is that of the precision matrix; otherwise, of the covariance matrix.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

### nfMethod

### Details

See Gelman et al., Appendix A or the BUGS manual for mathematical details. The rate matrix as used here is defined as the inverse of the scale matrix,  $S^{-1}$ , given in Gelman et al.

### Value

dmnorm\_chol gives the density and rmnorm\_chol generates random deviates.

### Author(s)

Christopher Paciorek

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

#### See Also

Distributions for other standard distributions

#### Examples

```
mean <- c(-10, 0, 10)
covmat <- matrix(c(1, .9, .3, .9, 1, -0.1, .3, -0.1, 1), 3)
ch <- chol(covmat)
x <- rmnorm_chol(1, mean, ch, prec_param = FALSE)
dmnorm_chol(x, mean, ch, prec_param = FALSE)</pre>
```

nfMethod

access (call) a member function of a nimbleFunction

## Description

Internal function for accessing a member function (method) of a nimbleFunction. Normally a user will write nfmethod(x) instead of nfMethod(nf, method)(x).

#### Usage

```
nfMethod(nf, methodName)
```

#### Arguments

nf	a specialized nimbleFunction, i.e. one that has already had setup parameters
	processed
methodName	a character string giving the name of the member function to call

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### Details

nimbleFunctions have a default member function called run, and may have other member functions provided via the methods argument to nimbleFunction. As an internal step, the NIMBLE compiler turns nf\$method(x) into nfMethod(nf, method)(x), but a NIMBLE user or programmer would not normally need to use nfMethod directly.

### Value

a function that can be called.

### Author(s)

NIMBLE development team

nfVar

Access or set a member variable of a nimbleFunction

### Description

Access or set a member variable of a specialized nimbleFunction, i.e. a variable passed to or created during the setup function that is used in run code or preserved by setupOutputs. Works in R for any variable and in NIMBLE for numeric variables.

#### Usage

nfVar(nf, varName)

nfVar(nf, varName) <- value</pre>

#### Arguments

nf	a specialized nimbleFunction, i.e. a function returned by executing a function
	returned from nimbleFunction with setup arguments
varName	a character string naming a variable in the setup function.
value	value to set the variable to.

#### Details

Internal way to access or set a member variable of a nimbleFunction created during setup. Normally in NIMBLE code you would use nf\$var instead of nfVar(nf, var).

When nimbleFunction is called and a setup function is provided, then nimbleFunction returns a function. That function is a generator that should be called with arguments to the setup function and returns another function with run and possibly other member functions. The member functions can use objects created or passed to setup. During internal processing, the NIMBLE compiler turns some cases of nf\$var into nfVar(nf, var). These provide direct access to setup variables (member data). nfVar is not typically called by a NIMBLE user or programmer.

For internal access to methods of nf, see nfMethod.

For more information, see ?nimbleFunction and the NIMBLE User Manual.

### nimble-internal

## Value

whatever varName is in the nimbleFunction nf.

### Author(s)

NIMBLE development team

### Examples

```
nfGen1 <- nimbleFunction(</pre>
    setup = function(A) {
    B <- matrix(rnorm(4), nrow = 2)</pre>
    setupOutputs(B) ## preserves B even though it is not used in run-code
   },
   run = function() {
      print('This is A', A, '\n')
})
nfGen2 <- nimbleFunction(</pre>
  setup = function() {
    nf1 <- nfGen1(1000)
  },
  run = function() {
      print('accessing A:', nfVar(nf1, 'A'))
      nfVar(nf1, 'B')[2,2] <<- -1000
      print('accessing B:', nfVar(nf1, 'B'))
   })
nf2 <- nfGen2()</pre>
nf2$run()
```

nimble-internal Functions and Classes Internal to NIMBLE

### Description

Functions and classes used internally in NIMBLE and not expected to be called directly by users. Some functions and classes not intended for direct use are documented and/or exported because they are used within Reference Class methods for classes programmatically generated by NIMBLE.

### Author(s)

NIMBLE Development Team

nimble-math

### Description

Mathematical functions for use in BUGS code and in nimbleFunction programming (i.e., nimble-Function run code). See Chapter 5 of the User Manual for more details.

## Author(s)

NIMBLE Development Team

nimble-R-functions NIMBLE language functions for R-like vector construction

## Description

The functions c, rep, seq, which, diag, length, seq\_along, is.na, is.nan, any, and all can be used in nimbleFunctions and compiled using compileNimble.

#### Usage

```
nimC(...)
nimRep(x, ...)
nimSeq(from, to, by, length.out)
```

## Arguments

	values to be concatenated.
x	vector of values to be replicated (rep), or logical array or vector (which), or object whose length is wanted (length), or input value (diag), or vector of values to be tested/checked (is.na, is.nan, any, all).
from	starting value of sequence.
to	end value of sequence.
by	increment of the sequence.
length.out	desired length of the sequence.

#### nimbleCode

#### Details

For c, rep, seq, these functions are NIMBLE's version of similar R functions, e.g., nimRep for rep. In a nimbleFunction, either the R name (e.g., rep) or the NIMBLE name (e.g., nimRep) can be used. If the R name is used, it will be converted to the NIMBLE name. For which, length, diag, seq\_along, is.na, is.nan, any, all simply use the standard name without "nim". These functions largely mimic (see exceptions below) the behavior of their R counterparts, but they can be compiled in a nimbleFunction using compileNimble.

nimC is NIMBLE's version of c and behaves identically.

nimRep is NIMBLE's version of rep. It should behave identically to rep. There are no NIMBLE versions of rep.int or rep\_len.

nimSeq is NIMBLE's version of seq. It behaves like seq with support for from, to, by and length.out arguments. The along.with argument is not supported. There are no NIMBLE versions of seq.int, seq\_along or seq\_len, with the exception that seq\_along can take a nimble-FunctionList as an argument to provide the index range of a for-loop (User Manual Ch. 13).

which behaves like the R version but without support for arr.ind or useNames arguments.

diag behaves like the R version but without support for the nrow and ncol arguments.

length behaves like the R version.

seq\_along behaves like the R version.

is.na behaves like the R version but does not correctly handle NA values from R that are type 'logical', so convert these using as.numeric() before passing from R to NIMBLE.

is.nan behaves like the R version, but treats NA of type 'double' as being NaN and NA of type 'logical' as not being NaN.

any behaves like the R version but takes only one argument and treats NAs as FALSE.

all behaves like the R version but takes only one argument and treats NAs as FALSE.

nimbleCode

Turn BUGS model code into an object for use in nimbleModel or readBUGSmodel

### Description

Simply keeps model code as an R call object, the form needed by nimbleModel and optionally usable by readBUGSmodel.

#### Usage

```
nimbleCode(code)
```

#### Arguments

code

expression providing the code for the model

### Details

It is equivalent to use the R function quote. nimbleCode is simply provided as a more readable alternative for NIMBLE users not familiar with quote.

## Author(s)

Daniel Turek

### Examples

```
code <- nimbleCode({
    x ~ dnorm(mu, sd = 1)
    mu ~ dnorm(0, sd = prior_sd)
})</pre>
```

nimbleExternalCall Create a nimbleFunction that wraps a call to external compiled code

### Description

Given C header information, a function that takes scalars or pointers can be called from a compiled nimbleFunction. If non-scalar return values are needed, an argument can be selected to behave as the return value in nimble.

### Usage

```
nimbleExternalCall(
   prototype,
   returnType,
   Cfun,
   headerFile,
   oFile,
   where = getNimbleFunctionEnvironment()
)
```

## Arguments

prototype	Argument type information. This can be provided as an R function using nimbleFunction type declarations or as a list of nimbleType objects.
returnType	Return object type information. This can be provided similarly to prototype as either a nimbleFunction type declaration or as a nimbleType object. In the latter case, the name will be ignored. If there is no return value, this should be void().
Cfun	Name of the external function (character).
headerFile	Name (possibly including file path) of the header file where Cfun is declared.

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oFile	Name (possibly including path) of the .o file where Cfun has been compiled. Spaces in the path may cause problems.
where	An optional where argument passed to setRefClass for where the reference class definition generated for this nimbleFunction will be stored. This is needed due to R package namespace issues but should never need to be provided by a user.

#### Details

The only argument types allowed in Cfun are double, int, and bool, corresponding to nimbleFunction types double, integer, and logical, respectively.

If the dimensionality is greater than zero, the arguments in Cfun should be pointers. This means it will typically be necessary to pass additional integer arguments telling Cfun the size(s) of non-scalar arguments.

The return argument can only be a scalar or void. Since non-scalar arguments are passed by pointer, you can use an argument to return results from Cfun. If you wish to have a nimbleFunction that uses one argument of Cfun as a return object, you can wrap the result of nimbleExternalCall in another nimbleFunction that allocates the return object. This is useful for using Cfun in a nimbleModel. See example below.

Note that a nimbleExternalCall can only be executed in a compiled nimbleFunction, not an uncompiled one.

If you have problems with spaces in file paths (e.g. for oFile), try compiling everything locally by including dirName = "." as an argument to compileNimble.

Note that if you use Rcpp to generate object files, NIMBLE's use of the --preclean option to R CMD SHLIB can cause failures, so you may need to run nimbleOptions(precleanCompilation=FALSE) to prevent removal of needed object files.

#### Value

A nimbleFunction that takes the indicated input arguments, calls Cfun, and returns the result.

#### Author(s)

Perry de Valpine

#### See Also

nimbleRcall for calling arbitrary R code from compiled nimbleFunctions.

## Examples

```
## Not run:
sink('add1.h')
cat('
extern "C" {
 void my_internal_function(double *p, double*ans, int n);
 }
')
```

```
sink()
sink('add1.cpp')
cat('
#include <cstdio>
 #include "add1.h"
 void my_internal_function(double *p, double *ans, int n) {
   printf("In my_internal_function\\n");
     /* cat reduces the double slash to single slash */
   for(int i = 0; i < n; i++)</pre>
     ans[i] = p[i] + 1.0;
}
')
sink()
system('g++ add1.cpp -c -o add1.o')
Radd1 <- nimbleExternalCall(function(x = double(1), ans = double(1),</pre>
n = integer()){}, Cfun = 'my_internal_function',
headerFile = file.path(getwd(), 'add1.h'), returnType = void(),
oFile = file.path(getwd(), 'add1.o'))
## If you need to use a function with non-scalar return object in model code,
## you can wrap it in another nimbleFunction like this:
model_add1 <- nimbleFunction(</pre>
     run = function(x = double(1)) {
         ans <- numeric(length(x))</pre>
         Radd1(x, ans, length(x))
         return(ans)
         returnType(double(1))
     })
demoCode <- nimbleCode({</pre>
     for(i in 1:4) {x[i] ~ dnorm(0,1)} ## just to get a vector
    y[1:4] <- model_add1(x[1:4])</pre>
})
demoModel <- nimbleModel(demoCode, inits = list(x = rnorm(4)),</pre>
check = FALSE, calculate = FALSE)
CdemoModel <- compileNimble(demoModel, showCompilerOutput = TRUE)</pre>
## End(Not run)
```

nimbleFunction create a nimbleFunction

## Description

create a nimbleFunction from a setup function, run function, possibly other methods, and possibly inheritance via contains

#### Usage

```
nimbleFunction(
   setup = NULL,
   run = function() {
```

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nimbleFunction

```
},
methods = list(),
globalSetup = NULL,
contains = NULL,
buildDerivs = list(),
name = NA,
check = getNimbleOption("checkNimbleFunction"),
where = getNimbleFunctionEnvironment()
)
```

#### Arguments

setup	An optional R function definition for setup processing.
run	An optional NIMBLE function definition that executes the primary job of the nimbleFunction
methods	An optional named list of NIMBLE function definitions for other class methods.
globalSetup	For internal use only
contains	An optional object returned from nimbleFunctionVirtual that defines arguments and returnTypes for run and/or methods, to which the current nimble-Function must conform
buildDerivs	A list of names of function methods for which to build derivatives capabilities.
name	An optional name used internally, for example in generated C++ code. Usually this is left blank and NIMBLE provides a name.
check	Boolean indicating whether to check the run code for function calls that NIM- BLE cannot compile. Checking can be turned off for all calls to nimbleFunction using nimbleOptions(checkNimbleFunction = FALSE).
where	An optional where argument passed to setRefClass for where the reference class definition generated for this nimbleFunction will be stored. This is needed due to R package namespace issues but should never need to be provided by a user.

### Details

This is the main function for defining nimbleFunctions. A lot of information is provided in the NIMBLE User Manual, so only a brief summary will be given here.

If a setup function is provided, then nimbleFunction returns a generator: a function that when called with arguments for the setup function will execute that function and return a specialized nimbleFunction. The run and other methods can be called using \$ like in other R classes, e.g. nf\$run(). The methods can use objects that were created in or passed to the setup function.

If no setup function is provided, then nimbleFunction returns a function that executes the run function. It is not a generator in this case, and no other methods can be provided.

If one wants a generator but does not need any setup arguments or code, setup = TRUE can be used.

See the NIMBLE User Manual for examples.

For more information about the contains argument, see the section on nimbleFunctionLists.

### Author(s)

NIMBLE development team

nimbleFunctionBase-class

 $Class \ nimble Function Base$ 

#### Description

Classes used internally in NIMBLE and not expected to be called directly by users.

nimbleFunctionList-class

Create a list of nimbleFunctions

### Description

Create an empty list of nimbleFunctions that all will inherit from a base class.

#### Details

See the User Manual for information about creating and populating a nimbleFunctionList.

### Author(s)

NIMBLE development team

nimbleFunctionVirtual create a virtual nimbleFunction, a base class for other nimbleFunctions

### Description

define argument types and returnType for the run function and any methods, to be used in the contains argument of nimbleFunction

### Usage

```
nimbleFunctionVirtual(
   contains = NULL,
   run = function() {
   },
   methods = list(),
   name = NA,
   methodControl = list()
)
```

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### nimbleList

#### Arguments

contains	Not yet functional
run	A NIMBLE function that will only be used to inspect its argument types and returnType.
methods	An optional named list of NIMBLE functions that will also only be used for inspecting argument types and returnTypes.
name	An optional name used internally by the NIMBLE compiler. This is usually omitted and NIMBLE provides one.
methodControl	An optional list that allows specification of methods with defaults.

#### Details

See the NIMBLE User Manual section on nimbleFunctionLists for explanation of how to use a virtual nimbleFunction.

### Value

An object that can be passed as the contains argument to nimbleFunction or as the argument to nimbleFunctionList

### Author(s)

NIMBLE development team

### See Also

nimbleFunction

nimbleList create a nimbleList

### Description

create a nimbleList from a nimbleList definition

## Usage

```
nimbleList(
    ...,
    name = as.character(NA),
    predefined = FALSE,
    where = getNimbleFunctionEnvironment()
)
```

### Arguments

	arbitrary set of names and types for the elements of the list or a single R list of type nimbleType.
name	optional character providing a name used internally, for example in generated C++ code. Usually this is left blank and NIMBLE provides a name.
predefined	logical for internal use only.
where	optional argument passed to setRefClass for where the reference class defini- tion generated for this nimbleFunction will be stored. This is needed due to R package namespace issues but should never need to be provided by a user.

### Details

This function creates a definition for a nimbleList. The types argument defines the names, types, and dimensions of the elements of the nimbleList. Elements of nimbleLists can be either basic types (e.g., integer, double) or other nimbleList definitions. The types argument can be either a series of expressions of the form name = type(dim), or a list of nimbleType objects.

nimbleList returns a definition, which can be used to create instances of this type of nimbleList via the new() member function.

Definitions can be created in R's general environment or in nimbleFunction setup code. Instances can be created using the new() function in R's global environment, in nimbleFunction setup code, or in nimbleFunction run code.

Instances of nimbleList definitions can be used as arguments to run code of nimbleFunctions, and as the return type of nimbleFunctions.

#### Author(s)

NIMBLE development team

#### **Examples**

```
## this nimbleList definition is identical to the one created above
exampleNimListDef <- nimbleList(nimbleListTypes)</pre>
```

nimbleMCMC

Executes one or more chains of NIMBLE's default MCMC algorithm, for a model specified using BUGS code

### nimbleMCMC

#### Description

nimbleMCMC is designed as the most straight forward entry point to using NIMBLE's default MCMC algorithm. It provides capability for running multiple MCMC chains, specifying the number of MCMC iterations, thinning, and burn-in, and which model variables should be monitored. It also provides options to return the posterior samples, to return summary statistics calculated from the posterior samples, and to return a WAIC value.

## Usage

```
nimbleMCMC(
  code,
  constants = list(),
  data = list(),
  inits,
  dimensions = list(),
 model,
 monitors,
  thin = 1,
  niter = 10000,
  nburnin = 0,
  nchains = 1,
  check = TRUE,
  setSeed = FALSE,
  progressBar = getNimbleOption("MCMCprogressBar"),
  samples = TRUE,
  samplesAsCodaMCMC = FALSE,
  summary = FALSE,
  WAIC = FALSE
)
```

### Arguments

code	The quoted code expression representing the model, such as the return value from a call to nimbleCode). Not required if model is provided.
constants	Named list of constants in the model. Constants cannot be subsequently modi- fied. For compatibility with JAGS and BUGS, one can include data values with constants and nimbleModel will automatically distinguish them based on what appears on the left-hand side of expressions in code.
data	Named list of values for the data nodes. Values that are NA will not be flagged as data.
inits	Argument to specify initial values for each MCMC chain. See details.
dimensions	Named list of dimensions for variables. Only needed for variables used with empty indices in model code that are not provided in constants or data.
model	A compiled or uncompiled NIMBLE model object. When provided, this model will be used to configure the MCMC algorithm to be executed, rather than using the code, constants, data and inits arguments to create a new model object.

	However, if also provided, the inits argument will still be used to initialize this model prior to running each MCMC chain.
monitors	A character vector giving the node names or variable names to monitor. The samples corresponding to these nodes will returned, and/or will have summary statistics calculated. Default value is all top-level stochastic nodes of the model.
thin	Thinning interval for collecting MCMC samples. Thinning occurs after the ini- tial nburnin samples are discarded. Default value is 1.
niter	Number of MCMC iterations to run. Default value is 10000.
nburnin	Number of initial, pre-thinning, MCMC iterations to discard. Default value is 0.
nchains	Number of MCMC chains to run. Default value is 1.
check	Logical argument, specifying whether to check the model object for missing or invalid values. Default value is TRUE.
setSeed	Logical or numeric argument. If a single numeric value is provided, R's random number seed will be set to this value at the onset of each MCMC chain. If a numeric vector of length nchains is provided, then each element of this vector is provided as R's random number seed at the onset of the corresponding MCMC chain. Otherwise, in the case of a logical value, if TRUE, then R's random number seed for the ith chain is set to be i, at the onset of each MCMC chain. Note that specifying the argument setSeed = $\emptyset$ does not prevent setting the RNG seed, but rather sets the random number generation seed to $\emptyset$ at the beginning of each MCMC chain. Default value is FALSE.
progressBar	Logical argument. If TRUE, an MCMC progress bar is displayed during exe- cution of each MCMC chain. Default value is defined by the nimble package option MCMCprogressBar
samples	Logical argument. If TRUE, then posterior samples are returned from each MCMC chain. These samples are optionally returned as coda mcmc objects, depending on the samplesAsCodaMCMC argument. Default value is TRUE. See details.
samplesAsCodaM	
	Logical argument. If TRUE, then a coda mcmc object is returned instead of an R matrix of samples, or when nchains > 1 a coda mcmc.list object is returned containing nchains mcmc objects. This argument is only used when samples is TRUE. Default value is FALSE. See details.
summary	Logical argument. When TRUE, summary statistics for the posterior samples of each parameter are also returned, for each MCMC chain. This may be returned in addition to the posterior samples themselves. Default value is FALSE. See details. z
WAIC	Logical argument. When TRUE, the WAIC (Watanabe, 2010) of the model is calculated and returned. If multiple chains are run, then a single WAIC value is calculated using the posterior samples from all chains. Default value is FALSE. Note that the version of WAIC used is the default WAIC conditional on random effects/latent states and without any grouping of data nodes. See help(waic) for more details. If a different version of WAIC is desired, do not use nimbleMCMC. Instead, specify the controlWAIC argument to configureMCMC or buildMCMC, and then use runMCMC.

#### nimbleMCMC

#### Details

The entry point for this function is providing the code, constants, data and inits arguments, to create a new NIMBLE model object, or alternatively providing an exisiting NIMBLE model object as the model argument.

At least one of samples, summary or WAIC must be TRUE, since otherwise, nothing will be returned. Any combination of these may be TRUE, including possibly all three, in which case posterior samples, summary statistics, and WAIC values are returned for each MCMC chain.

When samples = TRUE, the form of the posterior samples is determined by the samplesAsCodaMCMC argument, as either matrices of posterior samples, or coda mcmc and mcmc.list objects.

Posterior summary statistics are returned individually for each chain, and also as calculated from all chains combined (when nchains > 1).

The inits argument can be one of three things:

(1) a function to generate initial values, which will be executed once to initialize the model object, and once to generate initial values at the beginning of each MCMC chain, or (2) a single named list of initial values which, will be used to initialize the model object and for each MCMC chain, or (3) a list of length nchains, each element being a named list of initial values. The first element will be used to initialize the model object, and once element of the list will be used for each MCMC chain.

The inits argument may also be omitted, in which case the model will not be provided with initial values. This is not recommended.

The niter argument specifies the number of pre-thinning MCMC iterations, and the nburnin argument specifies the number of pre-thinning MCMC samples to discard. After discarding these burn-in samples, thinning of the remaining samples will take place. The total number of posterior samples returned will be floor((niter-nburnin)/thin).

#### Value

A list is returned with named elements depending on the arguments passed to nimbleMCMC, unless only one among samples, summary, and WAIC are requested, in which case only that element is returned. These elements may include samples, summary, and WAIC. When nchains = 1, posterior samples are returned as a single matrix, and summary statistics as a single matrix. When nchains > 1, posterior samples are returned as a list of matrices, one matrix for each chain, and summary statistics are returned as a list containing nchains+1 matrices: one matrix corresponding to each chain, and the final element providing a summary of all chains, combined. If samplesAsCodaMCMC is TRUE, then posterior samples are provided as coda mcmc and mcmc.list objects. When WAIC is TRUE, a WAIC summary object is returned.

#### Author(s)

Daniel Turek

#### See Also

configureMCMC buildMCMC runMCMC

### Examples

## End(Not run)

nimbleModel

Create a NIMBLE model from BUGS code

#### Description

Processes BUGS model code and optional constants, data, and initial values. Returns a NIMBLE model (see modelBaseClass) or model definition.

### Usage

```
nimbleModel(
    code,
    constants = list(),
    data = list(),
    inits = list(),
    dimensions = list(),
    returnDef = FALSE,
    where = globalenv(),
    debug = FALSE,
    check = getNimbleOption("checkModel"),
    calculate = TRUE,
    name = NULL,
    buildDerivs = getNimbleOption("buildModelDerivs"),
    userEnv = parent.frame()
)
```

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#### nimbleModel

### Arguments

code	code for the model in the form returned by ${\tt nimbleCode}$ or (equivalently) ${\tt quote}$
constants	named list of constants in the model. Constants cannot be subsequently modi- fied. For compatibility with JAGS and BUGS, one can include data values with constants and nimbleModel will automatically distinguish them based on what appears on the left-hand side of expressions in code.
data	named list of values for the data nodes. Data values can be subsequently mod- ified. Providing this argument also flags nodes as having data for purposes of algorithms that inspect model structure. Values that are NA will not be flagged as data.
inits	named list of starting values for model variables. Unlike JAGS, should only be a single list, not a list of lists.
dimensions	named list of dimensions for variables. Only needed for variables used with empty indices in model code that are not provided in constants or data.
returnDef	logical indicating whether the model should be returned (FALSE) or just the model definition (TRUE).
where	argument passed to setRefClass, indicating the environment in which the ref- erence class definitions generated for the model and its modelValues should be created. This is needed for managing package namespace issues during package loading and does not normally need to be provided by a user.
debug	logical indicating whether to put the user in a browser for debugging. Intended for developer use.
check	logical indicating whether to check the model object for missing or invalid values. Default is given by the NIMBLE option 'checkModel'. See nimbleOptions for details.
calculate	logical indicating whether to run calculate on the model after building it; this will calculate all deterministic nodes and logProbability values given the current state of all nodes. Default is TRUE. For large models, one might want to disable this, but note that deterministic nodes, including nodes introduced into the model by NIMBLE, may be NA.
name	optional character vector giving a name of the model for internal use. If omitted, a name will be provided.
buildDerivs	logical indicating whether to build derivative capabilities for the model.
userEnv	environment in which if-then-else statements in BUGS code will be evaluated if needed information not found in constants; intended primarily for internal use only

## Details

See the User Manual or help(modelBaseClass) for information about manipulating NIMBLE models created by nimbleModel, including methods that operate on models, such as getDependencies.

The user may need to provide dimensions for certain variables as in some cases NIMBLE cannot automatically determine the dimensions and sizes of variables. See the User Manual for more information.

As noted above, one may lump together constants and data (as part of the constants argument (unlike R interfaces to JAGS and BUGS where they are provided as the data argument). One may not provide lumped constants and data as the data argument.

For variables that are a mixture of data nodes and non-data nodes, any values passed in via inits for components of the variable that are data will be ignored. All data values should be passed in through data (or constants as just discussed).

### Author(s)

NIMBLE development team

#### See Also

readBUGSmodel for creating models from BUGS-format model files

### Examples

```
code <- nimbleCode({
    x ~ dnorm(mu, sd = 1)
    mu ~ dnorm(0, sd = prior_sd)
})
constants = list(prior_sd = 1)
data = list(x = 4)
Rmodel <- nimbleModel(code, constants = constants, data = data)</pre>
```

nimbleOptions NIMBLE Options Settings

#### Description

Allow the user to set and examine a variety of global \_options\_ that affect the way in which NIM-BLE operates. Call nimbleOptions() with no arguments to see a list of available opions.

#### Usage

```
nimbleOptions(...)
```

#### Arguments

• • •

any options to be defined as one or more name = value pairs or as a single list of name=value pairs.

#### Details

nimbleOptions mimics options. Invoking nimbleOptions() with no arguments returns a list with the current values of the options. To access the value of a single option, one should use getNimbleOption().

### nimbleRcall

### Value

When invoked with no arguments, returns a list with the current values of all options. When invoked with one or more arguments, returns a list of the the updated options with their updated values.

### Author(s)

Christopher Paciorek

#### Examples

nimbleRcall	Make an R function callable from compiled nimbleFunctions (includ-
	ing nimbleModels).

#### Description

Normally compiled nimbleFunctions call other compiled nimbleFunctions. nimbleRcall enables any R function (with viable argument types and return values) to be called (and evaluated in R) from compiled nimbleFunctions.

#### Usage

```
nimbleRcall(
   prototype,
   returnType,
   Rfun,
   where = getNimbleFunctionEnvironment()
)
```

#### Arguments

prototype Argument type information for Rfun. This can be provided as an R function using nimbleFunction type declarations or as a list of nimbleType objects.

returnType	Return object type information. This can be provided similarly to prototype as either a nimbleFunction type declaration or as a nimbleType object. In the latter case, the name will be ignored. If there is no return value this should be void().
Rfun	The name of an R function to be called from compiled nimbleFunctions.
where	An optional where argument passed to setRefClass for where the reference class definition generated for this nimbleFunction will be stored. This is needed due to R package namespace issues but should never need to be provided by a user.

#### Details

The nimbleFunction returned by nimbleRcall can be used in other nimbleFunctions. When called from a compiled nimbleFunction (including from a model), arguments will be copied according to the declared types, the function named by Rfun will be called, and the returned object will be copied if necessary. The example below shows use of an R function in a compiled nimbleModel.

A nimbleFunction returned by nimbleRcall can only be used in a compiled nimbleFunction. Rfun itself should work in an uncompiled nimbleFunction.

### Value

A nimbleFunction that wraps a call to Rfun with type-declared arguments and return object.

#### Author(s)

Perry de Valpine

#### See Also

nimbleExternalCall for calling externally provided C (or other) compiled code.

### Examples

```
## Not run:
## Say we want an R function that adds 2 to every value in a vector
add2 <- function(x) {
    x + 2
}
Radd2 <- nimbleRcall(function(x = double(1)){}, Rfun = 'add2',
returnType = double(1))
demoCode <- nimbleCode({
    for(i in 1:4) {x[i] ~ dnorm(0,1)}
    z[1:4] <- Radd2(x[1:4])
})
demoModel <- nimbleModel(demoCode, inits = list(x = rnorm(4)),
check = FALSE, calculate = FALSE)
CdemoModel <- compileNimble(demoModel)</pre>
```

## End(Not run)

#### Description

Create a nimbleType object, with information on the name, type, and dimension of an object to be placed in a nimbleList.

#### Arguments

name	The name of the object, given as a character string.
type	The type of the object, given as a character string.
dim	The dimension of the object, given as an integer. This can be left blank if the object is a nimbleList.

## Details

This function creates nimbleType objects, which can be used to define the elements of a nimbleList.

The type argument can be chosen from among character, double, integer, and logical, or can be the name of a previously created nimbleList definition.

See the NIMBLE User Manual for additional examples.

### Author(s)

NIMBLE development team

#### Examples

```
nimbleTypeList <- list()
nimbleTypeList[[1]] <- nimbleType(name = 'x', type = 'integer', dim = 0)
nimbleTypeList[[2]] <- nimbleType(name = 'Y', type = 'double', dim = 2)</pre>
```

nimCat

cat function for use in nimbleFunctions

### Description

cat function for use in nimbleFunctions

#### Usage

nimCat(...)

#### Arguments

. . .

an arbitrary set of arguments that will be printed in sequence.

### Details

cat in nimbleFunction run-code imitates the R function cat. It prints its arguments in order. No newline is inserted, so include "n" if one is desired.

When an uncompiled nimbleFunction is executed, R's cat is used. In a compiled nimbleFunction, a C++ output stream is used that will generally format output similarly to R's cat. Non-scalar numeric objects can be included, although their output will be formatted slightly different in uncompiled and compiled nimbleFunctions.

In nimbleFunction run-time code, cat is identical to print except the latter appends a newline at the end.

nimCat is the same as cat, and the latter is converted to the former when a nimbleFunction is defined.

For numeric values, the number of digits printed is controlled by the system option nimbleOptions('digits').

#### See Also

print

### Examples

ans <- matrix(1:4, nrow = 2) ## R code, not NIMBLE code
nimCat('Answer is ', ans) ## would work in R or NIMBLE</pre>

nimCopy

Copying function for NIMBLE

#### Description

Copies values from a NIMBLE model or modelValues object to another NIMBLE model or modelValues. Work in R and NIMBLE. The NIMBLE keyword copy is identical to nimCopy

### Usage

```
nimCopy(
  from,
  to,
  nodes = NULL,
  nodesTo = NULL,
  row = NA,
  rowTo = NA,
  logProb = FALSE,
  logProbOnly = FALSE
)
```

### nimCopy

#### Arguments

from	Either a NIMBLE model or modelValues object
to	Either a NIMBLE model or modelValues object
nodes	Vector of one or more node names of object from that will be copied from
nodesTo	Vector of one or more node names of object to that will be copied to. If nodesTo is NULL, will automatically be set to nodes
row	If from is a modelValues, the row that will be copied from
rowTo	If to is a modelValues, the row which will be copied to. If rowTo is NA, will automatically be set to row
logProb	A logical value indicating whether the log probabilities of the given nodes should also be copied (i.e. if nodes = 'x' and logProb = TRUE, then both 'x' and 'logProb_x' will be copied)
logProbOnly	A logical value indicating whether only the log probabilities of the given nodes should be copied (i.e. if nodes = 'x' and logProbOnly = TRUE, then only 'logProb_x' will be copied)

## Details

This function copies values from one or more nodes (possibly including log probabilities for nodes) between models and modelValues objects. For modelValues objects, the row must be specified. This function allows one to conveniently copy multiple nodes, avoiding having to write a loop.

#### Author(s)

Clifford Anderson-Bergman

## Examples

```
# Building model and modelValues object
simpleModelCode <- nimbleCode({</pre>
for(i in 1:100)
x[i] ~ dnorm(0,1)
})
rModel <- nimbleModel(simpleModelCode)</pre>
rModelValues <- modelValues(rModel)</pre>
#Setting model nodes
rModel$x <- rnorm(100)</pre>
#Using nimCopy in R.
nimCopy(from = rModel, to = rModelValues, nodes = 'x', rowTo = 1)
#Use of nimCopy in a simple nimbleFunction
cCopyGen <- nimbleFunction(</pre>
setup = function(model, modelValues, nodeNames){},
run = function(){
nimCopy(from = model, to = modelValues, nodes = nodeNames, rowTo = 1)
}
)
```

### nimDerivs

```
rCopy <- cCopyGen(rModel, rModelValues, 'x')
## Not run:
cModel <- compileNimble(rModel)
cCopy <- compileNimble(rCopy, project = rModel)
cModel[['x']] <- rnorm(100)
cCopy$run() ## execute the copy with the compiled function
## End(Not run)</pre>
```

nimDerivs Nimble Derivatives

#### Description

Computes the value, 1st order (Jacobian), and 2nd order (Hessian) derivatives of a given nimbleFunction method and/or model log probabilities

### Usage

nimDerivs(call = NA, wrt = NULL, order = nimC(0, 1, 2), model = NA, ...)

#### Arguments

call	a call to a nimbleFunction method with arguments included. Can also be a call to model\$calculate(nodes), or to calculate(model, nodes).
wrt	a character vector of either: names of function arguments (if taking deriva- tives of a nimbleFunction method), or node names (if taking derivatives of model\$calculate(nodes)) to take derivatives with respect to. If left empty, derivatives will be taken with respect to all arguments to nimFxn.
order	an integer vector with values within the set $0, 1, 2$ , corresponding to whether the function value, Jacobian, and Hessian should be returned respectively. Defaults to $c(0, 1, 2)$ .
model	(optional) for derivatives of a nimbleFunction that involves model. calculations, the uncompiled model that is used. This is needed in order to be able to correctly restore values into the model when order does not include 0 (or in all cases when double-taping).
	additional arguments intended for internal use only.

### Details

Derivatives for uncompiled nimbleFunctions are calculated using the numDeriv package. If this package is not installed, an error will be issued. Derivatives for matrix valued arguments will be returned in column-major order.

### nimDim

## Value

an ADNimbleList with elements value, jacobian, and hessian.

#### Examples

```
## Not run:
model <- nimbleModel(code = ...)
calcDerivs <- nimDerivs(model$calculate(model$getDependencies('x')),
    wrt = 'x')
```

## End(Not run)

nimDim

return sizes of an object whether it is a vector, matrix or array

### Description

R's regular dim function returns NULL for a vector. It is useful to have this function that treats a vector similarly to a matrix or array. Works in R and NIMBLE. In NIMBLE dim is identical to nimDim, not to R's dim

### Usage

nimDim(obj)

### Arguments

obj

objects for which the sizes are requested

## Value

a vector of sizes in each dimension

### Author(s)

NIMBLE development team

### Examples

```
x <- rnorm(4)
dim(x)
nimDim(x)
y <- matrix(x, nrow = 2)
dim(y)
nimDim(y)
```

nimEigen

#### Description

Computes eigenvalues and eigenvectors of a numeric matrix.

## Usage

nimEigen(x, symmetric = FALSE, only.values = FALSE)

#### Arguments

x	a numeric matrix (double or integer) whose spectral decomposition is to be com- puted.
symmetric	if TRUE, the matrix is guarranteed to be symmetric, and only its lower triangle (diagonal included) is used. Otherwise, the matrix is checked for symmetry. Default is FALSE.
only.values	if TRUE, only the eigenvalues are computed, otherwise both eigenvalues and eigenvectors are computed. Setting only.values = TRUE can speed up eigendecompositions, especially for large matrices. Default is FALSE.

### Details

Computes the spectral decomposition of a numeric matrix using the Eigen C++ template library. In a nimbleFunction, eigen is identical to nimEigen. If the matrix is symmetric, a faster and more accurate algorithm will be used to compute the eigendecomposition. Note that non-symmetric matrices can have complex eigenvalues, which are not supported by NIMBLE. If a complex eigenvalue or a complex element of an eigenvector is detected, a warning will be issued and that element will be returned as NaN.

Additionally, returnType(eigenNimbleList()) can be used within a link{nimbleFunction} to specify that the function will return a nimbleList generated by the nimEigen function. eigenNimbleList() can also be used to define a nested nimbleList element. See the User Manual for usage examples.

### Value

The spectral decomposition of x is returned as a nimbleList with elements:

- values vector containing the eigenvalues of x, sorted in decreasing order. Since x is required to be symmetric, all eigenvalues will be real numbers.
- vectors. matrix with columns containing the eigenvectors of x, or an empty matrix if only.values is TRUE.

### Author(s)

NIMBLE development team

### nimIntegrate

## See Also

nimSvd for singular value decompositions in NIMBLE.

#### Examples

```
eigenvaluesDemoFunction <- nimbleFunction(
   setup = function(){
      demoMatrix <- diag(4) + 2
   },
   run = function(){
      eigenvalues <- eigen(demoMatrix, symmetric = TRUE)$values
      returnType(double(1))
      return(eigenvalues)
})</pre>
```

nimIntegrate

Integration of One-Dimensional Functions

## Description

NIMBLE wrapper around R's builtin integrate. Adaptive quadrature of functions of one variable over a finite or infinite interval.

### Usage

```
nimIntegrate(
    f,
    lower,
    upper,
    param,
    subdivisions = 100L,
    rel.tol = .Machine$double.eps^0.25,
    abs.tol = .Machine$double.eps^0.25,
    stop.on.error = TRUE
)
```

### Arguments

f	nimbleFunction of one input for which the integral is desired. See below for details on requirements for how f must be defined.
lower	an optional scalar lower bound for the input of the function.
upper	an optional scalar upper bound for the input of the function.
param	additional parameter(s) to the function that are fixed with respect to the inte- gration. If f takes no additional arguments (beyond the variable of integration), this must be provided but need not be used in f. Can be of length one or more. parameters.

subdivisions	the maximum number of subintervals.
rel.tol	relative accuracy requested.
abs.tol	absolute accuracy requested.
stop.on.error	logical. If TRUE (the default) an error stops the function. Otherwise some errors will give a result with the error code given in the third element of the result vector.

### Details

The function f should take two arguments, the first of type double(1), i.e., vector. f should be vectorized in that it should also return a double(1) object, containing the result of applying the function to each element of the first argument. (The result can be calculated using vectorized NIMBLE code or using a loop.) The second argument is required to also be of type double(1), containing any additional parameter(s) to the function that are not being integrated over. This argument can be unused in the function if the function does not need additional parameters. Note that this must be of type double(1) even if param contains a single element (NIMBLE will manage the lengths behind the scenes).

Note that unlike with R's integrate, additional parameters must be passed as part of a vector, specified via param, and cannot be passed as individual named arguments.

### Value

A vector with three values, the first the estimate of the integral, the second an estimate of the modulus of the absolute error, and the third a result code corresponding to the message returned by integrate. The numerical result code can be interpreted as follows:

- 0: "OK"
- 1: "maximum number of subdivisions reached"
- 2: "roundoff error was detected"
- 3: "extremely bad integrand behaviour"
- 4: "roundoff error is detected in the extrapolation table"
- 5: "the integral is probably divergent"
- 6: "the input is invalid"

#### Author(s)

Christopher Paciorek, Paul van Dam-Bates, Perry de Valpine

## See Also

integrate

## nimMatrix

## Examples

```
integrand <- nimbleFunction(</pre>
   run = function(x = double(1), theta = double(1)) {
       return(x*theta[1])
  returnType(double(1))
 }
)
fun <- nimbleFunction(</pre>
   run = function(theta = double(0), lower = double(0), upper = double(0)) {
       param = c(theta, 0) # cannot be scalar, so pad with zero.
       output = integrate(integrand, lower, upper, param)
       returnType(double(1))
       return(output)
 })
fun(3.1415927, 0, 1)
## Not run:
cfun <- compileNimble(fun)</pre>
cfun(3.1415927, 0, 1)
## End(Not run)
```

nimMatrix

#### Creates matrix or array objects for use in nimbleFunctions

## Description

In a nimbleFunction, matrix and array are identical to nimMatrix and nimArray, respectively

### Usage

```
nimMatrix(
 value = 0,
 nrow = NA,
 ncol = NA,
 init = TRUE,
 fillZeros = TRUE,
 recycle = TRUE,
 type = "double"
)
nimArray(
 value = 0,
 dim = c(1, 1),
 init = TRUE,
 fillZeros = TRUE,
```

```
recycle = TRUE,
nDim,
type = "double"
)
```

#### Arguments

value	value(s) for initialization (default = 0). This can be a vector, matrix or array, but it will be used as a vector.
nrow	the number of rows in a matrix (default $= 1$ )
ncol	the number of columns in a matrix (default = $1$ )
init	logical, whether to initialize values (default = TRUE)
fillZeros	logical, whether to initialize any elements not filled by (possibly recycled) value with 0 (or FALSE for nimLogical) (default = TRUE)
recycle	logical, whether value should be recycled to fill the entire contents of the new object (default = TRUE)
type	<pre>character representing the data type, i.e. 'double', 'integer', or 'logical' (default = 'double')</pre>
dim	vector of dimension sizes in an array (default = $c(1, 1)$ )
nDim	number of dimensions in an array. This is only necessary for compileNimble if the length of dim cannot be determined during compilation.

#### Details

These functions are similar to R's matrix and array functions, but they can be used in a nimbleFunction and compiled using compileNimble. Largely for compilation purposes, finer control is provided over initialization behavior, similarly to nimNumeric, nimInteger, and nimLogical. If init = FALSE, no initialization will be done, and value, fillZeros and recycle will be ignored. If init=TRUE and recycle=TRUE, then fillZeros will be ignored, and value will be repeated (according to R's recycling rule) as much as necessary to fill the object. If init=TRUE and recycle=FALSE, then if fillZeros=TRUE, values of 0 (or FALSE for nimLogical) will be filled in after value. Compiled code will be more efficient if unnecessary initialization is not done, but this may or may not be noticeable depending on the situation.

When used in a nimbleFunction (in run or other member function), matrix and array are immediately converted to nimMatrix and nimArray, respectively.

The nDim argument is only necessary for a use like dim <-c(2, 3, 4); A <-nimArray(0, dim = dim, nDim = 3). It is necessary because the NIMBLE compiler must determine during compilation that A will be a 3-dimensional numeric array. However, the compiler doesn't know for sure what the length of dim will be at run time, only that it is a vector. On the other hand, A <-nimArray(0, dim = c(2, 3, 4)) is allowed because the compiler can directly determine that a vector of length three is constructed inline for the dim argument.

### Author(s)

Daniel Turek and Perry de Valpine

## nimNumeric

# See Also

nimNumeric nimInteger nimLogical

```
nimNumeric
```

Creates numeric, integer or logical vectors for use in nimbleFunctions

## Description

In a nimbleFunction, numeric, integer and logical are identical to nimNumeric, nimInteger and nimLogical, respectively.

### Usage

```
nimNumeric(
  length = 0,
  value = 0,
  init = TRUE,
 fillZeros = TRUE,
  recycle = TRUE
)
nimInteger(
  length = 0,
  value = 0,
  init = TRUE,
  fillZeros = TRUE,
  recycle = TRUE
)
nimLogical(
  length = 0,
  value = 0,
  init = TRUE,
 fillZeros = TRUE,
  recycle = TRUE
)
```

## Arguments

length	the length of the vector (default = $0$ )
value	value(s) for initializing the vector (default = 0). This may be a vector, matrix or array but will be used as a vector.
init	logical, whether to initialize elements of the vector (default = TRUE)
fillZeros	logical, whether to initialize any elements not filled by (possibly recycled) value with 0 (or FALSE for nimLogical) (default = TRUE)
recycle	logical, whether value should be recycled to fill the entire length of the new vector (default = TRUE)

## Details

These functions are similar to R's numeric, integer, logical functions, but they can be used in a nimbleFunction and then compiled using compileNimble. Largely for compilation purposes, finer control is provided over initialization behavior. If init = FALSE, no initialization will be done, and value, fillZeros and recycle will be ignored. If init=TRUE and recycle=TRUE, then fillZeros will be ignored, and value will be repeated (according to R's recycling rule) as much as necessary to fill a vector of length length. If init=TRUE and recycle=FALSE, then if fillZeros=TRUE, values of 0 (or FALSE for nimLogical) will be filled in after value up to length length. Compiled code will be more efficient if unnecessary initialization is not done, but this may or may not be noticeable depending on the situation.

When used in a nimbleFunction (in run or other member function), numeric, integer and logical are immediately converted to nimNumeric, nimInteger and nimLogical, respectively.

### Author(s)

Daniel Turek, Christopher Paciorek, Perry de Valpine

## See Also

nimMatrix, nimArray

nimOptim

General-purpose Optimization

## Description

NIMBLE wrapper around R's builtin optim, with flexibility for additional methods.

#### Usage

```
nimOptim(
   par,
   fn,
   gr = "NULL",
   he = "NULL",
   ...,
   method = "Nelder-Mead",
   lower = -Inf,
   upper = Inf,
   control = nimOptimDefaultControl(),
   hessian = FALSE
)
```

#### nimOptim

### Arguments

par	Initial values for the parameters to be optimized over.
fn	A function to be minimized (or maximized), with first argument the vector of parameters over which minimization is to take place. It should return a scalar result.
gr	A function to return the gradient for the "BFGS", "CG" and "L-BFGS-B" meth- ods. If not provided, a finite-difference approximation to derivatives will be used.
he	A function to return the Hessian matrix of second derivatives. Used (but not required) in "nlminb" or (optionally) user-provided methods.
	IGNORED
method	The method to be used. See 'Details' section of optim. One of: "Nelder-Mead", "BFGS", "CG", "L-BFGS-B", "nlminb", or "bobyqa". Note that the R methods "SANN", "Brent" are not supported. It is also possible to provide a new method; see details.
lower	Vector or scalar of lower bounds for parameters.
upper	Vector or scalar of upper bounds for parameters.
control	A list of control parameters. See Details section of optim. For code in a nimbleFunction to be compiled, this must be an optimControlNimbleList, which has fields for most elements in the control list for R's optim.
hessian	Logical. Should a Hessian matrix be returned?

### Details

This function for use in nimbleFunctions for compilation by compileNimble provides capabilities similar to R's optim and nlminb. For the supported methods provided by optim, a compiled nimbleFunction will directly call the C code used by R for these methods.

If optim appears in a nimbleFunction, it will be converted to nimOptim.

Note that if a gradient function (gr) is not provided, optim provides a finite difference approximation for use by optimization methods that need gradients. nimble's compiled version of nimOptim does the same thing, although results might not be completely identical.

For method="nlminb", a compiled nimbleFunction will run R's nlminb directly in R, with fn, gr (if provided) and he (if provided) that call back into compiled code. For method="bobyqa", a compiled nimbleFunction will run R's nloptr::bobyqa directly in R, with fn that calls back into compiled code.

An experimental feature is the capability to provide one's own optimization method in R and register it for use by nimOptim. One must write a function that takes arguments par, fn, gr, he, lower, upper, control, and hessian. The function must return a list with elements par, value, convergence, counts, evaluations, message, and hessian (which may be NULL). If hessian=TRUE but the function does not return a matrix in the hessian element of its return list, nimOptim will fill in that element using finite differences of the gradient. In general the function will be a wrapper around the actual R optimization function.

The control list passed from a nimbleFunction to the optimization function will include a minimum of options, including abstol, reltol, maxit, and trace. This means that the user's R

(wrapper) function must map between those minimum options and the equivalent inputs to the optimization function. Other options for a specific method may be set within the R (wrapper) function but cannot be passed from nimOptim.

The elements parscale and fnscale in control are used in a special way. They are implemented by nimOptim such that for \*any\* the method is expected to do minimization and nimOptim will arrange for it to minimize fn(par)/fnscale in the parameter space par/parscale.

To use the optimizer with nimOptim, an optimizer fun must be registered by nimOptimMethod("method\_name", fun), and then "method\_name" can be used as the method argument to nimOptim to use fun. An optimizer may be found by nimOptimMethod("method\_name") and may be removed by nimOptimMethod("method\_name", NULL).

Support for method="nlminb" is provided in this way, and can be studied as an example via nimOptimMethod("nlminb").

The system for providing one's own optimizer is not considered stable and is subject to change in future versions.

### Value

optimResultNimbleList

# See Also

optim

#### Examples

```
## Not run:
objectiveFunction <- nimbleFunction(</pre>
    run = function(par = double(1)) {
        return(sum(par) * exp(-sum(par ^ 2) / 2))
        returnType(double(0))
    }
)
optimizer <- nimbleFunction(</pre>
    run = function(method = character(0), fnscale = double(0)) {
        control <- optimDefaultControl()</pre>
        control$fnscale <- fnscale</pre>
        par <- c(0.1, -0.1)
        return(optim(par, objectiveFunction, method = method, control = control))
        returnType(optimResultNimbleList())
    }
)
cOptimizer <- compileNimble(optimizer)</pre>
cOptimizer(method = 'BFGS', fnscale = -1)
## End(Not run)
```

nimOptimDefaultControl

Creates a default control argument for nimOptim.

# Description

Creates a default control argument for nimOptim.

## Usage

nimOptimDefaultControl()

# Value

optimControlNimbleList

# See Also

nimOptim, optim

nimOptimMethod

Set or get an optimization function to be used by nimOptim

# Description

Add, check, or remove an R optimization function to/from NIMBLE's set of registered optimization functions that can be called from nimOptim.

## Usage

```
nimOptimMethod(name, value)
```

## Arguments

name	character string, giving the name of optimization method that can be referred to by the method argument of nimOptim (aka optim in a nimbleFunction).
value	An optimization function with specifications described below and in nimOptim. If value is NULL, then name will be found in NIMBLE's set of registered optimizer names. If value is missing, the registered optimizer for name will be returned.

### Details

When programming in nimbleFunctions, optim, which is converted automatically to nimOptim, provides a generalization of R's optim methods for optimization. If one of the supported original optim methods is not chosen with the method argument to nimOptim, an arbitrary method name can be given. If that name has been registered as a name by a call to nimOptimMethod, then the corresponding function (value) will be called for optimization.

The function value must perform minimization. If the call to nimOptim includes a control list with either fnscale (which, if negative, turns the problem into a maximization) or parscale, these will be managed by nimOptim outside of the optimizer such that the optimization should be minimization.

The function value must take named arguments par (initial parameter vector), fn (objective function), gr (optional gradient function), he (optional Hessian function), lower (vector of lower bounds), upper (vector of upper bounds), control (arbitrary control list), and hessian (logical indicating whether a Hessian at the optimum is requested). It must return a list with elements elements par (parameter values of the optimium, i.e., "arg min"), value (function value at the minimum), convergence (should be 0 if convergence occurred), counts (optional vector of counts of calls to fn, gr, and he), evaluations (optional total function evaluations), message (optional character message), and hessian (optional Hessian matrix, which may be NULL).

If the call to nimOptim has hessian=TRUE, that will be passed as hessian=TRUE to the optimizer. However, if the optimizer returns a NULL in the hessian element of the return list, then nimOptim will calculate the Hessian by finite element differences. Hence, an optimizer need not provide a Hessian capability.

The control list passed from nimOptim to the optimizer will have only a limited set of the optim control list options. These will include abstol, reltol, maxit, and trace. The optimizer may use these as it wishes. Other control options for a particular optimizer must be managed in some other way.

Note that it is possible to use browser() inside of value, or to set debug(value), to enter a browser when the optimizer (value) is called and then inspect its arguments to make sense of the situation.

This whole feature is particularly helpful when the nimbleFunction using nimOptim has been compiled by compileNimble. Many optimizers are available through R, so nimOptim arranges to call a named (registered) optimizer in R, while providing fn and optionally gr or he as functions that will call the compiled (by nimble) versions of the corresponding functions provided in the call to nimOptim.

R's optimizer nlminb is automatically registered under the name "nlminb".

nimPrint

print function for use in nimbleFunctions

## Description

print function for use in nimbleFunctions

### Usage

nimPrint(...)

### nimStop

#### Arguments

. . .

an abitrary set of arguments that will be printed in sequence.

#### Details

The keyword print in nimbleFunction run-time code will be automatically turned into nimPrint. This is a function that prints its arguments in order using cat in R, or using std::cout in C++ code generated by compiling nimbleFunctions. Non-scalar numeric objects can be included, although their output will be formatted slightly different in uncompiled and compiled nimbleFunctions.

For numeric values, the number of digits printed is controlled by the system option nimbleOptions('digits').

### See Also

cat

### Examples

ans <- matrix(1:4, nrow = 2) ## R code, not NIMBLE code nimPrint('Answer is ', ans) ## would work in R or NIMBLE

nimStop	Halt execution of a nimbleFunction function method. Part of the NIM-
	BLE language

#### Description

Halt execution of a nimbleFunction function method. Part of the NIMBLE language

## Usage

nimStop(msg)

#### Arguments

msg

Character object to be output as an error message

### Details

The NIMBLE stop is similar to the native R stop, but it takes only one argument, the error message to be output. During uncompiled NIMBLE execution, nimStop simply calls R's stop function. During compiled execution it calls the error function from the R headers. stop is an alias for nimStop in the NIMBLE language

#### Author(s)

Perry de Valpine

nimSvd

## Description

Computes singular values and, optionally, left and right singular vectors of a numeric matrix.

### Usage

```
nimSvd(x, vectors = "full")
```

### Arguments

x	a symmetric numeric matrix (double or integer) whose spectral decomposition is to be computed.
vectors	character that determines whether to calculate left and right singular vectors. Can take values 'none', 'thin' or 'full'. Defaults to 'full'. See 'Details'.

### Details

Computes the singular value decomposition of a numeric matrix using the Eigen C++ template library.

The vectors character argument determines whether to compute no left and right singular vectors ('none'), thinned left and right singular vectors ('thin'), or full left and right singular vectors ('full'). For a matrix x with dimensions n and p, setting vectors = 'thin' will does the following (quoted from eigen website): In case of a rectangular n-by-p matrix, letting m be the smaller value among n and p, there are only m singular vectors; the remaining columns of U and V do not correspond to actual singular vectors. Asking for thin U or V means asking for only their m first columns to be formed. So U is then a n-by-m matrix, and V is then a p-by-m matrix. Notice that thin U and V are all you need for (least squares) solving.

Setting vectors = 'full' will compute full matrices for U and V, so that U will be of size n-by-n, and V will be of size p-by-p.

In a nimbleFunction, svd is identical to nimSvd.

returnType(svdNimbleList()) can be used within a link{nimbleFunction} to specify that the function will return a nimbleList generated by the nimSvd function. svdNimbleList() can also be used to define a nested nimbleList element. See the User Manual for usage examples.

## Value

The singular value decomposition of x is returned as a nimbleList with elements:

- d length m vector containing the singular values of x, sorted in decreasing order.
- v matrix with columns containing the left singular vectors of x, or an empty matrix if vectors = 'none'.
- u matrix with columns containing the right singular vectors of x, or an empty matrix if vectors = 'none'.

### nodeFunctions

## Author(s)

NIMBLE development team

## See Also

nimEigen for spectral decompositions.

# Examples

```
singularValuesDemoFunction <- nimbleFunction(
   setup = function(){
      demoMatrix <- diag(4) + 2
   },
   run = function(){
      singularValues <- svd(demoMatrix)$d
      returnType(double(1))
      return(singularValues)
})</pre>
```

nodeFunctions

calculate, calculateDiff, simulate, or get the current log probabilities (densities) a set of nodes in a NIMBLE model

## Description

calculate, calculateDiff, simulate, or get the current log probabilities (densities) of one or more nodes of a NIMBLE model and (for calculate and getLogProb) return the sum of their log probabilities (or densities). Part of R and NIMBLE.

#### Usage

```
calculate(model, nodes, nodeFxnVector, nodeFunctionIndex)
calculateDiff(model, nodes, nodeFxnVector, nodeFunctionIndex)
getLogProb(model, nodes, nodeFxnVector, nodeFunctionIndex)
simulate(model, nodes, includeData = FALSE, nodeFxnVector, nodeFunctionIndex)
```

### Arguments

model	A NIMBLE model, either the compiled or uncompiled version
nodes	A character vector of node names, with index blocks allowed, such as 'x', 'y[2]', or 'z[1:3, 2:4]'
nodeFxnVector	An optional vector of nodeFunctions on which to operate, in lieu of model and nodes

nodeFunctionIndex

For internal NIMBLE use only

includeData A logical argument specifying whether data nodes should be simulated into (only relevant for simulate)

## Details

Standard usage is as a method of a model, in the form model\$calculate(nodes), but the usage as a simple function with the model as the first argument as above is also allowed.

These functions expands the nodes and then process them in the model in the order provided. Expanding nodes means turning 'y[1:2]' into c('y[1]', y[2]') if y is a vector of scalar nodes. Calculation is defined for a stochastic node as executing the log probability (density) calculation and for a deterministic node as calculating whatever function was provided on the right-hand side of the model declaration.

Difference calculation (calculateDiff) executes the operation(s) on the model as calculate, but it returns the sum of the difference between the new log probabilities and the previous ones.

Simulation is defined for a stochastic node as drawing a random value from its distribution, and for deterministic node as equivalent to calculate.

getLogProb collects and returns the sum of the log probabilities of nodes, using the log probability values currently stored in the model (as generated from the most recent call to calculate on each node)

These functions can be used from R or in NIMBLE run-time functions that will be compiled. When executed in R (including when an uncompiled nimbleFunction is executed), they can be slow because the nodes are expanded each time. When compiled in NIMBLE, the nodes are expanded only once during compilation, so execution will be much faster.

It is common to want the nodes to be provided in topologically sorted order, so that they will be calculated or simulated following the order of the model graph. Functions such as model\$getDependencies(nodes, ...) return nodes in topologically sorted order. They can be directly sorted by model\$topologicallySortNodes(nodes), but if so it is a good idea to expand names first by model\$topologicallySortNodes(model\$expandNodeNames(nodes))

### Value

calculate and getLogProb return the sum of the log probabilities (densities) of the calculated nodes, with a contribution of 0 from any deterministic nodes

calculateDiff returns the sum of the difference between the new and old log probabilities (densities) of the calculated nodes, with a contribution of 0 from any deterministic nodes.

simulate returns NULL.

#### Author(s)

NIMBLE development team

optimControlNimbleList

Data type for the control parameter of nimOptim

# Description

nimbleList definition for the type of nimbleList input as the control parameter to nimOptim. See optim for details.

## Usage

optimControlNimbleList

# Format

An object of class list of length 1.

## See Also

optim, nimOptim

optimDefaultControl Creates a deafult control argument for optim (just an empty list).

# Description

Creates a deafult control argument for optim (just an empty list).

## Usage

```
optimDefaultControl()
```

# Value

an empty list.

### See Also

nimOptim, optim

optimResultNimbleList Data type for the return value of nimOptim

### Description

nimbleList definition for the type of nimbleList returned by nimOptim.

#### Usage

optimResultNimbleList

#### Format

An object of class list of length 1.

#### Fields

par The best set of parameters found.

value The value of fn corresponding to par.

counts A two-element integer vector giving the number of calls to fn and gr respectively.

convergence An integer code. 0 indicates successful completion. Possible error codes are 1 indicates that the iteration limit maxit had been reached. 10 indicates degeneracy of the Nelder-Mead simplex. 51 indicates a warning from the "L-BFGS-B" method; see component message for further details. 52 indicates an error from the "L-BFGS-B" method; see component message for further details.

message A character string giving any additional information returned by the optimizer, or NULL.

hessian Only if argument hessian is true. A symmetric matrix giving an estimate of the Hessian at the solution found.

### See Also

optim, nimOptim

parameterTransform Automated transformations of model nodes to unconstrained scales

## Description

Provide general transformations of constrained continuous-valued model nodes (parameters) to unconstrained scales. It handles the cases of interval-bounded parameters (e.g. uniform or beta distributions), semi-interval-bounded parameters (e.g. exponential or gamma distributions), and the multivariate Wishart, inverse Wishart, Dirichlet, and LKJ distributions. Utilities are provided to transform parameters to an unconstrained scale, back-transform from the unconstrained scale to the original scale of the constrained parameterization, and to calculate the natural logarithm of the determinant of the Jacobian matrix of the inverse transformation, calculated at any location in the transformed (unconstrained) space.

### parameterTransform

### Usage

parameterTransform(model, nodes = character(0), control = list())

## Arguments

model	A nimble model object. See details.
nodes	A character vector specifying model node names to undergo transformation. See details.
control	An optional list allowing for additional control of the transformation. This currently supports a single element allowDeterm.

### Details

The parameterTransform nimbleFunction is an unspecialized function. Calling parameterTransform(model, nodes) will generate and return a specialized nimbleFunction, which provides transformation functionality for the specified hierarchical model and set of model nodes. The nodes argument can represent multiple model nodes arising from distinct prior distributions, which will be simultaneously transformed according to their respective distributions and constraints.

If the nodes argument is missing or has length zero, then no nodes will be transformed. A specialized nimbleFunction is created, but will not transform or operate on any model nodes.

The control argument is a list that supports one additional setting. If control\$allowDeterm=FALSE (the default), deterministic nodes are not allowed in the nodes argument. If control\$allowDeterm=TRUE, deterministic nodes are allowed and assumed to have no constraints on valid values.

This specialized nimbleFunction has the following methods:

transform: Transforms a numeric vector of values from the original constrained model scale to a vector of values on the unconstrained scale.

inverseTransform: Transforms a numeric vector of values from the unconstrained scale to the original constrained parameterization scale.

The unconstrained scale may have different dimensionality from the original constrained scale of the model parameters. For example, a d-dimensional dirichlet distribution is constrained to reside on a simplex in d-dimensional space. In contrast, the corresponding unconstrained parameterization is unrestrained in (d-1) dimensional space. The specialized parameterTransform nimbleFunction also provides utilities to return the dimensionality of the original (constrained) parameterization, and the transformed (unconstrained) parameterization:

getOriginalLength: Returns the dimensionality (number of scalar elements) of the original constrained parameterization.

getTransformedLength: Returns the dimensionality (number of scalar elements) comprising the transformed unconstrained parameterization.

The specialized parameterTransform nimbleFunction also provides a method for calculating the natural logarithm of the jacobian of the inverse transformation, calculated at any point in the transformed (unconstrained) space:

## logDetJacobian

The parameterTransformation function has no facility for handling discrete-valued parameters.

### Author(s)

Daniel Turek

## See Also

buildLaplace

## Examples

```
## Not run:
code <- nimbleCode({</pre>
    a ~ dnorm(0, 1)
    b \sim dgamma(1, 1)
    c \sim dunif(2, 10)
    d[1:3] ~ dmnorm(mu[1:3], cov = C[1:3,1:3])
    e[1:3,1:3] ~ dwish(R = C[1:3,1:3], df = 5)
})
constants <- list(mu=rep(0,3), C=diag(3))</pre>
Rmodel <- nimbleModel(code, constants)</pre>
## create a specialized parameterTransform function:
nodes <- c('a', 'b', 'c', 'd', 'e')
pt <- parameterTransform(Rmodel, nodes)</pre>
vals <- c(1, 10, 5,
                       1,2,3, as.numeric(diag(3)))
## transform values to unconstrained scale:
transformedVals <- pt$transform(vals)</pre>
## back-transform to original constrained scale of parameterization
pt$inverseTransform(transformedVals) ## return is same as original vals
## dimensionality of original constrained scale = 1 + 1 + 1 + 3 + 9
pt$getOriginalLength()
                             ## 15
## dimensionality of transformed (unconstrained) scale = 1 + 1 + 1 + 3 + 6
pt$getTransformedLength()
                            ## 12
## log of the jacobian of the inverse transformation matrix:
pt$logDetJacobian(transformedVals)
## End(Not run)
```

pow\_int

Power function for integer-valued exponent

## printErrors

# Description

pow function with exponent required to be integer

### Usage

pow\_int(a, b)

## Arguments

а	Base
b	Exponent

# Details

This is required in nimble models and nimbleFunctions if derivatives will be tracked but tracked only with respect to a, such that b might be any (positive, 0, or negative) integer. This contrasts with pow(a, b) (equivalent to a^b), which requires b > 0 if derivatives will be tracked, even if they will only be requested with respect to a.

## Value

a^b

printErrors Print error messages after failed compilation

# Description

Retrieves the error file from R's tempdir and prints to the screen.

# Usage

```
printErrors(excludeWarnings = TRUE)
```

#### Arguments

excludeWarnings

logical indicating whether compiler warnings should be printed; generally such warnings can be ignored.

### Author(s)

Christopher Paciorek

```
rankSample
```

#### Description

Takes a set of non-negative weights (do not need to sum to 1) and returns a sample with size elements of the integers 1:length(weights), where the probability of being sampled is proportional to the value of weights. An important note is that the output vector will be sorted in ascending order. Also, right now it works slightly odd syntax (see example below). Later releases of NIMBLE will contain more natural syntax.

#### Usage

```
rankSample(weights, size, output, silent = FALSE)
```

### Arguments

weights	A vector of numeric weights. Does not need to sum to 1, but must be non-negative
size	Size of sample
output	An R object into which the values will be placed. See example below for proper use
silent	Logical indicating whether to suppress logging information

### Details

If invalid weights provided (i.e. negative weights or weights sum to 1), sets output = rep(1, size) and prints warning. rankSample can be used inside nimble functions.

rankSample first samples from the joint distribution size uniform(0,1) distributions by conditionally sampling from the rank statistics. This leads to a sorted sample of uniform(0,1)'s. Then, a cdf vector is constructed from weights. Because the sample of uniforms is sorted, rankSample walks down the cdf in linear time and fills out the sample.

#### Author(s)

Clifford Anderson-Bergman

### Examples

```
set.seed(1)
sampInts = NA #sampled integers will be placed in sampInts
rankSample(weights = c(1, 1, 2), size = 10, sampInts)
sampInts
# [1] 1 1 2 2 2 2 2 3 3 3
rankSample(weights = c(1, 1, 2), size = 10000, sampInts)
table(sampInts)
#sampInts
```

## readBUGSmodel

```
1
         2
              3
#
#2434 2492 5074
#Used in a nimbleFunction
sampGen <- nimbleFunction(setup = function(){</pre>
x = 1:2
},
run = function(weights = double(1), k = integer() ){
rankSample(weights, k, x)
returnType(integer(1))
return(x)
})
rSamp <- sampGen()</pre>
rSamp$run(1:4, 5)
#[1] 3 3 4 4 4
```

readBUGSmodel

*Create a NIMBLE BUGS model from a variety of input formats, including BUGS model files* 

## Description

readBUGSmodel processes inputs providing the model and values for constants, data, initial values of the model in a variety of forms, returning a NIMBLE BUGS R model

#### Usage

```
readBUGSmodel(
  model,
  data = NULL,
  inits = NULL,
  useInits = TRUE,
  debug = FALSE,
  returnComponents = FALSE,
  check = getNimbleOption("checkModel"),
  calculate = TRUE,
  buildDerivs = getNimbleOption("buildModelDerivs")
)
```

### Arguments

```
model
```

one of (1) a character string giving the file name containing the BUGS model code, with relative or absolute path, (2) an R function whose body is the BUGS model code, or (3) the output of nimbleCode. If a file name, the file can contain a 'var' block and 'data' block in the manner of the JAGS versions of the BUGS examples but should not contain references to other input data files nor a const block. The '.bug' or '.txt' extension can be excluded.

data	(optional) (1) character string giving the file name for an R file providing the input constants and data as R code [assigning individual objects or as a named list], with relative or absolute path, or (2) a named list providing the input constants and data. If neither is provided, the function will look for a file named 'name_of_model-data' including extensions .R, .r, or .txt.
inits	(optional) (1) character string giving the file name for an R file providing starting values as R code [assigning individual objects or as a named list], with relative or absolute path, or (2) a named list providing the starting values. Unlike JAGS, this should provide a single set of starting values, and therefore if provided as a list should be a simple list and not a list of lists.
dir	(optional) character string giving the directory where the (optional) files are located
useInits	boolean indicating whether to set the initial values, either based on inits or by finding the '-inits' file corresponding to the input model file
debug	logical indicating whether to put the user in a browser for debugging when readBUGSmodel calls nimbleModel. Intended for developer use.
returnComponent	S
	logical indicating whether to return pieces of model object without building the model. Default is FALSE.
check	logical indicating whether to check the model object for missing or invalid values. Default is given by the NIMBLE option 'checkModel'. See nimbleOptions for details.
calculate	logical indicating whether to run calculate on the model after building it; this will calculate all deterministic nodes and logProbability values given the current state of all nodes. Default is TRUE. For large models, one might want to disable this, but note that deterministic nodes, including nodes introduced into the model by NIMBLE, may be NA.
buildDerivs	logical indicating whether to build derivative capabilities for the model.

# Details

Note that readBUGSmodel should handle most common ways of providing information on a model as used in BUGS and JAGS but does not handle input model files that refer to additional files containing data. Please see the BUGS examples provided with NIMBLE in the classic-bugs directory of the installed NIMBLE package or JAGS (https://sourceforge.net/projects/mcmc-jags/ files/Examples/) for examples of supported formats. Also, readBUGSmodel takes both constants and data via the 'data' argument, unlike nimbleModel, in which these are distinguished. The reason for allowing both to be given via 'data' is for backwards compatibility with the BUGS examples, in which constants and data are not distinguished.

# Value

returns a NIMBLE BUGS R model

## Author(s)

Christopher Paciorek

### registerDistributions

## See Also

nimbleModel

## Examples

## Reading a model defined in the R session

```
code <- nimbleCode({
    x ~ dnorm(mu, sd = 1)
    mu ~ dnorm(0, sd = prior_sd)
})
data = list(prior_sd = 1, x = 4)
model <- readBUGSmodel(code, data = data, inits = list(mu = 0))
model$x
model[['mu']]
model$calculate('x')
## Reading a classic BUGS model
pumpModel <- readBUGSmodel('pump.bug', dir = getBUGSexampleDir('pump'))
pumpModel$getVarNames()
pumpModel$x</pre>
```

registerDistributions Add user-supplied distributions for use in NIMBLE BUGS models

#### Description

Register distributional information so that NIMBLE can process user-supplied distributions in BUGS model code

# Usage

```
registerDistributions(
  distributionsInput,
  userEnv = parent.frame(),
  verbose = nimbleOptions("verbose")
)
```

## Arguments

distributionsInput

either a list or character vector specifying the user-supplied distributions. If a list, it should be a named list of lists in the form of that shown in nimble:::distributionsInputList with each list having required field BUGSdist and optional fields Rdist, altParams, discrete, pqAvail, types, and with the name of the list the same as that of the density function. Alternatively, simply a character vector providing the names of the density functions for the user-supplied distributions.

userEnv	environment in which to look for the nimbleFunctions that provide the distribu-
	tion; this will generally not need to be set by the user as it will default to the
	environment from which this function was called.
verbose	logical indicating whether to print additional logging information

### Details

When distributionsInput is a list of lists, see below for more information on the structure of the list. When distributionsInput is a character vector, the distribution is assumed to be of standard form, with parameters assumed to be the arguments provided in the density nimbleFunction, no alternative parameterizations, and the distribution assumed to be continuous with range from minus infinity to infinity. The availability of distribution and quantile functions is inferred from whether appropriately-named functions exist in the global environment.

One usually does not need to explicitly call registerDistributions as it will be called automatically when the user-supplied distribution is used for the first time in BUGS code. However, if one wishes to provide alternative parameterizations, to provide a range, or to indicate a distribution is discrete, then one still must explicitly register the distribution using registerDistributions with the argument in the list format.

Format of the component lists when distributionsInput is a list of lists:

- BUGSdist. A character string in the form of the density name (starting with 'd') followed by the names of the parameters in parentheses. When alternative parameterizations are given in Rdist, this should be an exhaustive list of the unique parameter names from all possible parameterizations, with the default parameters specified first.
- Rdist. An optional character vector with one or more alternative specifications of the density; each alternative specification can be an alternative name for the density, a different ordering of the parameters, different parameter name(s), or an alternative parameterization. In the latter case, the character string in parentheses should provide a given reparameterization as comma-separated name = value pairs, one for each default parameter, where name is the name of the default parameter and value is a mathematical expression relating the default parameter to the alternative parameters or other default parameters. The default parameters should correspond to the input arguments of the nimbleFunctions provided as the density and random generation functions. The mathematical expression can use any of the math functions allowed in NIM-BLE (see the User Manual) as well as user-supplied nimbleFunctions (which must have no setup code). The names of your nimbleFunctions for the distribution functions must match the function name in the Rdist entry (or if missing, the function name in the BUGSdist entry).
- discrete. An optional logical indicating if the distribution is that of a discrete random variable. If not supplied, distribution is assumed to be for a continuous random variable.
- pqAvail. An optional logical indicating if distribution (CDF) and quantile (inverse CDF) functions are provided as nimbleFunctions. These are required for one to be able to use truncated versions of the distribution. Only applicable for univariate distributions. If not supplied, assumed to be FALSE.
- altParams. A character vector of comma-separated 'name = value' pairs that provide the mathematical expressions relating non-canonical parameters to canonical parameters (canonical parameters are those passed as arguments to your distribution functions). These inverse

functions are used for MCMC conjugacy calculations when a conjugate relationship is expressed in terms of non-default parameters (such as the precision for normal-normal conjugacy). If not supplied, the system will still function but with a possible loss of efficiency in certain algorithms.

- types. A character vector of comma-separated 'name = input' pairs indicating the type and dimension of the random variable and parameters (including default and alternative parameters). 'input' should take the form 'double(d)' or 'integer(d)', where 'd' is 0 for scalars, 1 for vectors, 2 for matrices. Note that since NIMBLE uses doubles for numerical calculations and the default type is double(0), one should generally use 'double' and one need only specify the type for non-scalars. 'name' should be either 'value' to indicate the random variable itself or the parameter name to indicate a given parameter.
- range. A vector of two values giving the range of the distribution for possible use in future algorithms (not used currently). When the lower or upper limit involves a strict inequality (e.g., \$x>0\$), you should simply treat it as a non-strict inequality (\$x>=0\$, and set the lower value to 0). Also we do not handle ranges that are functions of parameters, so simply use the smallest/largest possible values given the possible parameter values. If not supplied this is taken to be (-Inf, Inf).

## Author(s)

**Christopher Paciorek** 

### Examples

```
dmyexp <- nimbleFunction(</pre>
   run = function(x = double(0), rate = double(0), \log = integer(0)) {
       returnType(double(0))
       logProb <- log(rate) - x*rate</pre>
       if(log) {
           return(logProb)
       } else {
           return(exp(logProb))
       }
   })
rmyexp <- nimbleFunction(</pre>
   run = function(n = integer(0), rate = double(0)) {
       returnType(double(0))
       if(n != 1) nimPrint("rmyexp only allows n = 1; using n = 1.")
       dev <- runif(1, 0, 1)
       return(-log(1-dev) / rate)
   }
   )
registerDistributions(list(
    dmyexp = list(
              BUGSdist = "dmyexp(rate, scale)",
              Rdist = "dmyexp(rate = 1/scale)",
              altParams = "scale = 1/rate",
              pqAvail = FALSE)))
code <- nimbleCode({</pre>
   y \sim dmyexp(rate = r)
    r \sim dunif(0, 100)
```

```
})
m <- nimbleModel(code, inits = list(r = 1), data = list(y = 2))</pre>
m$calculate('y')
m$r <- 2
m$calculate('y')
m$resetData()
m$simulate('y')
m$y
# alternatively, simply specify a character vector with the
# name of one or more 'd' functions
deregisterDistributions('dmyexp')
registerDistributions('dmyexp')
# or simply use in BUGS code without registration
deregisterDistributions('dmyexp')
m <- nimbleModel(code, inits = list(r = 1), data = list(y = 2))</pre>
# example of Dirichlet-multinomial registration to illustrate
# use of 'types' (note that registration is not actually needed
# in this case)
ddirchmulti <- nimbleFunction(</pre>
    run = function(x = double(1), alpha = double(1), size = double(0),
                   log = integer(0, default = 0)) {
        returnType(double(0))
        logProb <- lgamma(size) - sum(lgamma(x)) + lgamma(sum(alpha)) -</pre>
            sum(lgamma(alpha)) + sum(lgamma(alpha + x)) - lgamma(sum(alpha) +
                                                                    size)
        if(log) return(logProb)
        else return(exp(logProb))
    })
rdirchmulti <- nimbleFunction(</pre>
    run = function(n = integer(0), alpha = double(1), size = double(0)) {
        returnType(double(1))
        if(n != 1) print("rdirchmulti only allows n = 1; using n = 1.")
        p <- rdirch(1, alpha)</pre>
        return(rmulti(1, size = size, prob = p))
    })
registerDistributions(list(
    ddirchmulti = list(
        BUGSdist = "ddirchmulti(alpha, size)",
        types = c('value = double(1)', 'alpha = double(1)')
        )
    ))
```

```
resize
```

## Rmatrix2mvOneVar

## Description

Adds or removes rows to a modelValues object. If rows are added to a modelValues object, the default values are NA. Works in both R and NIMBLE.

## Usage

```
resize(container, k)
```

## Arguments

container	modelValues object
k	number of rows that modelValues is set to

## Details

See the User Manual or help(modelValuesBaseClass) for infomation about modelValues objects

## Author(s)

Clifford Anderson-Bergman

### Examples

Rmatrix2mvOneVar Set values of one variable of a modelValues object from an R matrix

# Description

Normally a modelValues object is accessed one "row" at a time. This function allows all rows for one variable to set from a matrix with one dimension more than the variable to be set.

#### Usage

Rmatrix2mvOneVar(mat, mv, varName, k)

run.time

## Arguments

mat	Input matrix
m∨	modelValues object to be modified.
varName	Character string giving the name of the variable on mv to be set
k	Number of rows to use

# Details

This function may be deprecated in the future when a more natural system for interacting with modelValues objects is developed.

RmodelBaseClass-class Class RmodelBaseClass

# Description

Classes used internally in NIMBLE and not expected to be called directly by users.

run.time

*Time execution of NIMBLE code* 

## Description

Time execution of NIMBLE code

## Usage

run.time(code)

### Arguments

code code to be timed

# Details

Function for use in nimbleFunction run code; when nimbleFunctions are run in R, this simply wraps system.time.

# Author(s)

NIMBLE Development Team

runCrossValidate

# Description

Takes a NIMBLE model MCMC configuration and conducts k-fold cross-validation of the MCMC fit, returning a measure of the model's predictive performance.

# Usage

```
runCrossValidate(
    MCMCconfiguration,
    k,
    foldFunction = "random",
    lossFunction = "MSE",
    MCMCcontrol = list(),
    returnSamples = FALSE,
    nCores = 1,
    nBootReps = 200,
    silent = FALSE
)
```

## Arguments

MCMCconfiguration

C	a NIMBLE MCMC configuration object, returned by a call to configureMCMC.
k	number of folds that should be used for cross-validation.
foldFunction	one of (1) an R function taking a single integer argument i, and returning a character vector with the names of the data nodes to leave out of the model for fold i, or (2) the character string "random", indicating that data nodes will be randomly partitioned into k folds. Note that choosing "random" and setting k equal to the total number of data nodes in the model will perform leave-one-out cross-validation. Defaults to "random". See 'Details'.
lossFunction	one of (1) an R function taking a set of simulated data and a set of observed data, and calculating the loss from those, or (2) a character string naming one of NIMBLE's built-in loss functions. If a character string, must be one of "predictive" to use the log predictive density as a loss function or "MSE" to use the mean squared error as a loss function. Defaults to "MSE". See 'Details' for information on creating a user-defined loss function.
MCMCcontrol	(optional) an R list with parameters governing the MCMC algorithm, See 'De- tails' for specific parameters.
returnSamples	logical indicating whether to return all posterior samples from all MCMC runs. This can result in a very large returned object (there will be k sets of posterior samples returned). Defaults to FALSE.
nCores	number of cpu cores to use in parallelizing the CV calculation. Only MacOS and Linux operating systems support multiple cores at this time. Defaults to 1.

nBootReps	number of bootstrap samples to use when estimating the Monte Carlo error of
	the cross-validation metric. Defaults to 200. If no Monte Carlo error estimate
	is desired, nBootReps can be set to NA, which can potentially save significant computation time.
silent	Boolean specifying whether to show output from the algorithm as it's running (default = FALSE).

## Details

k-fold CV in NIMBLE proceeds by separating the data in a nimbleModel into k folds, as determined by the foldFunction argument. For each fold, the corresponding data are held out of the model, and MCMC is run to estimate the posterior distribution and simultaneously impute posterior predictive values for the held-out data. Then, the posterior predictive values are compared to the known, held-out data values via the specified lossFunction. The loss values are averaged over the posterior samples for each fold, and these averaged values for each fold are then averaged over all folds to produce a single out-of-sample loss estimate. Additionally, estimates of the Monte Carlo error for each fold are returned.

#### Value

an R list with four elements:

- CVvalue. The CV value, measuring the model's ability to predict new data. Smaller relative values indicate better model performance.
- CVstandardError. The standard error of the CV value, giving an indication of the total Monte Carlo error in the CV estimate.
- foldCVInfo. An list of fold CV values and standard errors for each fold.
- samples. An R list, only returned when returnSamples = TRUE. The i'th element of this list will be a matrix of posterior samples from the model with the i'th fold of data left out. There will be k sets of samples.

#### The foldFunction Argument

If the default 'random' method is not used, the foldFunction argument must be an R function that takes a single integer-valued argument i. i is guaranteed to be within the range [1, k]. For each integer value i, the function should return a character vector of node names corresponding to the data nodes that will be left out of the model for that fold. The returned node names can be expanded, but don't need to be. For example, if fold i is inteded to leave out the model nodes x[1], x[2] and x[3] then the function could return either c('x[1]', 'x[2]', 'x[3]') or 'x[1:3]'.

### The lossFunction Argument

If you don't wish to use NIMBLE's built-in "MSE" or "predictive" loss functions, you may provide your own R function as the lossFunction argument to runCrossValidate. A user-supplied lossFunction must be an R function that takes two arguments: the first, named simulatedDataValues, will be a vector of simulated data values. The second, named actualDataValues, will be a vector of observed data values corresponding to the simulated data values in simulatedDataValues. The loss function should return a single scalar number. See 'Examples' for an example of a user-defined loss function.

## runCrossValidate

#### The MCMCcontrol Argument

The MCMCcontrol argument is a list with the following elements:

- niter. An integer argument determining how many MCMC iterations should be run for each loss value calculation. Defaults to 10000, but should probably be manually set.
- nburnin. The number of samples from the start of the MCMC chain to discard as burn-in for each loss value calculation. Must be between 0 and niter. Defaults to 10

### Author(s)

Nicholas Michaud and Lauren Ponisio

#### Examples

```
## Not run:
## We conduct CV on the classic "dyes" BUGS model.
dyesCode <- nimbleCode({</pre>
 for (i in 1:BATCHES) {
    for (j in 1:SAMPLES) {
     y[i,j] ~ dnorm(mu[i], tau.within);
    }
   mu[i] ~ dnorm(theta, tau.between);
 }
 theta ~ dnorm(0.0, 1.0E-10);
 tau.within ~ dgamma(0.001, 0.001); sigma2.within <- 1/tau.within;</pre>
 tau.between ~ dgamma(0.001, 0.001); sigma2.between <- 1/tau.between;</pre>
})
dyesData <- list(y = matrix(c(1545, 1540, 1595, 1445, 1595,</pre>
                               1520, 1440, 1555, 1550, 1440,
                               1630, 1455, 1440, 1490, 1605,
                               1595, 1515, 1450, 1520, 1560,
                               1510, 1465, 1635, 1480, 1580,
                               1495, 1560, 1545, 1625, 1445),
                               nrow = 6, ncol = 5))
dyesConsts <- list(BATCHES = 6,</pre>
                   SAMPLES = 5)
dyesInits <- list(theta = 1500, tau.within = 1, tau.between = 1)</pre>
dyesModel <- nimbleModel(code = dyesCode,</pre>
                          constants = dyesConsts,
                          data = dyesData,
                          inits = dyesInits)
# Define the fold function.
# This function defines the data to leave out for the i'th fold
```

 $\ensuremath{\texttt{\#}}$  as the i'th row of the data matrix y. This implies we will have

```
# 6 folds.
dyesFoldFunction <- function(i){</pre>
 foldNodes_i <- paste0('y[', i, ', ]') # will return 'y[1,]' for i = 1 e.g.</pre>
 return(foldNodes_i)
}
# We define our own loss function as well.
# The function below will compute the root mean squared error.
RMSElossFunction <- function(simulatedDataValues, actualDataValues){</pre>
 dataLength <- length(simulatedDataValues) # simulatedDataValues is a vector</pre>
 SSE <- 0
 for(i in 1:dataLength){
    SSE <- SSE + (simulatedDataValues[i] - actualDataValues[i])^2</pre>
 }
 MSE <- SSE / dataLength
 RMSE <- sqrt(MSE)</pre>
 return(RMSE)
}
dyesMCMCconfiguration <- configureMCMC(dyesModel)</pre>
crossValOutput <- runCrossValidate(MCMCconfiguration = dyesMCMCconfiguration,</pre>
                                     k = 6,
                                     foldFunction = dyesFoldFunction,
                                     lossFunction = RMSElossFunction,
                                     MCMCcontrol = list(niter = 5000,
                                                          nburnin = 500))
## End(Not run)
```

runLaplace

Combine steps of running Laplace or adaptive Gauss-Hermite quadrature approximation

## Description

Use an approximation (compiled or uncompiled) returned from 'buildLaplace' or 'buildAGHQ' to find the maximum likelihood estimate and return it with random effects estimates and/or standard errors.

# Usage

```
runLaplace(
    laplace,
    pStart,
    originalScale = TRUE,
    randomEffectsStdError = TRUE,
```

## runLaplace

```
jointCovariance = FALSE
)
runAGHQ(
   AGHQ,
   pStart,
   originalScale = TRUE,
   randomEffectsStdError = TRUE,
   jointCovariance = FALSE
)
```

## Arguments

laplace	A (compiled or uncompiled) nimble laplace approximation object returned from 'buildLaplace' or 'buildAGHQ'. These return the same type of approximation algorithm object. 'buildLaplace' is simply 'buildAGHQ' with 'nQuad=1'.
pStart	Initial values for parameters to begin optimization search for the maximum like- lihood estimates. If omitted, the values currently in the (compiled or uncom- piled) model object will be used.
originalScale	If TRUE, return all results on the original scale of the parameters and/or random effects as written in the model. Otherwise, return all results on potentially unconstrained transformed scales that are used in the actual computations. Transformed scales (parameterizations) are used if any parameter or random effect has contraint(s) on its support (range of allowed values). Default = TRUE.
randomEffectsStdError	
	If TRUE, include standard errors for the random effects estimates. Default = TRUE.
jointCovariance	
	If TRUE, return the full joint covariance matrix (inverse of the Hessian) of parameters and random effects. Default = FALSE.
AGHQ	Same as laplace.

#### Details

Adaptive Gauss-Hermite quadrature is a generalization of Laplace approximation. runLaplace simply calles runAGHQ and provides a convenient name.

These functions manage the steps of calling the 'findMLE' method to obtain the maximum likelihood estimate of the parameters and then the 'summaryLaplace' function to obtain standard errors, (optionally) random effects estimates (conditional modes), their standard errors, and the full parameter-random effects covariance matrix.

Note that for 'nQuad > 1' (see buildAGHQ), i.e., AGHQ with higher order than Laplace approximation, maximum likelihood estimation is available only if all random effects integrations are univariate. With multivariate random effects integrations, one can use 'nQuad > 1' only to calculate marginal log likelihoods at given parameter values. This is useful for checking the accuracy of the log likelihood at the MLE obtained for Laplace approximation ('nQuad == 1'). 'nQuad' can be changed using the 'updateSettings' method of the approximation object.

See summaryLaplace, which is called for the summary components.

## Value

A list with elements MLE and summary.

MLE is the result of the findMLE method, which contains the parameter estimates and Hessian matrix. This is considered raw output, and one should normally use instead the contents of summary. (For example not that the Hessian matrix in MLE may not correspond to the same scale as the parameter estimates if a transformation was used to operate in an unconstrained parameter space.)

summary is the result of summaryLaplace (or equivalently summaryAGHQ), which contains parameter estimates and standard errors, and optionally other requested components. All results in this object will be on the same scale (parameterization), either original or transformed, as requested.

runMCMC Run one or more chains of an MCMC algorithm and return samples, summary and/or WAIC

# Description

Takes as input an MCMC algorithm (ideally a compiled one for speed) and runs the MCMC with one or more chains, any returns any combination of posterior samples, posterior summary statistics, and a WAIC value.

#### Usage

```
runMCMC(
 mcmc,
  niter = 10000,
  nburnin = 0,
  thin,
  thin2,
  nchains = 1,
  inits,
  setSeed = FALSE,
  progressBar = getNimbleOption("MCMCprogressBar"),
  samples = TRUE,
  samplesAsCodaMCMC = FALSE,
  summary = FALSE,
 WAIC = FALSE,
  perChainWAIC = FALSE
)
```

## Arguments

mcmc	A NIMBLE MCMC algorithm. See details.
niter	Number of iterations to run each MCMC chain. Default value is 10000.
nburnin	Number of initial, pre-thinning, MCMC iterations to discard. Default value is 0.

thin	Thinning interval for collecting MCMC samples, corresponding to monitors. Thinning occurs after the initial nburnin samples are discarded. Default value is 1.
thin2	Thinning interval for collecting MCMC samples, corresponding to the second, optional set of monitors2. Thinning occurs after the initial nburnin samples are discarded. Default value is 1.
nchains	Number of MCMC chains to run. Default value is 1.
inits	Optional argument to specify initial values for each chain. See details.
setSeed	Logical or numeric argument. If a numeric vector of length nchains is provided, then each element of this vector is provided as R's random number seed at the onset of the corresponding MCMC chain. Otherwise, in the case of a logical value, if TRUE, then R's random number seed for the ith chain is set to be i, at the onset of each MCMC chain, and if FALSE, the random number seed is never set or modified. The case of providing a single numeric value for this argument is not supported, except in the case when nchains = 1. If the same starting seed is desired for each chain, use setSeed = rep(seed, nchains). Default value is FALSE.
progressBar	Logical argument. If TRUE, an MCMC progress bar is displayed during exe- cution of each MCMC chain. Default value is defined by the nimble package option MCMCprogressBar.
samples	Logical argument. If TRUE, then posterior samples are returned from each MCMC chain. These samples are optionally returned as coda mcmc objects, depending on the samplesAsCodaMCMC argument. Default value is TRUE. See details.
samplesAsCodaM	ICMC
	Logical argument. If TRUE, then a coda mcmc object is returned instead of an R matrix of samples, or when nchains > 1 a coda mcmc.list object is returned containing nchains mcmc objects. This argument is only used when samples is TRUE. Default value is FALSE. See details.
summary	Logical argument. When TRUE, summary statistics for the posterior samples of each parameter are also returned, for each MCMC chain. This may be returned in addition to the posterior samples themselves. Default value is FALSE. See details.
WAIC	Logical argument. When TRUE, the WAIC (Watanabe, 2010) of the model is calculated and returned. Note that in order for the WAIC to be calculated, the mcmc object must have also been created with the argument 'enableWAIC = TRUE'. If multiple chains are run, then a single WAIC value is calculated using the posterior samples from all chains. Default value is FALSE. See help(waic).
perChainWAIC	Logical argument. When TRUE and multiple chains are run, the WAIC for each chain is returned as a means of helping assess the stability of the WAIC estimate. Default value is FALSE.

# Details

At least one of samples, summary or WAIC must be TRUE, since otherwise, nothing will be returned. Any combination of these may be TRUE, including possibly all three, in which case posterior samples and summary statistics are returned for each MCMC chain, and an overall WAIC value is calculated and returned.

When samples = TRUE, the form of the posterior samples is determined by the samplesAsCodaMCMC argument, as either matrices of posterior samples, or coda mcmc and mcmc.list objects.

Posterior summary statistics are returned individually for each chain, and also as calculated from all chains combined (when nchains > 1).

If provided, the inits argument can be one of three things:

(1) a function to generate initial values, which will be executed to generate initial values at the beginning of each MCMC chain, or (2) a single named list of initial values which, will be used for each chain, or (3) a list of length nchains, each element being a named list of initial values which be used for one MCMC chain.

The inits argument may also be omitted, in which case the current values in the model object will be used as the initial values of the first chain, and subsequent chains will begin using starting values where the previous chain ended.

Other aspects of the MCMC algorithm, such as the specific sampler assignments, must be specified in advance using the MCMC configuration object (created using configureMCMC), which is then used to build an MCMC algorithm (using buildMCMC) argument.

The niter argument specifies the number of pre-thinning MCMC iterations, and the nburnin argument specifies the number of pre-thinning MCMC samples to discard. After discarding these burn-in samples, thinning of the remaining samples will take place. The total number of posterior samples returned will be floor((niter-nburnin)/thin).

The MCMC option mcmc\$run(..., reset = FALSE), used to continue execution of an MCMC chain, is not available through runMCMC().

### Value

A list is returned with named elements depending on the arguments passed to nimbleMCMC, unless this list contains only a single element, in which case only that element is returned. These elements may include samples, summary, and WAIC, and when the MCMC is monitoring a second set of nodes using monitors2, also samples2. When nchains = 1, posterior samples are returned as a single matrix, and summary statistics as a single matrix. When nchains > 1, posterior samples are returned as a list of matrices, one matrix for each chain, and summary statistics are returned as a list containing nchains+1 matrices: one matrix corresponding to each chain, and the final element providing a summary of all chains, combined. If samplesAsCodaMCMC is TRUE, then posterior samples are provided as coda mcmc and mcmc.list objects. When WAIC is TRUE, a WAIC summary object is returned.

# Author(s)

Daniel Turek

#### See Also

configureMCMC buildMCMC nimbleMCMC

### sampler\_BASE

## Examples

```
## Not run:
code <- nimbleCode({
    mu ~ dnorm(0, sd = 1000)
    sigma ~ dunif(0, 1000)
    for(i in 1:10) {
        x[i] ~ dnorm(mu, sd = sigma)
    }
})
Rmodel <- nimbleModel(code)
Rmodel$setData(list(x = c(2, 5, 3, 4, 1, 0, 1, 3, 5, 3)))
Rmcmc <- buildMCMC(Rmodel)
Cmodel <- compileNimble(Rmodel)
Cmcmc <- compileNimble(Rmcmc, project = Rmodel)
inits <- function() list(mu = rnorm(1,0,1), sigma = runif(1,0,10))
samplesList <- runMCMC(Cmcmc, niter = 10000, nchains = 3, inits = inits)</pre>
```

## End(Not run)

sampler\_BASE

MCMC Sampling Algorithms

#### Description

Details of the MCMC sampling algorithms provided with the NIMBLE MCMC engine; HMC samplers are in the nimbleHMC package and particle filter samplers are in the nimbleSMC package.

#### Usage

```
sampler_BASE()
```

sampler\_prior\_samples(model, mvSaved, target, control)
sampler\_posterior\_predictive(model, mvSaved, target, control)
sampler\_binary(model, mvSaved, target, control)
sampler\_categorical(model, mvSaved, target, control)
sampler\_noncentered(model, mvSaved, target, control)
sampler\_RW(model, mvSaved, target, control)
sampler\_RW\_block(model, mvSaved, target, control)
sampler\_RW\_llFunction(model, mvSaved, target, control)

sampler\_slice(model, mvSaved, target, control) sampler\_ess(model, mvSaved, target, control) sampler\_AF\_slice(model, mvSaved, target, control) sampler\_crossLevel(model, mvSaved, target, control) sampler\_RW\_llFunction\_block(model, mvSaved, target, control) sampler\_RW\_multinomial(model, mvSaved, target, control) sampler\_RW\_dirichlet(model, mvSaved, target, control) sampler\_RW\_wishart(model, mvSaved, target, control) sampler\_RW\_lkj\_corr\_cholesky(model, mvSaved, target, control) sampler\_RW\_block\_lkj\_corr\_cholesky(model, mvSaved, target, control) sampler\_CAR\_normal(model, mvSaved, target, control) sampler\_CAR\_proper(model, mvSaved, target, control) sampler\_polyagamma(model, mvSaved, target, control) sampler\_RJ\_fixed\_prior(model, mvSaved, target, control) sampler\_RJ\_indicator(model, mvSaved, target, control) sampler\_RJ\_toggled(model, mvSaved, target, control) sampler\_CRP\_concentration(model, mvSaved, target, control) sampler\_CRP(model, mvSaved, target, control) sampler\_slice\_CRP\_base\_param(model, mvSaved, target, control)

#### Arguments

model	(uncompiled) model on which the MCMC is to be run
mvSaved	modelValues object to be used to store MCMC samples
target	node(s) on which the sampler will be used
control	named list that controls the precise behavior of the sampler, with elements spe- cific to samplertype. The default values for control list are specified in the setup code of each sampling algorithm. Descriptions of each sampling algorithm, and the possible customizations for each sampler (using the control argument) ap- pear below.

### sampler\_BASE

#### Hamiltonian Monte Carlo samplers

Hamiltonian Monte Carlo (HMC) samplers are provided separately in the nimbleHMC R package. After loading nimbleHMC, see help(HMC) for details.

#### Particle filter samplers

As of Version 0.10.0 of NIMBLE, the RW\_PF and RW\_PF\_block samplers are provided separately in the 'nimbleSMC' package. After loading nimbleSMC, see help(samplers) for details.

#### sampler\_base

base class for new samplers

When you write a new sampler for use in a NIMBLE MCMC (see User Manual), you must include contains = sampler\_BASE.

#### binary sampler

The binary sampler performs Gibbs sampling for binary-valued (discrete 0/1) nodes. This can only be used for nodes following either a dbern(p) or dbinom(p, size=1) distribution.

The binary sampler accepts no control list arguments.

#### categorical sampler

The categorical sampler performs Gibbs sampling for a single node, which generally would follow a categorical (dcat) distribution. The categorical sampler can be assigned to other distributions as well, in which case the number of possible outcomes (1, 2, 3, ..., k) of the distribution must be specified using the 'length' control argument.

The categorical sampler accepts the following control list elements:

- length. A character string or a numeric argument. When a character string, this should be
  the name of a parameter of the distribution of the target node being sampled. The length of
  this distribution parameter (considered as a 1-dimensional vector) will be used to determine
  the number of possible outcomes of the target node's distribution. When a numeric value,
  this value will be used as the number of possible outcomes of the target node's distribution.
  (default = "prob")
- check. A logical argument. When FALSE, no check for a 'dcat' prior distribution for the target node takes place. (default = TRUE)

#### **RW** sampler

The RW sampler executes adaptive Metropolis-Hastings sampling with a normal proposal distribution (Metropolis, 1953), implementing the adaptation routine given in Shaby and Wells, 2011. This sampler can be applied to any scalar continuous-valued stochastic node, and can optionally sample on a log scale.

The RW sampler accepts the following control list elements:

• log. A logical argument, specifying whether the sampler should operate on the log scale. (default = FALSE)

- reflective. A logical argument, specifying whether the normal proposal distribution should reflect to stay within the range of the target distribution. (default = FALSE)
- adaptive. A logical argument, specifying whether the sampler should adapt the scale (proposal standard deviation) throughout the course of MCMC execution to achieve a theoretically desirable acceptance rate. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation. Every adaptInterval MCMC iterations (prior to thinning), the RW sampler will perform its adaptation procedure. This updates the scale variable, based upon the sampler's achieved acceptance rate over the past adaptInterval iterations. (default = 200)
- adaptFactorExponent. Exponent controling the rate of decay of the scale adaptation factor. See Shaby and Wells, 2011, for details. (default = 0.8)
- scale. The initial value of the normal proposal standard deviation. If adaptive = FALSE, scale will never change. (default = 1)

The RW sampler cannot be used with options log=TRUE and reflective=TRUE, i.e. it cannot do reflective sampling on a log scale.

After an MCMC algorithm has been configured and built, the value of the proposal standard deviation of a RW sampler can be modified using the setScale method of the sampler object. This use the scalar argument to modify the current value of the proposal standard deviation, as well as modifying the initial (pre-adaptation) value to which the proposal standard deviation is reset, at the onset of a new MCMC chain.

### **RW\_block sampler**

The RW\_block sampler performs a simultaneous update of one or more model nodes, using an adaptive Metropolis-Hastings algorithm with a multivariate normal proposal distribution (Roberts and Sahu, 1997), implementing the adaptation routine given in Shaby and Wells, 2011. This sampler may be applied to any set of continuous-valued model nodes, to any single continuous-valued multivariate model node, or to any combination thereof.

The RW\_block sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should adapt the scale (a coefficient for the entire proposal covariance matrix) and propCov (the multivariate normal proposal covariance matrix) throughout the course of MCMC execution. If only the scale should undergo adaptation, this argument should be specified as TRUE. (default = TRUE)
- adaptScaleOnly. A logical argument, specifying whether adaption should be done only for scale (TRUE) or also for provCov (FALSE). This argument is only relevant when adaptive = TRUE. When adaptScaleOnly = FALSE, both scale and propCov undergo adaptation; the sampler tunes the scaling to achieve a theoretically good acceptance rate, and the proposal covariance to mimic that of the empirical samples. When adaptScaleOnly = TRUE, only the proposal scale is adapted. (default = FALSE)
- adaptInterval. The interval on which to perform adaptation. Every adaptInterval MCMC iterations (prior to thinning), the RW\_block sampler will perform its adaptation procedure, based on the past adaptInterval iterations. (default = 200)
- adaptFactorExponent. Exponent controling the rate of decay of the scale adaptation factor. See Shaby and Wells, 2011, for details. (default = 0.8)

- scale. The initial value of the scalar multiplier for propCov. If adaptive = FALSE, scale will never change. (default = 1)
- propCov. The initial covariance matrix for the multivariate normal proposal distribution. This element may be equal to the character string 'identity', in which case the identity matrix of the appropriate dimension will be used for the initial proposal covariance matrix. (default = 'identity')
- tries. The number of times this sampler will repeatedly operate on each MCMC iteration. Each try consists of a new proposed transition and an accept/reject decision of this proposal. Specifying tries > 1 can help increase the overall sampler acceptance rate and therefore chain mixing. (default = 1)

After an MCMC algorithm has been configured and built, the value of the proposal standard deviation of a RW\_block sampler can be modified using the setScale method of the sampler object. This use the scalar argument to will modify the current value of the proposal standard deviation, as well as modifying the initial (pre-adaptation) value which the proposal standard deviation is reset to, at the onset of a new MCMC chain.

Operating analogous to the setScale method, the RW\_block sampler also has a setPropCov method. This method accepts a single matrix-valued argument, which will modify both the current and initial (used at the onset of a new MCMC chain) values of the multivariate normal proposal covariance.

Note that modifying elements of the control list may greatly affect the performance of this sampler. In particular, the sampler can take a long time to find a good proposal covariance when the elements being sampled are not on the same scale. We recommend providing an informed value for propCov in this case (possibly simply a diagonal matrix that approximates the relative scales), as well as possibly providing a value of scale that errs on the side of being too small. You may also consider decreasing adaptFactorExponent and/or adaptInterval, as doing so has greatly improved performance in some cases.

## Barker proposal sampler

The Barker proposal sampler implements a (multivariate) gradient-based sampling scheme, following the work of Livingstone and Zanella (2022) and Vogrinc et al. (2023). This sampler may be applied to any set of continuous-valued model nodes, to any single continuous-valued multivariate model node, or to any combination thereof. The sampler uses an gradient-based adaptive Metropolis-Hastings algorithm with a multivariate normal proposal distribution, which can use a full proposal covariance matrix (recommended for most problems) or a diagonal matrix. To use the Barker sampler, you must set buildDerivs = TRUE when creating your model via nimbleModel.

The Barker sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should adapt the scalar global scale (a coefficient scaling the entire proposal covariance matrix) and (possibly) the multivariate normal proposal covariance matrix throughout the course of MCMC execution. If only the scale should undergo adaptation, this argument should be specified as TRUE. (default = TRUE)
- adaptScaleOnly. A logical argument, specifying whether adaption should be done only for the global scale and not for the covariance matrix. This argument is only relevant when adaptive = TRUE. When adaptScaleOnly = TRUE, only the scale is adapted, tuned to achieve a theoretically good acceptance rate (specified by targetAcceptanceRate). (default = FALSE)

- adaptCov. A logical argument, specifying whether adaption should be done for the full proposal covariance matrix (TRUE) or only for the diagonal of the matrix (the proposal variances) (FALSE). This argument is only relevant when adaptive = TRUE and adaptScaleOnly = FALSE. The full covariance matrix or diagonal values are tuned to mimic the full covariance or the variances, respectively, of the empirical samples from the posterior.
- scale. Initial multiplier that scales the step-size of the proposal steps. If adaptation is turned off, this determines the step-size. (default = 1)
- propCov. Initial value for proposal covariance. This can be the string "identity" (indicating the identity matrix), a single number that scales the identity matrix, a vector of values that provides the diagonal values (variances) of the matrix (of length equal to the number of parameters in the transformed space), or a full proposal covariance matrix (with number of rows and columns equal to the number of parameters in the transformed space). (default = 1)
- adaptInterval. The interval on which to perform adaptation of the scale (and diagonal variance values when adaptCov = FALSE). At the moment only the value 1 is allowed.
- adaptIntervalCov. The interval on which to perform adaptation of the full proposal covariance. This only has effect when adaptCov = TRUE. The default of 10 was chosen based on performance on various examples but other values may improve mixing in specific cases. Note that if invariantWeight = FALSE, changing this value also has the effect of modifying the influence of the most recent set of empirical samples relative to the current proposal covariance. (default = 10)
- adaptDelayCov. The number of initial iterations in which the off-diagonal elements of the proposal covariance are not adapted. In experiments, adapting the full covariance from the first iteration can produce an algorithm that performs poorly as the covariances may be adapted while the chain is still burning in, during whih the samples are not reflective of the posterior. Only relevant if adaptCov = TRUE. The default of 100 was chosen based on performance on various examples but other values may improve mixing in specific cases. (default = 100)
- adaptFactorExponent. Exponent controlling the rate of decay of the scale adaptation factor. As suggested in Livingstone and Zanella (2022), the default is 0.6.
- targetAcceptanceRate. Acceptance rate targeted when adapting the global scale. As suggested in Vogrinc et al. (2023) the default is 0.574, as in the MALA algorithm.
- bimodal. A logical argument indicating whether to use the bimodal proposal of Vogrinc et al. (2023) (TRUE) or simply a normal distribution (FALSE). (default = TRUE)
- sigma. The value of sigma in the bimodal Barker proposal suggested in Vogrinc et al. (2023). Only used if bimodal = TRUE. (default = 0.1)
- invariantWeight. A logical argument indicating whether to modify the relative weight of the most recent set of empirical samples relative to the current proposal covariance such that changing adaptIntervalCov has little effect on the weighting. While in principle setting this to TRUE makes sense, in experiments this tended to make MCMC performance worse, so the default is FALSE.

The Barker proposal provides a gradient-based Metropolis-Hastings algorithm demonstrated to be more robust to tuning parameters than other gradient-based methods, in particular the Metropolis-adjusted Langevin algorithm (MALA). The approach tends to do a better job of adjusting to hetero-geneity in the scaling of the target elements and to bad (particularly overly large) initial proposal variance(s) than random walk Metropolis-Hastings (i.e., the RW\_block sampler).

For some problems without strong dependence, adapting only the diagonal of the proposal covariance (adaptCov = FALSE) may perform well, but for most problems, use of the full proposal covariance matrix is expected to perform better. The implementation of the proposal covariance for the Barker proposal is derived based on the use of preconditioning to transform the parameters to be approximately linearly independent. This is equivalent to and implemented as a dense proposal covariance matrix.

Adaptation of the full proposal covariance matrix (i.e., of the off-diagonal elements) starting from the first iteration of the MCMC can cause poor MCMC performance by adapting the covariances based on samples in which the MCMC is burning in, which can prevent the sampler from burning in and from finding a good proposal covariance in a reasonable number of iterations. For this reason, by default the sampler only adapts the global scale and proposal variances for the first adaptDelayCov iterations, defaulting to 100 iterations.

The Barker proposal uses the gradient of the log posterior density with respect to the parameters, using nimble's automatic differentiation (AD) system. Given this, elements of the target vector that are constrained in some fashion (either by their prior or relative to other elements, such as sampling the elements of a Dirichlet-distributed vector or the elements of a positive definite matrix) are transformed to an unconstrained space using nimble's automatic parameter transformation system. Thus the proposal covariance is with respect to this transformed space.

To use this sampler instead of 'RW\_block' as the default multivariate sampler for continuous distributions, set nimbleOptions(MCMCuseBarkerAsDefaultMV = TRUE)

After an MCMC algorithm has been configured and built, the value of the global scale of a Barker sampler can be modified using the setScale method of the sampler object. This use the scalar argument to will modify the current value of the scale, as well as modifying the initial (pre-adaptation) value which the scale is reset to, at the onset of a new MCMC chain.

Operating analogous to the setScale method, the Barker sampler also has a setPropVar (for when adaptCov = FALSE) and setPropCov (for when adaptCov = TRUE). These method accept a single vector- and matrix-valued argument, respectively, which will modify both the current and initial (used at the onset of a new MCMC chain) values of the multivariate normal proposal variances or covariance, respectively.

## **RW\_llFunction sampler**

Sometimes it is useful to control the log likelihood calculations used for an MCMC updater instead of simply using the model. For example, one could use a sampler with a log likelihood that analytically (or numerically) integrates over latent model nodes. Or one could use a sampler with a log likelihood that comes from a stochastic approximation such as a particle filter, allowing composition of a particle MCMC (PMCMC) algorithm (Andrieu et al., 2010). The RW\_IIFunction sampler handles this by using a Metropolis-Hastings algorithm with a normal proposal distribution and a user-provided log-likelihood function. To allow compiled execution, the log-likelihood function must be provided as a specialized instance of a nimbleFunction. The log-likelihood function may use the same model as the MCMC as a setup argument, but if so the state of the model should be unchanged during execution of the function (or you must understand the implications otherwise).

The RW\_llFunction sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should adapt the scale (proposal standard deviation) throughout the course of MCMC execution. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation. (default = 200)

- scale. The initial value of the normal proposal standard deviation. (default = 1)
- IlFunction. A specialized nimbleFunction that accepts no arguments and returns a scalar double number. The return value must be the total log-likelihood of all stochastic dependents of the target nodes and, if includesTarget = TRUE, of the target node(s) themselves or whatever surrogate is being used for the total log-likelihood. This is a required element with no default.
- includesTarget. Logical variable indicating whether the return value of llFunction includes the log-likelihood associated with target. This is a required element with no default.

## slice sampler

The slice sampler performs slice sampling of the scalar node to which it is applied (Neal, 2003). This sampler can operate on either continuous-valued or discrete-valued scalar nodes. The slice sampler performs a 'stepping out' procedure, in which the slice is iteratively expanded to the left or right by an amount sliceWidth. This sampler is optionally adaptive, governed by a control list element, whereby the value of sliceWidth is adapted towards the observed absolute difference between successive samples.

The slice sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler will adapt the value of sliceWidth throughout the course of MCMC execution. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation. (default = 200)
- sliceWidth. The initial value of the width of each slice, and also the width of the expansion during the iterative 'stepping out' procedure. (default = 1)
- sliceMaxSteps. The maximum number of expansions which may occur during the 'stepping out' procedure. (default = 100)
- maxContractions. The maximum number of contractions of the interval that may occur during sampling (this prevents infinite looping in unusual situations). (default = 100)
- maxContractionsWarning. A logical argument specifying whether to warn when the maximum number of contractions is reached. (default = TRUE)

#### ess sampler

The ess sampler performs elliptical slice sampling of a single node, which must follow either a univariate or multivariate normal distribution (Murray, 2010). The algorithm is an extension of slice sampling (Neal, 2003), generalized to context of the Gaussian distribution. An auxiliary variable is used to identify points on an ellipse (which passes through the current node value) as candidate samples, which are accepted contingent upon a likelihood evaluation at that point. This algorithm requires no tuning parameters and therefore no period of adaptation, and may result in very efficient sampling from Gaussian distributions.

The ess sampler accepts the following control list arguments.

- maxContractions. The maximum number of contractions of the interval that may occur during sampling (this prevents infinite looping in unusual situations). (default = 100)
- maxContractionsWarning. A logical argument specifying whether to warn when the maximum number of contractions is reached. (default = TRUE)

## **AF\_slice** sampler

The automated factor slice sampler conducts a slice sampling algorithm on one or more model nodes. The sampler uses the eigenvectors of the posterior covariance between these nodes as an orthogonal basis on which to perform its 'stepping Out' procedure. The sampler is adaptive in updating both the width of the slices and the values of the eigenvectors. The sampler can be applied to any set of continuous or discrete-valued model nodes, to any single continuous or discrete-valued multivariate model node, or to any combination thereof. The automated factor slice sampler accepts the following control list elements:

- sliceWidths. A numeric vector of initial slice widths. The length of the vector must be equal to the sum of the lengths of all nodes being used by the automated factor slice sampler. Defaults to a vector of 1's.
- sliceAdaptFactorMaxIter. The number of iterations for which the factors (eigenvectors) will continue to adapt to the posterior correlation. (default = 15000)
- sliceAdaptFactorInterval. The interval on which to perform factor adaptation. (default = 200)
- sliceAdaptWidthMaxIter. The maximum number of iterations for which to adapt the widths for a given set of factors. (default = 512)
- sliceAdaptWidthTolerance. The tolerance for when widths no longer need to adapt, between 0 and 0.5. (default = 0.1)
- sliceMaxSteps. The maximum number of expansions which may occur during the 'stepping out' procedure. (default = 100)
- maxContractions. The maximum number of contractions of the interval that may occur during sampling (this prevents infinite looping in unusual situations). (default = 100)
- maxContractionsWarning. A logical argument specifying whether to warn when the maximum number of contractions is reached. (default = TRUE)

#### crossLevel sampler

This sampler is constructed to perform simultaneous updates across two levels of stochastic dependence in the model structure. This is possible when all stochastic descendents of node(s) at one level have conjugate relationships with their own stochastic descendents. In this situation, a Metropolis-Hastings algorithm may be used, in which a multivariate normal proposal distribution is used for the higher-level nodes, and the corresponding proposals for the lower-level nodes undergo Gibbs (conjugate) sampling. The joint proposal is either accepted or rejected for all nodes involved based upon the Metropolis-Hastings ratio. This sampler is a conjugate version of Scheme 3 in Knorr-Held and Rue (2002). It can also be seen as a Metropolis-based version of collapsed Gibbs sampling (in particular Sampler 3 of van Dyk and Park (2008)).

The requirement that all stochastic descendents of the target nodes must themselves have only conjugate descendents will be checked when the MCMC algorithm is built. This sampler is useful when there is strong dependence across the levels of a model that causes problems with convergence or mixing.

The crossLevel sampler accepts the following control list elements:

- adaptive. Logical argument, specifying whether the multivariate normal proposal distribution for the target nodes should be adaptived. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation. (default = 200)

- scale. The initial value of the scalar multiplier for propCov. (default = 1)
- propCov. The initial covariance matrix for the multivariate normal proposal distribution. This element may be equal to the character string 'identity' or any positive definite matrix of the appropriate dimensions. (default = 'identity')

#### **RW\_llFunction\_block sampler**

Sometimes it is useful to control the log likelihood calculations used for an MCMC updater instead of simply using the model. For example, one could use a sampler with a log likelihood that analytically (or numerically) integrates over latent model nodes. Or one could use a sampler with a log likelihood that comes from a stochastic approximation such as a particle filter, allowing composition of a particle MCMC (PMCMC) algorithm (Andrieu et al., 2010) (but see samplers listed below for NIMBLE's direct implementation of PMCMC). The RW\_11Function\_block sampler handles this by using a Metropolis-Hastings algorithm with a multivariate normal proposal distribution and a user-provided log-likelihood function. To allow compiled execution, the log-likelihood function must be provided as a specialized instance of a nimbleFunction. The log-likelihood function may use the same model as the MCMC as a setup argument, but if so the state of the model should be unchanged during execution of the function (or you must understand the implications otherwise).

The RW\_llFunction\_block sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should adapt the proposal covariance throughout the course of MCMC execution. (default is TRUE)
- adaptScaleOnly. A logical argument, specifying whether adaption should be done only for scale (TRUE) or also for provCov (FALSE). This argument is only relevant when adaptive = TRUE. When adaptScaleOnly = FALSE, both scale and propCov undergo adaptation; the sampler tunes the scaling to achieve a theoretically good acceptance rate, and the proposal covariance to mimic that of the empirical samples. When adaptScaleOnly = TRUE, only the proposal scale is adapted. (default = FALSE)
- adaptInterval. The interval on which to perform adaptation. (default = 200)
- adaptFactorExponent. Exponent controling the rate of decay of the scale adaptation factor. See Shaby and Wells, 2011, for details. (default = 0.8)
- scale. The initial value of the scalar multiplier for propCov. If adaptive = FALSE, scale will never change. (default = 1)
- propCov. The initial covariance matrix for the multivariate normal proposal distribution. This element may be equal to the character string 'identity', in which case the identity matrix of the appropriate dimension will be used for the initial proposal covariance matrix. (default = 'identity')
- IlFunction. A specialized nimbleFunction that accepts no arguments and returns a scalar double number. The return value must be the total log-likelihood of all stochastic dependents of the target nodes and, if includesTarget = TRUE, of the target node(s) themselves or whatever surrogate is being used for the total log-likelihood. This is a required element with no default.
- includesTarget. Logical variable indicating whether the return value of llFunction includes the log-likelihood associated with target. This is a required element with no default.

#### **RW\_multinomial sampler**

This sampler updates latent multinomial distributions, using Metropolis-Hastings proposals to move observations between pairs of categories. Each proposal moves one or more observations from one category to another category, and acceptance or rejection follows standard Metropolis-Hastings theory. The number of observations in the proposed move is randomly drawn from a discrete uniform distribution, which is bounded above by the 'maxMove' control argument. The RW\_multinomial sampler can make multiple independent attempts at transitions on each sampling iteration, which is govered by the 'tries' control argument.

The RW\_multinomial sampler accepts the following control list elements:

- maxMove. An integer argument, specifying the upper bound for the number of observations
  to propose moving, on each independent propose/accept/reject step. The number to move is
  drawn from a discrete uniform distribution, with lower limit one, and upper limit given by the
  minimum of 'maxMove' and the number of observations in the category. The default value
  for 'maxMove' is 1/20 of the total number of observations comprising the target multinomial
  distribution (given by the 'size' parameter of the distribution).
- tries. An integer argument, specifying the number of independent Metropolis-Hastings proposals (and subsequent acceptance or rejection) that are attempted each time the sampler operates. For example, if 'tries' is one, then a single proposal (of moving one or more observations to a different category) will be made, and either accepted or rejected. If tries is two, this process is repeated twice. The default value for 'tries' scales as the cube root of the total number of observations comprising the target multinomial distribution (given by the 'size' parameter of the distribution).

## **RW\_dirichlet** sampler

This sampler is designed for sampling non-conjugate Dirichlet distributions. The sampler performs a series of Metropolis-Hastings updates (on the log scale) to each component of a gammareparameterization of the target Dirichlet distribution. The acceptance or rejection of these proposals follows a standard Metropolis-Hastings procedure.

The RW\_dirichlet sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should independently adapt the scale (proposal standard deviation, on the log scale) for each componentwise Metropolis-Hasting update, to achieve a theoretically desirable acceptance rate for each. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation. Every adaptInterval MCMC iterations (prior to thinning), the sampler will perform its adaptation procedure. (default = 200)
- adaptFactorExponent. Exponent controling the rate of decay of the scale adaptation factor. See Shaby and Wells, 2011, for details. (default = 0.8)
- scale. The initial value of the proposal standard deviation (on the log scale) for each component of the reparameterized Dirichlet distribution. If adaptive = FALSE, the proposal standard deviations will never change. (default = 1)

## **RW\_wishart sampler**

This sampler is designed for sampling non-conjugate Wishart and inverse-Wishart distributions. More generally, it can update any symmetric positive-definite matrix (for example, scaled covariance or precision matrices). The sampler performs block Metropolis-Hastings updates following a transformation to an unconstrained scale (Cholesky factorization of the original matrix, then taking the log of the main diagonal elements.

The RW\_wishart sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should adapt the scale and proposal covariance for the multivariate normal Metropolis-Hasting proposals, to achieve a theoretically desirable acceptance rate for each. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation. Every adaptInterval MCMC iterations (prior to thinning), the sampler will perform its adaptation procedure. (default = 200)
- adaptFactorExponent. Exponent controling the rate of decay of the scale adaptation factor. See Shaby and Wells, 2011, for details. (default = 0.8)
- scale. The initial value of the scalar multiplier for the multivariate normal Metropolis-Hastings proposal covariance. If adaptive = FALSE, scale will never change. (default = 1)

#### RW\_block\_lkj\_corr\_cholesky sampler

This sampler is designed for sampling non-conjugate LKJ correlation Cholesky factor distributions. The sampler performs a blocked Metropolis-Hastings update following a transformation to an unconstrained scale (using the signed stickbreaking approach documented in Section 10.12 of the Stan Language Reference Manual, version 2.27).

The RW\_block\_lkj\_corr\_cholesky sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should adapt the scale (a coefficient for the entire proposal covariance matrix) and propCov (the multivariate normal proposal covariance matrix) throughout the course of MCMC execution. If only the scale should undergo adaptation, this argument should be specified as TRUE. (default = TRUE)
- adaptScaleOnly. A logical argument, specifying whether adaption should be done only for scale (TRUE) or also for provCov (FALSE). This argument is only relevant when adaptive = TRUE. When adaptScaleOnly = FALSE, both scale and propCov undergo adaptation; the sampler tunes the scaling to achieve a theoretically good acceptance rate, and the proposal covariance to mimic that of the empirical samples. When adaptScaleOnly = TRUE, only the proposal scale is adapted. (default = FALSE)
- adaptInterval. The interval on which to perform adaptation. Every adaptInterval MCMC iterations (prior to thinning), the RW\_block sampler will perform its adaptation procedure, based on the past adaptInterval iterations. (default = 200)
- adaptFactorExponent. Exponent controling the rate of decay of the scale adaptation factor. See Shaby and Wells, 2011, for details. (default = 0.8)
- scale. The initial value of the scalar multiplier for propCov. If adaptive = FALSE, scale will never change. (default = 1)
- propCov. The initial covariance matrix for the multivariate normal proposal distribution. This element may be equal to the character string 'identity', in which case the identity matrix of the appropriate dimension will be used for the initial proposal covariance matrix. (default = 'identity')

This is the default sampler for the LKJ distribution. However, blocked samplers may perform poorly if the adaptation configuration is poorly chosen. See the comments in the RW\_block section of this documentation.

## RW\_lkj\_corr\_cholesky sampler

This sampler is designed for sampling non-conjugate LKJ correlation Cholesky factor distributions. The sampler performs individual Metropolis-Hastings updates following a transformation to an unconstrained scale (using the signed stickbreaking approach documented in Section 10.12 of the Stan Language Reference Manual, version 2.27).

The RW\_lkj\_corr\_cholesky sampler accepts the following control list elements:

- adaptive. A logical argument, specifying whether the sampler should adapt the scales of the univariate normal Metropolis-Hasting proposals, to achieve a theoretically desirable acceptance rate for each. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation. Every adaptInterval MCMC iterations (prior to thinning), the sampler will perform its adaptation procedure. (default = 200)
- adaptFactorExponent. Exponent controling the rate of decay of the scale adaptation factor. See Shaby and Wells, 2011, for details. (default = 0.8)
- scale. The initial value of the scalar multiplier for the multivariate normal Metropolis-Hastings proposal covariance. If adaptive = FALSE, scale will never change. (default = 1)

Note that this sampler is likely run much more slowly than the blocked sampler for the LKJ distribution, as updating each single element will generally incur the full cost of updating all dependencies of the entire matrix.

## polyagamma sampler

The polyagamma sampler uses Pólya-gamma data augmentation to do conjugate sampling for the parameters in the linear predictor of a logistic regression model (Polson et al., 2013), analogous to the Albert-Chib data augmentation scheme for probit regression. This sampler is not assigned as a default sampler by configureMCMC and so can only be used if manually added to an MCMC configuration.

As an example, consider model code containing:

```
for(i in 1:n) {
    logit(prob[i]) <- beta0 + beta1*x1[i] + beta2*x2[i] + u[group[i]]
    y[i] ~ dbinom(prob = prob[i], size = size[i])
}
for(j in 1:num_groups)
    u[j] ~ dnorm(0, sd = sigma_group)</pre>
```

where beta0, beta1, and beta2 are fixed effects with normal priors, u is a random effect associated with groups of data, and group[i] gives the group index of the i-th observation, y[i]. In this model, the parameters beta0, beta1, beta2, and all the u[j] can be jointly sampled by the polyagamma sampler, i.e., they will be its target nodes.

After building a model (calling nimbleModel) containing the above code, one would configure the sampler as follows:

```
MCMCconf <- configureMCMC(model)
logistic_nodes <- c("beta0", "beta1", "beta2", "u")
# Optionally, remove default samplers.
MCMCconf$removeSamplers(logistic_nodes)
MCMCconf$addSampler(target = logistic_nodes, type = "polyagamma",
    control = list(fixedDesignColumns=TRUE))</pre>
```

As shown here, the stochastic dependencies (y[i] here) of the target nodes must follow dbin or dbern distributions. The logit transformation of their probability parameter must be a linear function (technically an affine function) of the target nodes, which themselves must have dnorm or dmnorm priors. Zero inflation to account for structural zeroes is also supported, allowed as discussed below. The stochastic dependencies will often but not always be the observations in the logistic regression and will be referred to as 'responses' henceforth. Internally, the sampler draws latent values from the Pólya-gamma distribution, one per response. These latent values are then used to draw from the multivariate normal conditional distribution of the target nodes.

Importantly, note that because the Pólya-gamma draws are not retained when an iteration of the sampler finishes, one generally wants to apply the sampler to all parameter nodes involved in the linear predictor of the logistic regression, to avoid duplicative Pólya-gamma draws of the latent values. If there are stochastic indices (e.g., if group[i] above is stochastic), the Pólya-gamma sampler can still be used, but the stochastic nodes cannot be sampled by it and must have separate sampler(s). It is also possible in some models that regression parameters can be split into (conditionally independent) groups that can be sampled independently, e.g., if one has distinct logistic regression specifications for different sets of responses in the model.

Sampling involves use of the design matrix. The design matrix includes one column corresponding to each regression covariate as well as one columnar block corresponding to each random effect. In the example above, the columns would include a vector of ones (to multiply beta0), the vectors x1 and x2, and a vector of indicators for each u[j] (with a 1 in row i if group[i] is j), resulting in 3+num\_groups columns. Note that the polyagamma sampler can determine the design matrix from the model, even when written as above such that the design matrix is not explicitly in the model code. It is also possible to write model code for the linear prediction using matrix multiplication and an explicit design matrix, but that is not necessary.

Often the design matrix is fixed in advance, but in some cases elements of the matrix may be stochastic and sampled during the MCMC. That would be the case if there are missing values (e.g., missing covariate values (declared as stochastic nodes)) or stochastic indexing (e.g., unknown assignment of responses to clusters, as mentioned above). Note that changes in the values of any of the beta or u[j] target nodes in the example above do not change the design matrix.

Recalculating the elements of the design matrix at every iteration is costly and will likely greatly slow the sampler. To alleviate this, users can specify which columns of the design matrix are fixed (non-stochastic) using the fixedDesignColumns control argument. If all columns are fixed, which will often be the case, this argument can be specified simply as TRUE. Note that the sampler does not determine if any or all columns are fixed, so users wishing to take advantage of the large speed gains from having fixed columns should provide this control argument. Columns indicated as fixed will be determined (if necessary) when the sampler is first run and retained for subsequent iterations.

By default, NIMBLE will determine the design matrix (and as discussed above will do so repeatedly at each iteration for any columns not indicated as being fixed). If the matrix has no stochastic elements, users may choose to provide the matrix directly to the sampler via the designMatrix control argument. This will save time in computing the matrix initially but likely will have limited

benefit relative to the cost of running many iterations of MCMC and therefore can be omitted in most cases.

The sampler allows for binomial responses with stochastic sizes. This would be the case in the above example if the size[i] values are themselves declared as unobserved stochastic nodes and thus are sampled by MCMC.

The sampler allows for zero inflation of the response probability in that the probability determined by the inverse logit transformation of the linear predictor can be multipled by one or more binary scalar nodes to produce the response probability. These binary nodes must be specified via the dbern distribution or the dbin distribution with size equal to one. This functionality is intended for use in cases where another part of the model introduces structural zeroes, such as in determining occupancy in ecological occupancy models. An example would be if the above were modified by  $y[i] \sim dbinom(prob = z[i] * p[i], size = size[i])$ , where each z[i] is either 0 or 1.

The polyagamma sampler accepts the following control list elements:

- fixedDesignColumns. Either a single logical value indicating if the design matrix is fixed (non-stochastic) or a logical vector indicating which columns are fixed. In the latter case, the columns must be ordered exactly as the ordering of target node elements given by model\$expandNodeNames(target, returnScalarComponents = TRUE), where target is the same as the target argument to configureMCMC\$addSampler above. (default = FALSE)
- designMatrix. The full design matrix with rows corresponding to the ordering of the responses and columns ordered exactly as the ordering of target node elements given by model\$expandNodeNames(target, returnScalarComponents = TRUE), where target is the same as the target argument to configureMCMC\$addSampler above. If provided, all columns are assumed to be fixed, ignoring the fixedDesignColumns control element.
- nonTargetNodes. Additional stochastic nodes involved in the linear predictor that are not to be sampled as part of the sampler. This must include any nodes specifying stochastic indexes (e.g., "group" if the group[i] values are stochastic) and any parameters considered known or that for any reason one does not want to sample. Providing nonTargetNodes is required in order to allow NIMBLE to check for the presence of zero inflation.
- check. A logical value indicating whether NIMBLE should check various conditions required for validity of the sampler. This is provided for rare cases where the checking may be overly conservative and a user is sure that the sampler is valid and wants to override the checking. (default = TRUE)

#### noncentered sampler

The noncentered sampler is designed to sample the mean or standard deviation of a set of centered random effects while also moving the random effects values to possibly allow better mixing. The noncentered sampler deterministically shifts or scales the dependent node values to be consistent with the proposed value of the target (the mean or the standard deviation) such that the effect is to sample in a noncentered parameterization (Yu and Meng 2011), via an on-the-fly reparameterization. This can improve mixing by updating the target node based on information in the model nodes whose parent nodes are the dependent nodes of the target (i.e., the "grandchild" nodes of the target; these will often be data nodes). This comes at the extra computational cost of calculating the logProbability of the "grandchild" nodes.

It is still necessary to have other samplers on the random effects values.

Mathematically, the noncentered sampler operates in one dimension of a transformed parameter space. When sampling a mean, all random effects will be shifted by the same amount as the mean. When sampling a standard deviation, all random effects (relative to their means) will be scaled by the same factor as the standard deviation. Consider a model that includes the following code:

for(i in 1:n)
 y[i] ~ dnorm(beta1\*x[i] + u[group[i]], sd = sigma\_obs)
for(j in 1:num\_groups)
 u[j] ~ dnorm(beta0, sd = sigma\_group)

where u is a random effect associated with groups of data, and group[i] gives the group index of the i-th observation. This model has a centered random effect, because the u[j] have the intercept beta0 as their mean. In basic univariate sampling, updates to beta0 or to sigma\_group do not change u[j], making only small moves possible if num\_groups is large. When the noncentered sampler considers a new value for beta0, it will shift all the u[j] so that (in this case) their prior probabilities do not change. If the noncentered sampler considers a new value for sigma\_group, it will rescale all the u[j] accordingly.

The effect of such a sampling strategy is to update beta0 and sigma\_group as if the model had been written in a different (noncentered) way. For updating beta0, it would be:

```
for(i in 1:n)
    y[i] ~ dnorm(beta0 + beta1*x[i] + u[group[i]], sd = sigma_obs)
for(j in 1:num_groups)
    u[j] ~ dnorm(0, sd = sigma_group)
```

For updating sigma\_group, it would be:

```
for(i in 1:n)
   y[i] ~ dnorm(beta1*x[i] + u[group[i]] * sigma_group, sd = sigma_obs)
for(j in 1:num_groups)
   u[j] ~ dnorm(beta0, sd = 1)
```

Whether centered or noncentered parameterizations result in better sampling can depend on the model and the data. Therefore Yu and Meng (2011) recommended an "interweaving" strategy of using both kinds of samplers. Adding the noncentered sampler (on either the mean or standard deviation or both) to an existing MCMC configuration for a model specified using the centered parameterization (and with a sampler already assigned to the target node) produces an overall sampling approach that is a variation on the interweaving strategy of Yu and Meng (2011). This provides the benefits of sampling in both the centered and noncentered parameterizations in a single MCMC.

There is a higher computational cost to the noncentered sampler (or to writing the model directly in one of the equivalent ways shown). The cost is that when updating beta0 or sigma\_group, the relevant log probabilities calculations will include (in this case) all the of y[i], i.e. the "grandchild" nodes of beta0 or sigma\_group.

The noncentered sampler is not assigned by default by configureMCMC but must be manually added. For example:

MCMCconf <- configureMCMC(model)
MCMCconf\$addSampler(target = "beta0", type = "noncentered",</pre>

```
control = list(param = "location", sampler = "RW"))
MCMCconf$addSampler(target = "sigma_group", type = "noncentered",
    control = list(param = "scale", sampler = "RW"))
```

While the target node will generally be either the mean (location) or standard deviation (scale) of a set of other nodes (e.g., random effects), it could in theory be used in other contexts and one can choose whether the transformation is a shift or a scale operation. In a shift operation (e.g., when the sampling target is a mean), the dependent nodes are set to their previous values plus the difference between the proposed value and previous value for the target. In a scale operation (e.g., when the sampling target is the standard deviation), the dependent nodes minus their means are multiplied by the ratio of the proposed value to the previous value for the target and the previous value for the target. Whether to shift or scale is determined from the param element of the control list.

The sampling algorithm for the target node can either be adaptive Metropolis random walk (which uses NIMBLE's RW sampler) or slice sampling (which uses NIMBLE's slice sampler), determined from the sampler element of the control list. In either case, the underlying sampling accounts for the Jacobian of the deterministic shifting or scaling of the dependent nodes (in the case of shifting, the Jacobian is equal to 1 and has no impact). When the target is the standard deviation of normally-distributed dependent nodes, the Jacobian cancels with the prior distribution for the dependent nodes, and the update is in effect based only on the prior for the target and the distribution of the "grandchild" nodes.

The noncentered sampler accepts the following control list elements:

- sampler. A character string, either "RW" or "slice" specifying the type of sampler to be used for the target node. (default = "RW")
- param. A character string, either "location" or "scale" specifying whether sampling is done as shifting or scaling the dependent nodes. (default = "location")

## **CAR\_normal sampler**

The CAR\_normal sampler operates uniquely on improper (intrinsic) Gaussian conditional autoregressive (CAR) nodes, those with a dcar\_normal prior distribution. It internally assigns one of three univariate samplers to each dimension of the target node: a posterior predictive, conjugate, or RW sampler; however these component samplers are specialized to operate on dimensions of a dcar\_normal distribution.

The CAR\_normal sampler accepts the following control list elements:

- carUseConjugacy. A logical argument, specifying whether to assign conjugate samplers for conjugate components of the target node. If FALSE, a RW sampler would be assigned instead. (default = TRUE)
- adaptive. A logical argument, specifying whether any component RW samplers should adapt the scale (proposal standard deviation), to achieve a theoretically desirable acceptance rate. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation for any component RW samplers. Every adaptInterval MCMC iterations (prior to thinning), component RW samplers will perform an adaptation procedure. This updates the scale variable, based upon the sampler's achieved acceptance rate over the past adaptInterval iterations. (default = 200)
- scale. The initial value of the normal proposal standard deviation for any component RW samplers. If adaptive = FALSE, scale will never change. (default = 1)

## **CAR\_proper sampler**

The CAR\_proper sampler operates uniquely on proper Gaussian conditional autoregressive (CAR) nodes, those with a dcar\_proper prior distribution. It internally assigns one of three univariate samplers to each dimension of the target node: a posterior predictive, conjugate, or RW sampler, however these component samplers are specialized to operate on dimensions of a dcar\_proper distribution.

The CAR\_proper sampler accepts the following control list elements:

- carUseConjugacy. A logical argument, specifying whether to assign conjugate samplers for conjugate components of the target node. If FALSE, a RW sampler would be assigned instead. (default = TRUE)
- adaptive. A logical argument, specifying whether any component RW samplers should adapt the scale (proposal standard deviation), to achieve a theoretically desirable acceptance rate. (default = TRUE)
- adaptInterval. The interval on which to perform adaptation for any component RW samplers. Every adaptInterval MCMC iterations (prior to thinning), component RW samplers will perform an adaptation procedure. This updates the scale variable, based upon the sampler's achieved acceptance rate over the past adaptInterval iterations. (default = 200)
- scale. The initial value of the normal proposal standard deviation for any component RW samplers. If adaptive = FALSE, scale will never change. (default = 1)

## **CRP** sampler

The CRP sampler is designed for fitting models involving Dirichlet process mixtures. It is exclusively assigned by NIMBLE's default MCMC configuration to nodes having the Chinese Restaurant Process distribution, dCRP. It executes sequential sampling of each component of the node (i.e., the cluster membership of each element being clustered). Internally, either of two samplers can be assigned, depending on conjugate or non-conjugate structures within the model. For conjugate and non-conjugate model structures, updates are based on Algorithm 2 and Algorithm 8 in Neal (2000), respectively.

- checkConjugacy. A logical argument, specifying whether to assign conjugate samplers if valid. (default = TRUE)
- printTruncation. A logical argument, specifying whether to print a warning when the MCMC attempts to use more clusters than the maximum number specified in the model. Only relevant where the user has specified the maximum number of clusters to be less than the number of observations. (default = TRUE)

## **CRP\_concentration sampler**

The CRP\_concentration sampler is designed for Bayesian nonparametric mixture modeling. It is exclusively assigned to the concentration parameter of the Dirichlet process when the model is specified using the Chinese Restaurant Process distribution, dCRP. This sampler is assigned by default by NIMBLE's default MCMC configuration and can only be used when the prior for the concentration parameter is a gamma distribution. The assigned sampler is an augmented beta-gamma sampler as discussed in Section 6 in Escobar and West (1995).

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#### sampler\_BASE

#### prior\_samples sampler

The prior\_samples sampler uses a provided set of numeric values (samples) to define the prior distribution of one or more model nodes. One every MCMC iteration, the prior\_samples sampler takes value(s) from the numeric values provided, and stores these value(s) into the target model node(s). This allows one to define the prior distribution of model parameters empirically, using a set of numeric samples, presumably obtained previously using MCMC. The target node may be either a single scalar node (scalar case), or a collection of model nodes.

The prior\_samples sampler provides two options for selection of the value to use on each MCMC iteration. The default behaviour is to take sequential values from the samples vector (scalar case), or in the case of multiple dimensions, sequential rows of the samples matrix are used. The alternative behaviour, by setting the control argument randomDraws = TRUE, will instead use random draws from the samples vector (scalar case), or randomly selected rows of the samples matrix in the multidimensional case.

If the default of sequential selection of values is used, and the number of MCMC iterations exceeds the length of the samples vector (scalar case) or the number of rows of the samples matrix, then samples will be recycled as necessary for the number of MCMC iterations. A message to this effect is also printed at the beginning of the MCMC chain.

Logically, prior\_samples samplers might want to operate first, in advance of other samplers, on every MCMC iteration. By default, at the time of MCMC building, all prior\_samples samplers are re-ordered to appear first in the list of MCMC samplers. This behaviour can be subverted, however, by setting nimbleOptions(MCMCorderPriorSamplesSamplersFirst = FALSE).

The prior\_samples sampler can be assigned to non-stochastic model nodes (nodes which are not assigned a prior distribution in the model). In fact, it is recommended that nodes being assigned a prior\_samples are not provided with a prior distribution in the model, and rather, that these nodes only appear on the right-hand-side of model declaration lines. In such case that a prior\_samples sampler is assigned to a nodes with a prior distribution, the prior distribution will be overridden by the sample values provided to the sampler; however, the node will still be a stochastic node for other purposes, and will contribute to the model joint-density (using the sample values provided relative to the prior distribution), will have an MCMC sampler assigned to it by default, and also may introduce potential for confusion. In this case, a message is issued at the time of MCMC building.

The prior\_samples sampler accepts the following control list elements:

- samples. A numeric vector or matrix. When the target node is a single scalar-valued node, samples should be a numeric vector. When the target node specifies d > 2 model dimensions, samples should be a matrix containing d columns. The samples control argument is required.
- randomDraws. A logical argument, specifying whether to use a random draw from samples on each iteration. If samples is a matrix, then a randomly-selected row of the samples matrix is used. When FALSE, sequential values (or sequential matrix rows) are used (default = FALSE).

#### posterior\_predictive sampler

The posterior\_predictive sampler operates only on posterior predictive stochastic nodes. A posterior predictive node is a node that is not itself data and has no data nodes in its entire downstream (descendant) dependency network. Note that such nodes play no role in inference for model parameters but have often been included in BUGS models to make predictions, including for posterior

predictive checks. As of version 0.13.0, NIMBLE samples model parameters without conditioning on the posterior predictive nodes and samples conditionally from the posterior predictive nodes as the last step of each MCMC iteration.

(Also note that NIMBLE allows posterior predictive values to be simulated independently of running MCMC, for example by writing a nimbleFunction to do so. This means that in many cases where terminal stochastic (posterior predictive) nodes have been included in BUGS models, they are not needed when using NIMBLE.)

The posterior\_predictive sampler functions by simulating new values for all downstream (dependent) nodes using their conditional distributions, as well as updating the associated model probabilities. A posterior\_predictive sampler will automatically be assigned to all trailing non-data stochastic nodes in a model, or when possible, to any node at a point in the model after which all downstream (dependent) stochastic nodes are non-data.

The posterior\_predictive sampler accepts no control list arguments.

## **RJ\_fixed\_prior** sampler

This sampler proposes addition/removal for variable of interest in the framework of variable selection using reversible jump MCMC, with a specified prior probability of inclusion. A normal proposal distribution is used to generate proposals for the addition of the variable. This is a specialized sampler used by configureRJ function, when the model code is written without using indicator variables. See help{configureRJ} for details. It is not intended for direct assignment.

## **RJ\_indicator** sampler

This sampler proposes transitions of a binary indicator variable, corresponding to a variable of interest, in the framework of variable selection using reversible jump MCMC. This is a specialized sampler used by configureRJ function, when the model code is written using indicator variables. See help{configureRJ} for details. It is not intended for direct assignment.

## **RJ\_toggled** sampler

This sampler operates in the framework of variable selection using reversible jump MCMC. Specifically, it conditionally performs updates of the target variable of interest using the originally-specified sampling configuration, when variable is "in the model". This is a specialized sampler used by configureRJ when adding a reversible jump MCMC. See help{configureRJ} for details. It is not intended for direct assignment.

# Author(s)

Daniel Turek

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#### See Also

configureMCMC addSampler buildMCMC runMCMC

## Examples

```
## y[1] ~ dbern() or dbinom():
# mcmcConf$addSampler(target = 'y[1]', type = 'binary')
# mcmcConf$addSampler(target = 'a', type = 'RW',
    control = list(log = TRUE, adaptive = FALSE, scale = 3))
#
# mcmcConf$addSampler(target = 'b', type = 'RW',
#
    control = list(adaptive = TRUE, adaptInterval = 200))
# mcmcConf$addSampler(target = 'p', type = 'RW',
     control = list(reflective = TRUE))
#
## a, b, and c all continuous-valued:
# mcmcConf$addSampler(target = c('a', 'b', 'c'), type = 'RW_block')
# mcmcConf$addSampler(target = 'p', type = 'RW_llFunction',
     control = list(llFunction = RllFun, includesTarget = FALSE))
#
# mcmcConf$addSampler(target = 'y[1]', type = 'slice',
#
    control = list(adaptive = FALSE, sliceWidth = 3))
# mcmcConf$addSampler(target = 'y[2]', type = 'slice',
#
     control = list(adaptive = TRUE, sliceMaxSteps = 1))
# mcmcConf$addSampler(target = 'x[1:10]', type = 'ess') ## x[1:10] ~ dmnorm()
# mcmcConf$addSampler(target = 'p[1:5]', type = 'RW_dirichlet') ## p[1:5] ~ ddirch()
## y[1] is a posterior predictive node:
# mcmcConf$addSampler(target = 'y[1]', type = 'posterior_predictive')
```

setAndCalculate

Creates a nimbleFunction for setting the values of one or more model nodes, calculating the associated deterministic dependents and log-Prob values, and returning the total sum log-probability.

# Description

This nimbleFunction generator must be specialized to any model object and one or more model nodes. A specialized instance of this nimbleFunction will set the values of the target nodes in the specified model, calculate the associated logProbs, calculate the values of any deterministic dependents, calculate the logProbs of any stochastic dependents, and return the sum log-probability associated with the target nodes and all stochastic dependent nodes.

## Usage

setAndCalculate(model, targetNodes)

setAndCalculateDiff(model, targetNodes)

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#### Arguments

model	An uncompiled or compiled NIMBLE model. This argument is required.
targetNodes	A character vector containing the names of one or more nodes or variables in
	the model. This argument is required.

## Details

Calling setAndCalculate(model, targetNodes) or setAndCalculate(model, targetNodes) will return a nimbleFunction object whose run function takes a single, required argument:

targetValues: A vector of numeric values which will be put into the target nodes in the specified model object. The length of this numeric vector much exactly match the number of target nodes.

The difference between setAndCalculate and setAndCalculateDiff is the return value of their run functions. In the former, run returns the sum of the log probabilities of the targetNodes with the provided targetValues, while the latter returns the difference between that sum with the new targetValues and the previous values in the model.

# Author(s)

Daniel Turek

# Examples

```
code <- nimbleCode({ for(i in 1:3) { x[i] ~ dnorm(0,1); y[i] ~ dnorm(0, 1)}})
Rmodel <- nimbleModel(code)
my_setAndCalc <- setAndCalculate(Rmodel, c('x[1]', 'x[2]', 'y[1]', 'y[2]'))
lp <- my_setAndCalc$run(c(1.2, 1.4, 7.6, 8.9))</pre>
```

setAndCalculateOne Creates a nimbleFunction for setting the value of a scalar model node, calculating the associated deterministic dependents and logProb values, and returning the total sum log-probability.

## Description

This nimbleFunction generator must be specialized to any model object and any scalar model node. A specialized instance of this nimbleFunction will set the value of the target node in the specified model, calculate the associated logProb, calculate the values of any deterministic dependents, calculate the logProbs of any stochastic dependents, and return the sum log-probability associated with the target node and all stochastic dependent nodes.

## Usage

setAndCalculateOne(model, targetNode)

## Arguments

model	An uncompiled or compiled NIMBLE model. This argument is required.
targetNode	The character name of any scalar node in the model object. This argument is
	required.

# Details

Calling setAndCalculateOne(model, targetNode) will return a function with a single, required argument:

targetValue: The numeric value which will be put into the target node, in the specified model object.

## Author(s)

Daniel Turek

## Examples

```
code <- nimbleCode({ for(i in 1:3) x[i] ~ dnorm(0, 1) })
Rmodel <- nimbleModel(code)
my_setAndCalc <- setAndCalculateOne(Rmodel, 'x[1]')
lp <- my_setAndCalc$run(2)</pre>
```

setSize

set the size of a numeric variable in NIMBLE

# Description

set the size of a numeric variable in NIMBLE. This works in R and NIMBLE, but in R it usually has no effect.

# Usage

```
setSize(numObj, ..., copy = TRUE, fillZeros = TRUE)
```

# Arguments

numObj	This is the object to be resized
	sizes, provided as scalars, in order, or as a single vector
сору	logical indicating whether values should be preserved (in column-major order)
fillZeros	logical indicating whether newly allocated space should be initialized with zeros (in compiled code)

## Details

Note that assigning the result of numeric, integer, logical, matrix, or array is often as good or better than using setSize. For example, 'x <- matrix(nrow = 5, ncol = 5)' is equivalent to 'setSize(x, 5, 5)' but the former allows more control over initialization.

This function is part of the NIMBLE language. Its purpose is to explicitly resize a multivariate object (vector, matrix or array), currently up to 4 dimensions. Explicit resizing is not needed when an entire object is assigned to. For example, in  $Y \le A \% \% B$ , where A and B are matrices, Y will be resized automatically. Explicit resizing is necessary when assignment will be by indexed elements or blocks, if the object is not already an appropriate size for the assignment. E.g. prior to  $Y[5:10] \le A \% \% B$ , one can use setSize to ensure that Y has a size (length) of at least 10.

This does work in uncompiled (R) and well as compiled execution, but in some cases it is only necessary for compiled execution. During uncompiled execution, it may not catch bugs due to resizing because some R objects will be dynamically resized during assignments anyway.

If preserving values in the resized object and/or initializing new values with 0 is not necessary, then setting these arguments to FALSE will yield slightly more efficient compiled code.

## Author(s)

NIMBLE development team

setupMargNodes

Organize model nodes for marginalization

#### Description

Process model to organize nodes for marginalization (integration over latent nodes or random effects) as by Laplace approximation.

## Usage

```
setupMargNodes(
  model,
  paramNodes,
  randomEffectsNodes,
  calcNodes0ther,
  split = TRUE,
  check = TRUE,
  allowDiscreteLatent = FALSE
)
```

#### Arguments

model	A nimble model such as returned by nimbleModel.
paramNodes	A character vector of names of stochastic nodes that are parameters of nodes to
	be marginalized over (randomEffectsNodes). See details for default.

#### randomEffectsNodes

	A character vector of nodes to be marginalized over (or "integrated out"). In the case of calculating the likelihood of a model with continuous random effects, the nodes to be marginalized over are the random effects, hence the name of this argument. However, one can marginalize over any nodes desired as long as they are continuous. See details for default.
calcNodes	A character vector of nodes to be calculated as the integrand for marginaliza- tion. Typically this will include randomEffectsNodes and some data nodes. Se details for default.
calcNodesOther	A character vector of nodes to be calculated as part of the log likelihood that are not connected to the randomEffectNodes and so are not actually part of the marginalization. These are somewhat extraneous to the purpose of this function, but it is convenient to handle them here because often the purpose of marginal- ization is to calculate log likelihoods, including from "other" parts of the model.
split	A logical indicating whether to split randomEffectsNodes into conditionally independent sets that can be marginalized separately (TRUE) or to keep them all in one set for a single marginalization calculation.
check	A logical indicating whether to try to give reasonable warnings of badly formed inputs that might be missing important nodes or include unnecessary nodes.
allowDiscreteLatent	
	A logical indicating whether to allow discrete latent states (default = FALSE)

A logical indicating whether to allow discrete latent states. (default = FALSE)

## Details

This function is used by buildLaplace to organize model nodes into roles needed for setting up the (approximate) marginalization done by Laplace approximation. It is also possible to call this function directly and pass the resulting list (possibly modified for your needs) to buildLaplace.

Any of the input node vectors, when provided, will be processed using nodes <- model\$expandNodeNames(nodes), where nodes may be paramNodes, randomEffectsNodes, and so on. This step allows any of the inputs to include node-name-like syntax that might contain multiple nodes. For example, paramNodes = 'beta[1:10]' can be provided if there are actually 10 scalar parameters, 'beta[1]' through 'beta[10]'. The actual node names in the model will be determined by the exapndNodeNames step.

This function does not do any of the marginalization calculations. It only organizes nodes into roles of parameters, random effects, integrand calculations, and other log likelihood calculations.

The checking done if 'check=TRUE' tries to be reasonable, but it can't cover all cases perfectly. If it gives an unnecessary warning, simply set 'check=FALSE'.

If paramNodes is not provided, its default depends on what other arguments were provided. If neither randomEffectsNodes nor calcNodes were provided, paramNodes defaults to all top-level, stochastic nodes, excluding any posterior predictive nodes (those with no data anywhere down-stream). These are determined by model\$getNodeNames(topOnly = TRUE, stochOnly = TRUE, includePredictive = FALSE). If randomEffectsNodes was provided, paramNodes defaults to stochastic parents of randomEffectsNodes. In these cases, any provided calcNodes or calcNodesOther are excluded from default paramNodes. If calcNodes but not randomEffectsNodes was provided, then the default for randomEffectsNodes is determined first, and then paramNodes defaults to stochastic parents of randomEffectsNodes. Finally, any stochastic parents of calcNodes (whether

## setupMargNodes

provided or default) that are not in calcNodes are added to the default for paramNodes, but only after paramNodes has been used to determine the defaults for randomEffectsNodes, if necessary.

Note that to obtain sensible defaults, some nodes must have been marked as data, either by the data argument in nimbleModel or by model\$setData. Otherwise, all nodes will appear to be posterior predictive nodes, and the default paramNodes may be empty.

For purposes of buildLaplace, paramNodes does not need to (but may) include deterministic nodes between the parameters and any calcNodes. Such deterministic nodes will be included in calculations automatically when needed.

If randomEffectsNodes is missing, the default is a bit complicated: it includes all latent nodes that are descendants (or "downstream") of paramNodes (if provided) and are either (i) ancestors (or "upstream") of data nodes (if calcNodes is missing), or (ii) ancestors or elements of calcNodes (if calcNodes and paramNodes are provided), or (iii) elements of calcNodes (if calcNodes is provided but paramNodes is missing). In all cases, discrete nodes (with warning if check=TRUE), posterior predictive nodes and paramNodes are excluded.

randomEffectsNodes should only include stochastic nodes.

If calcNodes is missing, the default is randomEffectsNodes and their descendants to the next stochastic nodes, excluding posterior predictive nodes. These are determined by model\$getDependencies(randomEffectsNincludePredictive=FALSE).

If calcNodesOther is missing, the default is all stochastic descendants of paramNodes, excluding posterior predictive nodes (from model\$getDependencies(paramNodes, stochOnly=TRUE, self=FALSE, includePosterior=FALSE)) that are not part of calcNodes.

For purposes of buildLaplace, neither calcNodes nor calcNodesOther needs to (but may) contain deterministic nodes between paramNodes and calcNodes or calcNodesOther, respectively. These will be included in calculations automatically when needed.

If split is TRUE, model\$getConditionallyIndependentSets is used to determine sets of the randomEffectsNodes that can be independently marginalized. The givenNodes are the paramNodes and calcNodes excluding any randomEffectsNodes and their deterministic descendants. The nodes (to be split into sets) are the randomEffectsNodes.

If split is a numeric vector, randomEffectsNodes will be split by split(randomEffectsNodes, control\$split). The last option allows arbitrary control over how randomEffectsNodes are blocked.

If check=TRUE, then defaults for each of the four categories of nodes are created even if the corresponding argument was provided. Then warnings are emitted if there are any extra (potentially unnecessary) nodes provided compared to the default or if there are any nodes in the default that were not provided (potentially necessary). These checks are not perfect and may be simply turned off if you are confident in your inputs.

(If randomEffectsNodes was provided but calcNodes was not provided, the default (for purposes of check=TRUE only) for randomEffectsNodes differs from the above description. It uses stochastic descendants of randomEffectsNodes in place of the "data nodes" when determining ancestors of data nodes. And it uses item (ii) instead of (iii) in the list above.)

# Value

A list is returned with elements:

• paramNodes: final processed version of paramNodes

- randomEffectsNodes: final processed version of randomEffectsNodes
- calcNodes: final processed version of calcNodes
- calcNodesOther: final processed version of calcNodesOther
- givenNodes: Input to model\$getConditionallyIndependentSets, if split=TRUE.
- randomEffectsSets: Output from model\$getConditionallyIndependentSets, if split=TRUE. This will be a list of vectors of node names. The node names in one list element can be marginalized independently from those in other list elements. The union of the list elements should be all of randomEffectsNodes. If split=FALSE, randomEffectsSets will be a list with one element, simply containing randomEffectsNodes. If split is a numeric vector, randomEffectsSets will be the result of split(randomEffectsNodes, control\$split).

# Author(s)

Wei Zhang, Perry de Valpine, Paul van Dam-Bates

setupOutputs	Explicitly declare objects created in setup code to be preserved and
	compiled as member data

# Description

Normally a nimbleFunction determines what objects from setup code need to be preserved for run code or other member functions. setupOutputs allows explicit declaration for cases when an object created in setup code is not used in member functions.

#### Arguments

. . .

An arbitrary set of names

## Details

Normally any object created in setup whose name appears in run or another member function is included in the saved results of setup code. When the nimbleFunction is compiled, such objects will become member data of the resulting C++ class. If it is desired to force an object to become member data even if it does not appear in a member function, declare it using setupOutputs. E.g., setupOutputs(a, b) declares that a and b should be preserved.

The setupOutputs line will be removed from the setup code. It is really a marker during nimble-Function creation of what should be preserved. simNodes

# Description

simulate, calculate, or get existing log probabilities for the current values in a NIMBLE model

## Usage

```
simNodes(model, nodes)
calcNodes(model, nodes)
```

getLogProbNodes(model, nodes)

## Arguments

model	A NIMBLE model
nodes	A set of nodes. If none are provided, default is all model\$getNodeNames()

# Details

These are basic nimbleFunctions that take a model and set of nodes and return a function that will call calculate, simulate, or getLogProb on those nodes. Each is equivalent to a direct call from R, but in nimbleFunction form they can be be compiled. For example, myCalc <- calcNodes(model, nodes); ans <- myCalc() is equivalent to ans <- model\$calculate(nodes), but one can also do CmyCalc <- compileNimble(myCalc) to get a faster version. Note that this will often be much faster than using 'calculate' from R with a compiled model, such as compiled\_model\$calculate(nodes) because of overhead in running 'calculate' from R.

In nimbleFunctions, one would generally use model\$calculate(nodes) in the run-time code (and similarly for 'simulate' and 'getLogProb').

# Author(s)

Perry de Valpine

simNodesMV

## Description

simulate, calculate, or get the existing log probabilities for values in a modelValues object using a NIMBLE model

## Usage

```
simNodesMV(model, mv, nodes)
calcNodesMV(model, mv, nodes)
getLogProbNodesMV(model, mv, nodes)
```

## Arguments

model	A nimble model.
mv	A modelValues object in which multiple sets of model variables and their cor- responding logProb values are or will be saved. mv must include the nodes pro- vided
nodes	A set of nodes. If none are provided, default is all model\$getNodeNames()

#### **Details**

simNodesMV simulates values in the given nodes and saves them in mv. calcNodesMV calculates these nodes for each row of mv and returns a vector of the total log probabilities (densities) for each row. getLogProbNodesMV is like calcNodesMV without actually doing the calculations.

Each of these will expand variables or index blocks and topologically sort them so that each node's parent nodes are processed before itself.

getLogProbMV should be used carefully. It is generally for situations where the logProb values are guaranteed to have already been calculated, and all that is needed is to query them. The risk is that a program may have changed the values in the nodes, in which case getLogProbMV would collect logProb values that are out of date with the node values.

#### Value

from simNodesMV: NULL. from calcNodesMV and getLogProbMV: a vector of the sum of log probabilities (densities) from any stochastic nodes in nodes.

#### **Run time arguments**

- m. (simNodesMV only). Number of simulations requested.
- saveLP. (calcNodesMVonly). Whether to save the logProb values in mv. Should be given as TRUE unless there is a good reason not to.

```
singleVarAccessClass-class
```

# Author(s)

Clifford Anderson-Bergman

## Examples

```
code <- nimbleCode({</pre>
for(i in 1:5)
x[i] ~ dnorm(0,1)
})
myModel <- nimbleModel(code)</pre>
myMV <- modelValues(myModel)</pre>
Rsim <- simNodesMV(myModel, myMV)</pre>
Rcalc <- calcNodesMV(myModel, myMV)</pre>
Rglp <- getLogProbNodesMV(myModel, myMV)</pre>
## Not run:
  cModel <- compileNimble(myModel)</pre>
  Csim <- compileNimble(Rsim, project = myModel)</pre>
  Ccalc <- compileNimble(Rcalc, project = myModel)</pre>
  Cglp <- compileNimble(Rglp, project = myModel)</pre>
  Csim$run(10)
  Ccalc$run(saveLP = TRUE)
  Cglp$run() #Gives identical answers to Ccalc because logProbs were saved
  Csim$run(10)
  Ccalc$run(saveLP = FALSE)
  Cglp$run() #Gives wrong answers because logProbs were not saved
  result <- as.matrix(Csim$mv)</pre>
```

## End(Not run)

singleVarAccessClass-class

Class singleVarAccessClass

## Description

Classes used internally in NIMBLE and not expected to be called directly by users.

StickBreakingFunction The Stick Breaking Function

# Description

Computes probabilities based on stick breaking construction.

# Usage

stick\_breaking(z, log = 0)

#### Arguments

Z	vector argument.
log	logical; if TRUE, weights are returned on the log scale.

## Details

The stick breaking function produces a vector of probabilities that add up to one, based on a series of individual probabilities in z, which define the breaking points relative to the remaining stick length. The first element of z determines the first probability based on breaking a proportion z[1] from a stick of length one. The second element of z determines the second probability based on breaking a proportion z[2] from the remaining stick (of length 1-z[1]), and so forth. Each element of z should be in (0, 1). The returned vector has length equal to the length of z plus 1. If z[k] is equal to 1 for any k, then the returned vector has length smaller than z. If one of the components is smaller than 0 or greater than 1, NaNs are returned.

## Author(s)

Claudia Wehrhahn

# References

Sethuraman, J. (1994). A constructive definition of Dirichlet priors. Statistica Sinica, 639-650.

# Examples

```
z <- rbeta(5, 1, 1)
stick_breaking(z)
## Not run:
cstick_breaking <- compileNimble(stick_breaking)
cstick_breaking(z)</pre>
```

## End(Not run)

summaryLaplace

Summarize results from Laplace or adaptive Gauss-Hermite quadrature approximation

## Description

Process the results of the 'findMLE' method of a nimble Laplace or AGHQ approximation into a more useful format.

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# summaryLaplace

# Usage

```
summaryLaplace(
  laplace,
  MLEoutput,
  originalScale = TRUE,
  randomEffectsStdError = TRUE,
  jointCovariance = FALSE
)
summaryAGHQ(
  AGHQ,
  MLEoutput,
  originalScale = TRUE,
  randomEffectsStdError = TRUE,
  jointCovariance = FALSE
)
```

## Arguments

laplace	The Laplace approximation object, typically the compiled one. This would be the result of compiling an object returned from 'buildLaplace'.	
MLEoutput	The maximum likelihood estimate using Laplace or AGHQ, returned from e.g. 'approx\$findMLE()', where approx is the algorithm object returned by 'build-Laplace' or 'buildAGHQ', or (more typically) the result of compiling that object with 'compileNimble'. See 'help(buildLaplace)' for more information.	
originalScale	Should results be returned using the original parameterization in the model code (TRUE) or the potentially transformed parameterization used internally by the Laplace approximation (FALSE). Transformations are used for any parameters and/or random effects that have constrained ranges of valid values, so that in the transformed parameter space there are no constraints. (default = TRUE)	
randomEffectsStdError		
	If TRUE, calculate the standard error of the estimates of random effects values. (default = TRUE)	
jointCovariance		
	If TRUE, calculate the joint covariance matrix of the parameters and random effects together. If FALSE, calculate the covariance matrix of the parameters. (default = FALSE)	
AGHQ	Same as laplace. Note that 'buildLaplace' and 'buildAGHQ' create the same kind of algorithm object that can be used interchangeably. 'buildLaplace' simply sets the number of quadrature points ('nQuad') to 1 to achieve Laplace approximation as a special case of AGHQ.	

# Details

The numbers obtained by this function can be obtained more directly by 'approx\$summary(...)'. The added benefit of 'summaryLaplace' is to arrange the results into data frames (for parameters and random effects), with row names for the model nodes, and also adding row and column names to the covariance matrix.

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# Value

A list with data frames 'params' and 'randomEffects', each with columns for 'estimate' and (possibly) 'se' (standard error) and row names for model nodes, a matrix 'vcov' with the covariance matrix with row and column names, and 'originalScale' with the input value of 'originalScale' so it is recorded for later use if wanted.

svdNimbleList svdNimbleList definition

## Description

nimbleList definition for the type of nimbleList returned by nimSvd.

# Usage

svdNimbleList

# Format

An object of class list of length 1.

## Author(s)

NIMBLE development team

# See Also

nimSvd

t

The t Distribution

## Description

Density, distribution function, quantile function and random generation for the t distribution with df degrees of freedom, allowing non-zero location, mu, and non-unit scale, sigma

#### Usage

dt\_nonstandard(x, df = 1, mu = 0, sigma = 1, log = FALSE)
rt\_nonstandard(n, df = 1, mu = 0, sigma = 1)
pt\_nonstandard(q, df = 1, mu = 0, sigma = 1, lower.tail = TRUE, log.p = FALSE)
qt\_nonstandard(p, df = 1, mu = 0, sigma = 1, lower.tail = TRUE, log.p = FALSE)

Arguments

x	vector of values.
df	vector of degrees of freedom values.
mu	vector of location values.
sigma	vector of scale values.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations.
q	vector of quantiles.
lower.tail	logical; if TRUE (default) probabilities are $P[X \le x]$ ; otherwise, $P[X > x]$ .
log.p	logical; if TRUE, probabilities p are given by user as log(p).
р	vector of probabilities.

# Details

See Gelman et al., Appendix A or the BUGS manual for mathematical details.

## Value

dt\_nonstandard gives the density, pt\_nonstandard gives the distribution function, qt\_nonstandard gives the quantile function, and rt\_nonstandard generates random deviates.

# Author(s)

**Christopher Paciorek** 

## References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

# See Also

Distributions for other standard distributions

# Examples

```
x <- rt_nonstandard(50, df = 1, mu = 5, sigma = 1)
dt_nonstandard(x, 3, 5, 1)</pre>
```

t

testBUGSmodel

# Description

testBUGSmodel builds a BUGS model in the NIMBLE system and simulates from the model, comparing the values of the nodes and their log probabilities in the uncompiled and compiled versions of the model

## Usage

```
testBUGSmodel(
  example = NULL,
  dir = NULL,
  model = NULL,
  data = NULL,
  inits = NULL,
  useInits = TRUE,
  expectModelWarning = FALSE,
  debug = FALSE,
  verbose = nimbleOptions("verbose")
)
```

# Arguments

example	(optional) example character vector indicating name of BUGS example to test; can be null if model is provided
dir	(optional) character vector indicating directory in which files are contained, by default the classic-bugs directory if the installed package is used; to use the current working directory, set this to ""
model	(optional) one of (1) a character string giving the file name containing the BUGS model code, (2) an R function whose body is the BUGS model code, or (3) the output of nimbleCode. If a file name, the file can contain a 'var' block and 'data' block in the manner of the JAGS versions of the BUGS examples but should not contain references to other input data files nor a const block. The '.bug' or '.txt' extension can be excluded.
data	(optional) one of (1) character string giving the file name for an R file provid- ing the input constants and data as R code [assigning individual objects or as a named list] or (2) a named list providing the input constants and data. If nei- ther is provided, the function will look for a file named example-data including extensions .R, .r, or .txt.
inits	(optional) (1) character string giving the file name for an R file providing the ini- tial values for parameters as R code [assigning individual objects or as a named list] or (2) a named list providing the values. If neither is provided, the function will look for a file named example-init or example-inits including extensions .R, .r, or .txt.

useInits	boolean indicating whether to test model with initial values provided via inits.	
expectModelWarning		
	boolean indicating whether nimbleModel is expected to produce a warning or character string giving part of expected warning.	
debug	logical indicating whether to put the user in a browser for debugging when testBUGSmodel calls readBUGSmodel. Intended for developer use.	
verbose	logical indicating whether to print additional logging information	

# Details

Note that testing without initial values may cause warnings when parameters are sampled from improper or fat-tailed distributions

## Author(s)

Christopher Paciorek

# Examples

## Not run: testBUGSmodel('pump')

## End(Not run)

valueInCompiledNimbleFunction

get or set value of member data from a compiled nimbleFunction using a multi-interface

# Description

Most nimbleFunctions written for direct user interaction allow standard R-object-like access to member data using \$ or `[[`. However, sometimes compiled nimbleFunctions contained within other compiled nimbleFunctions are interfaced with a light-weight system called a multi-interface. valueInCompiledNimbleFunction provides a way to get or set values in such cases.

## Usage

```
valueInCompiledNimbleFunction(cnf, name, value)
```

## Arguments

cnf	Compiled nimbleFunction object
name	Name of the member data
value	If provided, the value to assign to the member data. If omitted, the value of the member data is returned.

# Details

The member data of a nimbleFunction are the objects created in setup code that are used in run code or other member functions.

Whether multi-interfaces are used for nested nimbleFunctions is controlled by the buildInterfacesForCompiledNestedNir option in nimbleOptions.

To see an example of a multi-interface, see samplerFunctions in a compiled MCMC interface object.

## Author(s)

Perry de Valpine

values

Access or set values for a set of nodes in a model

## Description

Get or set values for a set of nodes in a model

## Usage

values(model, nodes, accessorIndex)

values(model, nodes, accessorIndex) <- value</pre>

# Arguments

model	a NIMBLE model object, either compiled or uncompiled
nodes	a vector of node names, allowing index blocks that will be expanded
accessorIndex	For internal NIMBLE use only
value	value to set the node(s) to

## Details

Access or set values for a set of nodes in a NIMBLE model.

Calling values(model, nodes) returns a vector of the concatenation of values from the nodes requested P <- values(model, nodes) is a newer syntax for getValues(P, model, values), which still works and modifies P in the calling environment.

Calling values(model, nodes) <- P sets the value of the nodes in the model, in sequential order from the vector P.

In both uses, when requested nodes are from matrices or arrays, the values will be handled following column-wise order.

The older function getValues(P, model, nodes) is equivalent to P <- values(model, nodes), and the older function setValues(P, model, nodes) is equivalent to values(model, nodes) <- P

These functions work in R and in NIMBLE run-time code that can be compiled.

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waic

# Value

A vector of values concatenated from the provided nodes in the model

## Author(s)

NIMBLE development team

waic

Using WAIC

# Description

Details of the WAIC measure for comparing models. NIMBLE implements an online WAIC algorithm, computed during the course of the MCMC iterations.

## Details

To obtain WAIC, set WAIC = TRUE in nimbleMCMC. If using a more customized workflow, set enableWAIC = TRUE in configureMCMC or (if skipping configureMCMC) in buildMCMC, followed by setting WAIC = TRUE in runMCMC, if using runMCMC to manage sample generation.

By default, NIMBLE calculates WAIC using an online algorithm that updates required summary statistics at each post-burnin iteration of the MCMC.

One can also use calculateWAIC to run an offline version of the WAIC algorithm after all MCMC sampling has been done. This allows calculation of WAIC from a matrix (or dataframe) of posterior samples and also retains compatibility with WAIC in versions of NIMBLE before 0.12.0. However, the offline algorithm is less flexible than the online algorithm and only provides conditional WAIC without the ability to group data points. See help(calculateWAIC) for details.

#### controlWAIC list

The controlWAIC argument is a list that controls the behavior of the WAIC algorithm and is passed to either configureMCMC or (if not using configureMCMC) buildMCMC. One can supply any of the following optional components:

online: Logical value indicating whether to calculate WAIC during the course of the MCMC. Default is TRUE and setting to FALSE is primarily for backwards compatibility to allow use of the old calculateWAIC method that calculates WAIC from monitored values after the MCMC finishes.

dataGroups: Optional list specifying grouping of data nodes, one element per group, with each list element containing the node names for the data nodes in that group. If provided, the predictive density values computed will be the joint density values, one joint density per group. Defaults to one data node per 'group'. See details.

marginalizeNodes: Optional set of nodes (presumably latent nodes) over which to marginalize to compute marginal WAIC (i.e., WAIC based on a marginal likelihood), rather than the default conditional WAIC (i.e., WAIC conditioning on all parent nodes of the data nodes). See details.

niterMarginal: Number of Monte Carlo iterations to use when marginalizing (default is 1000).

convergenceSet: Optional vector of numbers between 0 and 1 that specify a set of shorter Monte Carlo simulations for marginal WAIC calculation as fractions of the full (niterMarginal) Monte Carlo simulation. If not provided, NIMBLE will use 0.25, 0.50, and 0.75. NIMBLE will report the WAIC, lppd, and pWAIC that would have been obtained for these smaller Monte Carlo simulations, allowing assessment of the number of Monte Carlo samples needed for stable calculation of WAIC.

thin: Logical value for specifying whether to do WAIC calculations only on thinned samples (default is FALSE). Likely only useful for reducing computation when using marginal WAIC.

nburnin\_extra: Additional number of pre-thinning MCMC iterations to discard before calculating online WAIC. This number is discarded in addition to the usual MCMC burnin, nburnin. The purpose of this option is to allow a user to retain some samples for inspection without having those samples used for online WAIC calculation (default = 0).

## Extracting WAIC

The calculated WAIC and related quantities can be obtained in various ways depending on how the MCMC is run. If using nimbleMCMC and setting WAIC = TRUE, see the WAIC component of the output list. If using runMCMC and setting WAIC = TRUE, either see the WAIC component of the output list or use the getWAIC method of the MCMC object (in the latter case WAIC = TRUE is not required). If using the run method of the MCMC object, use the getWAIC method of the MCMC object.

The output of running WAIC (unless one sets online = FALSE) is a list containing the following components:

WAIC: The computed WAIC, on the deviance scale. Smaller values are better when comparing WAIC for two models.

lppd: The log predictive density component of WAIC.

pWAIC: The pWAIC estimate of the effective number of parameters, computed using the pWAIC2 method of Gelman et al. (2014).

To get further information, one can use the getWAICdetails method of the MCMC object. The result of running getWAICdetails is a list containing the following components:

marginal: Logical value indicating whether marginal (TRUE) or conditional (FALSE) WAIC was calculated.

niterMarginal: Number of Monte Carlo iterations used in computing marginal likelihoods if using marginal WAIC.

thin: Whether WAIC was calculated based only on thinned samples.

online: Whether WAIC was calculated during MCMC sampling.

nburnin\_extra: Number of additional iterations discarded as burnin, in addition to original MCMC burnin.

WAIC\_partialMC, lppd\_partialMC, pWAIC\_partialMC: The computed marginal WAIC, lppd, and pWAIC based on fewer Monte Carlo simulations, for use in assessing the sensitivity of the WAIC calculation to the number of Monte Carlo iterations.

niterMarginal\_partialMC: Number of Monte Carlo iterations used for the values in WAIC\_partialMC, lppd\_partialMC, pWAIC\_partialMC.

WAIC\_elements, lppd\_elements, pWAIC\_elements: Vectors of individual WAIC, lppd, and pWAIC values, one element per data node (or group of nodes in the case of specifying dataGroups). Of use in computing the standard error of the difference in WAIC between two models, following Vehtari et al. (2017).

#### **Online WAIC**

As of version 0.12.0, NIMBLE provides enhanced WAIC functionality, with user control over whether to use conditional or marginal versions of WAIC and whether to group data nodes. In addition, users are no longer required to carefully choose MCMC monitors. WAIC by default is now calculated in an online manner (updating the required summary statistics at each MCMC iteration), using all post-burnin samples. The WAIC (Watanabe, 2010) is calculated from Equations 5, 12, and 13 in Gelman et al. (2014) (i.e., using 'pWAIC2').

Note that there is not a unique value of WAIC for a model. By default, WAIC is calculated conditional on the parent nodes of the data nodes, and the density values used are the individual density values of the data nodes. However, by modifying the marginalizeNodes and dataGroups elements of the control list, users can request a marginal WAIC (using a marginal likelihood that integrates over user-specified latent nodes) and/or a WAIC based on grouping observations (e.g., all observations in a cluster) to use joint density values. See the MCMC Chapter of the NIMBLE User Manual for more details.

For more detail on the use of different predictive distributions, see Section 2.5 from Gelman et al. (2014) or Ariyo et al. (2019).

Note that based on a limited set of simulation experiments in Hug and Paciorek (2021) our tentative recommendation is that users only use marginal WAIC if also using grouping.

#### Author(s)

Joshua Hug and Christopher Paciorek

#### References

Watanabe, S. (2010). Asymptotic equivalence of Bayes cross validation and widely applicable information criterion in singular learning theory. *Journal of Machine Learning Research* 11: 3571-3594.

Gelman, A., Hwang, J. and Vehtari, A. (2014). Understanding predictive information criteria for Bayesian models. *Statistics and Computing* 24(6): 997-1016.

Ariyo, O., Quintero, A., Munoz, J., Verbeke, G. and Lesaffre, E. (2019). Bayesian model selection in linear mixed models for longitudinal data. *Journal of Applied Statistics* 47: 890-913.

Vehtari, A., Gelman, A. and Gabry, J. (2017). Practical Bayesian model evaluation using leave-oneout cross-validation and WAIC. *Statistics and Computing* 27: 1413-1432.

Hug, J.E. and Paciorek, C.J. (2021). A numerically stable online implementation and exploration of WAIC through variations of the predictive density, using NIMBLE. *arXiv e-print* <arXiv:2106.13359>.

#### See Also

calculateWAIC configureMCMC buildMCMC runMCMC nimbleMCMC

## Examples

```
code <- nimbleCode({
  for(j in 1:J) {
    for(i in 1:n)
      y[j, i] ~ dnorm(mu[j], sd = sigma)</pre>
```

waic

```
mu[j] ~ dnorm(mu0, sd = tau)
  }
  sigma ~ dunif(0, 10)
  tau ~ dunif(0, 10)
})
J <- 5
n <- 10
groups <- paste0('y[', 1:J, ', 1:', n, ']')
y <- matrix(rnorm(J*n), J, n)</pre>
Rmodel <- nimbleModel(code, constants = list(J = J, n = n), data = list(y = y),</pre>
                       inits = list(tau = 1, sigma = 1))
## Various versions of WAIC available via online calculation.
## Conditional WAIC without data grouping:
conf <- configureMCMC(Rmodel, enableWAIC = TRUE)</pre>
## Conditional WAIC with data grouping
conf <- configureMCMC(Rmodel, enableWAIC = TRUE, controlWAIC = list(dataGroups = groups))</pre>
## Marginal WAIC with data grouping:
conf <- configureMCMC(Rmodel, enableWAIC = TRUE, controlWAIC =</pre>
            list(dataGroups = groups, marginalizeNodes = 'mu'))
## Not run:
Rmcmc <- buildMCMC(conf)</pre>
Cmodel <- compileNimble(Rmodel)</pre>
Cmcmc <- compileNimble(Rmcmc, project = Rmodel)</pre>
output <- runMCMC(Cmcmc, niter = 1000, WAIC = TRUE)</pre>
output$WAIC
                          # direct access
## Alternatively call via the `getWAIC` method; this doesn't require setting
## `waic=TRUE` in `runMCMC`
Cmcmc$getWAIC()
Cmcmc$getWAICdetails()
```

```
## End(Not run)
```

waicDetailsNimbleList waicDetailsNimbleList definition

#### Description

waicDetailsNimbleList definition for the nimbleList type returned by WAIC computation.

#### Usage

```
waicDetailsNimbleList
```

#### Format

An object of class list of length 1.

#### Details

See help(waic) for details on the elements of the list.

waicNimbleList

#### Author(s)

NIMBLE development team

waicNimbleList waicNimbleList definition

## Description

waicNimbleList definition for the nimbleList type returned by WAIC computation.

#### Usage

waicNimbleList

#### Format

An object of class list of length 1.

#### Details

See help(waic) for details on the elements of the list.

#### Author(s)

NIMBLE development team

Wishart

The Wishart Distribution

## Description

Density and random generation for the Wishart distribution, using the Cholesky factor of either the scale matrix or the rate matrix.

#### Usage

dwish\_chol(x, cholesky, df, scale\_param = TRUE, log = FALSE)
rwish\_chol(n = 1, cholesky, df, scale\_param = TRUE)

#### Arguments

х	vector of values.
cholesky	upper-triangular Cholesky factor of either the scale matrix (when scale_param is TRUE) or rate matrix (otherwise).
df	degrees of freedom.
scale_param	logical; if TRUE the Cholesky factor is that of the scale matrix; otherwise, of the rate matrix.
log	logical; if TRUE, probability density is returned on the log scale.
n	number of observations (only n=1 is handled currently).

## Details

See Gelman et al., Appendix A or the BUGS manual for mathematical details. The rate matrix as used here is defined as the inverse of the scale matrix,  $S^{-1}$ , given in Gelman et al.

## Value

dwish\_chol gives the density and rwish\_chol generates random deviates.

## Author(s)

Christopher Paciorek

#### References

Gelman, A., Carlin, J.B., Stern, H.S., and Rubin, D.B. (2004) *Bayesian Data Analysis*, 2nd ed. Chapman and Hall/CRC.

## See Also

Distributions for other standard distributions

## Examples

```
df <- 40
ch <- chol(matrix(c(1, .7, .7, 1), 2))
x <- rwish_chol(1, ch, df = df)
dwish_chol(x, ch, df = df)</pre>
```

withNimbleOptions Temporarily set some NIMBLE options.

## Description

Temporarily set some NIMBLE options.

## Usage

```
withNimbleOptions(options, expr)
```

## Arguments

options	a list of options suitable for nimbleOptions.
expr	an expression or statement to evaluate.

## Value

expr as evaluated with given options.

# Examples

```
## Not run:
if (!(getNimbleOption('showCompilerOutput') == FALSE)) stop()
nf <- nimbleFunction(run = function(){ return(0); returnType(double()) })
cnf <- withNimbleOptions(list(showCompilerOutput = TRUE), {
    if (!(getNimbleOption('showCompilerOutput') == TRUE)) stop()
    compileNimble(nf)
})
if (!(getNimbleOption('showCompilerOutput') == FALSE)) stop()
## End(Not run)
```

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