## Package 'BayesNSGP'

#### October 12, 2022

Title Bayesian Analysis of Non-Stationary Gaussian Process Models

**Description** Enables off-the-shelf functionality for fully Bayesian, nonstationary Gaussian process modeling. The approach to nonstationary modeling involves a closed-form, convolution-based covariance function with spatially-varying parameters; these parameter processes can be specified either deterministically (using covariates or basis functions) or stochastically (using approximate Gaussian processes). Stationary Gaussian processes are a special case of our methodology, and we furthermore implement approximate Gaussian process inference to account for very large spatial data sets (Finley, et al (2017) <arXiv:1702.00434v2>). Bayesian inference is carried out using Markov chain Monte Carlo methods via the 'nimble' package, and posterior prediction for the Gaussian process at unobserved locations is provided as a post-processing step.

Version 0.1.2

Date 2022-01-07

Maintainer Daniel Turek <danielturek@gmail.com>
Author Daniel Turek, Mark Risser

Depends R (>= 3.4.0),nimble

Imports FNN,Matrix,methods,StatMatch

License GPL-3

Encoding UTF-8

RoxygenNote 7.1.1

NeedsCompilation no

Repository CRAN

**Date/Publication** 2022-01-09 01:52:42 UTC

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calcQF

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Calculate the Gaussian quadratic form for the NNGP approximation

## Description

calcQF calculates the quadratic form in the multivariate Gaussian based on the NNGP approximation, for a specific parameter combination. The quadratic form is  $t(u)C^{-1}v$ .

## Usage

```
calcQF(u, v, AD, nID)
```

u	Vector; left product.
V	Vector; right product
AD	N x (k+1) matrix; the first k columns are the 'A' matrix, and the last column is the 'D' vector. Represents the Cholesky of $C^{-1}$ .
nID	N x k matrix of neighbor indices.

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#### Value

A list with two components: (1) an N x 2 array containing the same spatial coordinates, ordered by MMD, and (2) the same thing, but with any NA values removed.

calculateAD\_ns

Calculate A and D matrices for the NNGP approximation

#### **Description**

calculateAD\_ns calculates A and D matrices (the Cholesky of the precision matrix) needed for the NNGP approximation.

## Usage

```
calculateAD_ns(
  dist1_3d,
  dist2_3d,
  dist12_3d,
  Sigma11,
  Sigma22,
  Sigma12,
  log_sigma_vec,
  log_tau_vec,
  nID,
  N,
  k,
  nu,
  d
)
```

```
dist1_3d
                  N x (k+1) x (k+1) array of distances in the x-coordinate direction.
                  N x (k+1) x (k+1) array of distances in the y-coordinate direction.
dist2_3d
dist12_3d
                  N x (k+1) x (k+1) array of cross-distances.
Sigma11
                  N-vector; 1-1 element of the Sigma() process.
Sigma22
                  N-vector; 2-2 element of the Sigma() process.
Sigma12
                  N-vector; 1-2 element of the Sigma() process.
log_sigma_vec
                  N-vector; process standard deviation values.
log_tau_vec
                  N-vector; nugget standard deviation values.
nID
                  N x k matrix of neighbor indices.
                  Scalar; number of data measurements.
Ν
k
                  Scalar; number of nearest neighbors.
nu
                  Scalar; Matern smoothness parameter.
                  Scalar; dimension of the spatial domain.
d
```

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#### Value

A N x (k+1) matrix; the first k columns are the 'A' matrix, and the last column is the 'D' vector.

calculateU\_ns

Calculate the (sparse) matrix U

#### **Description**

calculateU\_ns calculates the (sparse) matrix U (i.e., the Cholesky of the inverse covariance matrix) using a nonstationary covariance function. The output only contains non-zero values and is stored as three vectors: (1) the row indices, (2) the column indices, and (3) the non-zero values. NOTE: this code assumes the all inputs correspond to the ORDERED locations.

#### Usage

```
calculateU_ns(
  dist1_3d,
  dist2_3d,
  dist12_3d,
  Sigma11,
  Sigma22,
  Sigma12,
  log_sigma_vec,
  log_tau_vec,
  nu,
  nID,
  cond_on_y,
  Ν,
  k,
  d,
 M = 0
)
```

```
dist1_3d
                  N x (k+1) x (k+1) array of distances in the x-coordinate direction.
dist2_3d
                  N x (k+1) x (k+1) array of distances in the y-coordinate direction.
dist12_3d
                  N x (k+1) x (k+1) array of cross-distances.
Sigma11
                  N-vector; 1-1 element of the Sigma() process.
Sigma22
                  N-vector; 2-2 element of the Sigma() process.
                  N-vector; 1-2 element of the Sigma() process.
Sigma12
                  N-vector; process standard deviation values.
log_sigma_vec
                  N-vector; nugget standard deviation values.
log_tau_vec
                  Scalar; Matern smoothness parameter.
nu
```

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nID	N x k matrix of (ordered) neighbor indices.
cond_on_y	A matrix indicating whether the conditioning set for each (ordered) location is on the latent process $(y,1)$ or the observed values $(z,\emptyset)$ . Calculated in sgvSetup.
N	Scalar; number of data measurements.
k	Scalar; number of nearest neighbors.
d	Scalar; dimension of the spatial domain.
М	Scalar; number of prediction sites.

#### Value

Returns a sparse matrix representation of the Cholesky of the precision matrix for a fixed set of covariance parameters.

## **Description**

conditionLatentObs assigns  $q_y(i)$  vs  $q_z(i)$  following Section 5.1 in Katzfuss and Guinness (2018). This function only needs to be run once per SGV analysis.

#### Usage

```
conditionLatentObs(nID, coords_ord, N)
```

#### **Arguments**

nID N x k matrix of neighbor indices.

coords\_ord N x 2 matrix of locations.

N Scalar; number of locations (observed only!).

#### Value

A matrix indicating whether the conditioning set for each location is on the latent process (y, 1) or the observed values (z, 0).

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determineNeighbors

Determine the k-nearest neighbors for each spatial coordinate.

## Description

determineNeighbors returns an  $N \times k$  matrix of the nearest neighbors for spatial locations coords, with the ith row giving indices of the k nearest neighbors to the ith location, which are selected from among the 1,...(i-1) other spatial locations. The first row is -1's, since the first location has no neighbors. The i=2 through i=(k+1) rows each necessarily contain 1:i.

#### Usage

```
determineNeighbors(coords, k)
```

#### **Arguments**

coords N x 2 array of N 2-dimensional (x,y) spatial coordinates.

k Scalar; number of neighbors

#### Value

An N x k matrix of nearest neighbor indices

### **Examples**

```
coords <- cbind(runif(100), runif(100))
determineNeighbors(coords, 20)</pre>
```

dmnorm\_nngp

Function for the evaluating the NNGP approximate density.

## Description

dmnorm\_nngp (and rmnorm\_nngp) calculate the approximate NNGP likelihood for a fixed set of parameters (i.e., A and D matrices). Finally, the distributions must be registered within nimble.

#### Usage

```
dmnorm_nngp(x, mean, AD, nID, N, k, log)
```

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## Arguments

X	N-vector of data.
mean	N-vector with current values of the mean
AD	$N \ x \ (k+1)$ matrix; the first k columns are the 'A' matrix, and the last column is the 'D' vector.
nID	N x k matrix of neighbor indices.
N	Scalar; number of data measurements.
k	Scalar; number of nearest neighbors.
log	Scalar; should the density be on the log scale (1) or not (0).

## Value

The NNGP approximate density.

dmnorm_sgv	Function for the evaluating the SGV approximate density.

## Description

dmnorm\_sgv (and rmnorm\_sgv) calculate the approximate SGV likelihood for a fixed set of parameters (i.e., the U matrix). Finally, the distributions must be registered within nimble.

#### Usage

```
dmnorm_sgv(x, mean, U, N, k, log = 1)
```

## Arguments

X	Vector of measurements
mean	Vector of mean valuees
U	Matrix of size N x 3; representation of a sparse N x N Cholesky of the precision matrix. The first two columns contain row and column indices, respectively, and the last column is the nonzero elements of the matrix.
N	Number of measurements in x
k	Number of neighbors for the SGV approximation.
log	Logical; should the density be evaluated on the log scale.

## Value

Returns the SGV approximation to the Gaussian likelihood.

8 inverseEigen

nents	inverseEigen	Calculate covariance elements based on eigendecomposition components
-------	--------------	--

#### **Description**

inverseEigen calculates the inverse eigendecomposition – in other words, the covariance elements based on the eigenvalues and vectors. For a 2x2 anisotropy (covariance) matrix, we parameterize the three unique values in terms of the two log eigenvalues and a rotation parameter on the rescaled logit. The function is coded as a nimbleFunction (see the nimble package) but can also be used as a regular R function.

## Usage

```
inverseEigen(eigen_comp1, eigen_comp2, eigen_comp3, which_Sigma)
```

#### **Arguments**

eigen_comp1	N-vector; contains values of the log of the first anisotropy eigenvalue for a set of locations.
eigen_comp2	N-vector; contains values of the log of the second anisotropy eigenvalue for a set of locations.
eigen_comp3	N-vector; contains values of the rescaled logit of the anisotropy rotation for a set of locations.
which_Sigma	Scalar; one of (1,2,3), corresponding to which covariance component should be calculated (Sigma11, Sigma22, or Sigma12, respectively).

#### Value

A vector of anisotropy values (Sigma11, Sigma22, or Sigma12; depends on which\_Sigma) for the corresponding set of locations.

#### **Examples**

```
# Generate some eigendecomposition elements (all three are real-valued)
eigen_comp1 <- rnorm(10)
eigen_comp2 <- rnorm(10)
eigen_comp3 <- rnorm(10)
inverseEigen( eigen_comp1, eigen_comp2, eigen_comp3, 2) # Return the Sigma22 values</pre>
```

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matern_	corr

Calculate a stationary Matern correlation matrix

#### **Description**

matern\_corr calculates a stationary Matern correlation matrix for a fixed set of locations, based on a range and smoothness parameter. This function is primarily used for the "npGP" and "approxGP" models. The function is coded as a nimbleFunction (see the nimble package) but can also be used as a regular R function.

#### Usage

```
matern_corr(dist, rho, nu)
```

#### **Arguments**

dist N x N matrix; contains values of pairwise Euclidean distances in the x-y plane.

rho Scalar; "range" parameter used to rescale distances

nu Scalar; Matern smoothness parameter. nu = 0.5 corresponds to the Exponential

correlation; nu = Inf corresponds to the Gaussian correlation function.

#### Value

A correlation matrix for a fixed set of stations and fixed parameter values.

#### **Examples**

```
# Generate some coordinates
coords <- cbind(runif(100),runif(100))
nu <- 2
# Calculate distances -- can use nsDist to calculate Euclidean distances
dist_list <- nsDist(coords, isotropic = TRUE)
# Calculate the correlation matrix
corMat <- matern_corr(sqrt(dist_list$dist1_sq), 1, nu)</pre>
```

```
nimble_sparse_chol
```

nimble\_sparse\_chol

#### **Description**

```
nimble_sparse_chol
```

#### Usage

```
nimble_sparse_chol(i, j, x, n)
```

nimble\_sparse\_solve

## Arguments

i	Vector of row indices.
j	Vector of column indices.
x	Vector of values in the matrix

n Length of the vector

```
nimble_sparse_crossprod
```

nimble\_sparse\_crossprod

## Description

nimble\_sparse\_crossprod

## Usage

```
nimble_sparse_crossprod(i, j, x, z, n, subset, transp)
```

## Arguments

i	Vector of row indices.
j	Vector of column indices.
х	Vector of values in the matrix.
Z	Vector to calculate the cross-product with.
n	Length of the vector
subset	Optional vector of rows to include in the calculation.
4	0.4'1'

transp Optional indicator of using the transpose

## **Description**

```
nimble_sparse_solve
```

## Usage

```
nimble_sparse_solve(i, j, x, z)
```

- i Vector of row indices.
- j Vector of column indices.
- x Vector of values in the matrix.
- z Vector to calculate the cross-product with.

```
nimble\_sparse\_tcrossprod\\ nimble\_sparse\_tcrossprod
```

#### **Description**

```
nimble_sparse_tcrossprod
```

## Usage

```
nimble_sparse_tcrossprod(i, j, x, subset)
```

#### **Arguments**

i	Vector of row indices.
j	Vector of column indices.
X	Vector of values in the matrix.
subset	Optional vector of rows to include in the calculation.

nsCorr	Calculate a nonstationary Matern correlation matrix
--------	---

## Description

nsCorr calculates a nonstationary correlation matrix for a fixed set of locations, based on vectors of the unique anisotropy parameters for each station. Since the correlation function uses a spatially-varying Mahalanobis distance, this function requires coordinate- specific distance matrices (see below). The function is coded as a nimbleFunction (see the nimble package) but can also be used as a regular R function.

#### Usage

```
nsCorr(dist1_sq, dist2_sq, dist12, Sigma11, Sigma22, Sigma12, nu, d)
```

dist1_sq	N x N matrix; contains values of pairwise squared distances in the x-coordinate.
dist2_sq	N x N matrix; contains values of pairwise squared distances in the y-coordinate.
dist12	N x N matrix; contains values of pairwise signed cross- distances between the x- and y-coordinates. The sign of each element is important; see nsDist function for the details of this calculation. in the x-coordinate.
Sigma11	Vector of length N; contains the 1-1 element of the anisotropy process for each station.

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Sigma22	Vector of length N; contains the 2-2 element of the anisotropy process for each station.
Sigma12	Vector of length N; contains the 1-2 element of the anisotropy process for each station.
nu	Scalar; Matern smoothness parameter. $nu = 0.5$ corresponds to the Exponential correlation; $nu = Inf$ corresponds to the Gaussian correlation function.
d	Scalar; dimension of the spatial coordinates.

#### Value

A correlation matrix for a fixed set of stations and fixed parameter values.

#### **Examples**

nsCrosscorr

Calculate a nonstationary Matern cross-correlation matrix

#### **Description**

nsCrosscorr calculates a nonstationary cross-correlation matrix between two fixed sets of locations (a prediction set with M locations, and the observed set with N locations), based on vectors of the unique anisotropy parameters for each station. Since the correlation function uses a spatially-varying Mahalanobis distance, this function requires coordinate- specific distance matrices (see below). The function is coded as a nimbleFunction (see the nimble package) but can also be used as a regular R function.

#### Usage

```
nsCrosscorr(
   Xdist1_sq,
   Xdist2_sq,
   Xdist12,
   Sigma11,
   Sigma22,
```

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```
Sigma12,
PSigma11,
PSigma22,
PSigma12,
nu,
d
```

## Arguments

Xdist1_sq	M x N matrix; contains values of pairwise squared cross-distances in the x-coordinate.
Xdist2_sq	M x N matrix; contains values of pairwise squared cross-distances in the y-coordinate.
Xdist12	M x N matrix; contains values of pairwise signed cross/cross- distances between the x- and y-coordinates. The sign of each element is important; see nsDist function for the details of this calculation. in the x-coordinate.
Sigma11	Vector of length N; contains the 1-1 element of the anisotropy process for each observed location.
Sigma22	Vector of length N; contains the 2-2 element of the anisotropy process for each observed location.
Sigma12	Vector of length N; contains the 1-2 element of the anisotropy process for each observed location.
PSigma11	Vector of length N; contains the 1-1 element of the anisotropy process for each prediction location.
PSigma22	Vector of length N; contains the 2-2 element of the anisotropy process for each prediction location.
PSigma12	Vector of length N; contains the 1-2 element of the anisotropy process for each prediction location.
nu	Scalar; Matern smoothness parameter. nu = 0.5 corresponds to the Exponential correlation; nu = Inf corresponds to the Gaussian correlation function.
d	Scalar; dimension of the spatial domain.

## Value

A M x N cross-correlation matrix for two fixed sets of stations and fixed parameter values.

#### **Examples**

```
# Generate some coordinates and parameters
coords <- cbind(runif(100),runif(100))
Sigma11 <- rep(1, 100) # Identity anisotropy process
Sigma22 <- rep(1, 100)
Sigma12 <- rep(0, 100)
Pcoords <- cbind(runif(200),runif(200))
PSigma11 <- rep(1, 200) # Identity anisotropy process
PSigma22 <- rep(1, 200)</pre>
```

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```
PSigma12 <- rep(0, 200)
nu <- 2
# Calculate distances
Xdist_list <- nsCrossdist(coords, Pcoords)
# Calculate the correlation matrix
XcorMat <- nsCrosscorr(Xdist_list$dist1_sq, Xdist_list$dist2_sq, Xdist_list$dist12,
    Sigma11, Sigma22, Sigma12, PSigma11, PSigma22, PSigma12, nu, ncol(coords))</pre>
```

nsCrossdist

Calculate coordinate-specific cross-distance matrices

#### **Description**

nsCrossdist calculates coordinate-specific cross distances in x, y, and x-y for use in the nonstationary cross-correlation calculation. This function is useful for calculating posterior predictions.

#### Usage

```
nsCrossdist(coords, Pcoords, scale_factor = NULL, isotropic = FALSE)
```

## Arguments

coords N x 2 matrix; contains x-y coordinates of station (observed) locations.

Pcoords M x 2 matrix; contains x-y coordinates of prediction locations.

scale\_factor Scalar; optional argument for re-scaling the distances.

isotropic Logical; indicates whether distances should be calculated using Euclidean dis-

tance (isotropic = TRUE) or using the anisotropic formulation (isotropic =

FALSE).

#### Value

A list of distances matrices, with the following components:

dist1_sq	M x N matrix; contains values of pairwise squared cross- distances in the x-coordinate.
dist2_sq	M x N matrix; contains values of pairwise squared cross- distances in the y-coordinate.
dist12	$M\ x\ N$ matrix; contains values of pairwise signed cross- distances between the x- and y-coordinates.
scale_factor	Value of the scale factor used to rescale distances.

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#### **Examples**

```
# Generate some coordinates
coords <- cbind(runif(100),runif(100))
Pcoords <- cbind(runif(200),runif(200))
# Calculate distances
Xdist_list <- nsCrossdist(coords, Pcoords)</pre>
```

nsCrossdist3d

Calculate coordinate-specific cross-distance matrices, only for nearest neighbors and store in an array

#### Description

nsCrossdist3d generates and returns new 3-dimensional arrays containing the former dist1\_sq, dist2\_s1, and dist12 matrices, but only as needed for the k nearest-neighbors of each location. these 3D matrices (dist1\_3d, dist2\_3d, and dist12\_3d) are used in the new implementation of calculateAD\_ns().

#### Usage

```
nsCrossdist3d(
  coords,
  predCoords,
  P_nID,
  scale_factor = NULL,
  isotropic = FALSE
)
```

#### Arguments

coords N x d matrix; contains the x-y coordinates of stations.

predCoords M x d matrix

P\_nID N x k matrix; contains indices of nearest neighbors.

scale\_factor Scalar; optional argument for re-scaling the distances.

isotropic Logical; indicates whether distances should be calculated separately for each

coordinate dimension (FALSE) or simultaneously for all coordinate dimensions (TRUE). isotropic = FALSE can only be used for two-dimensional coordinate

systems.

#### Value

Arrays with nearest neighbor distances in each coordinate direction. When the spatial dimension d > 2, dist1\_3d contains squared Euclidean distances, and dist2\_3d and dist12\_3d are empty.

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#### **Examples**

```
# Generate some coordinates and neighbors
coords <- cbind(runif(100),runif(100))
predCoords <- cbind(runif(200),runif(200))
P_nID <- FNN::get.knnx(coords, predCoords, k = 10)$nn.index # Prediction NN
# Calculate distances
Pdist <- nsCrossdist3d(coords, predCoords, P_nID)</pre>
```

nsDist

Calculate coordinate-specific distance matrices

#### **Description**

nsDist calculates x, y, and x-y distances for use in the nonstationary correlation calculation. The sign of the cross-distance is important. The function contains an optional argument for re-scaling the distances such that the coordinates lie in a square.

#### Usage

```
nsDist(coords, scale_factor = NULL, isotropic = FALSE)
```

#### **Arguments**

isotropic

coords N x 2 matrix; contains the x-y coordinates of stations scale\_factor Scalar; optional argument for re-scaling the distances.

Logical; indicates whether distances should be calculated separately for each coordinate dimension (FALSE) or simultaneously for all coordinate dimensions

(TRUE). isotropic = TRUE can only be used for two-dimensional coordinate

systems.

#### Value

A list of distances matrices, with the following components:

dist1\_sq N x N matrix; contains values of pairwise squared distances in the x-coordinate.

dist2\_sq N x N matrix; contains values of pairwise squared distances in the y-coordinate.

N x N matrix; contains values of pairwise signed cross- distances between the x- and y-coordinates.

Value of the scale factor used to rescale distances.

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#### **Examples**

```
# Generate some coordinates
coords <- cbind(runif(100),runif(100))
# Calculate distances
dist_list <- nsDist(coords)
# Use nsDist to calculate Euclidean distances
dist_Euclidean <- sqrt(nsDist(coords, isotropic = TRUE)$dist1_sq)</pre>
```

nsDist3d Calculate coordinate-specific distance matrices, only for nearest neighbors and store in an array

#### **Description**

nsDist3d generates and returns new 3-dimensional arrays containing the former dist1\_sq, dist2\_sq, and dist12 matrices, but only as needed for the k nearest-neighbors of each location. these 3D matrices (dist1\_3d, dist2\_3d, and dist12\_3d) are used in the new implementation of calculateAD\_ns().

#### Usage

```
nsDist3d(coords, nID, scale_factor = NULL, isotropic = FALSE)
```

#### **Arguments**

coords N x 2 matrix; contains the x-y coordinates of stations.

N x k matrix; contains indices of nearest neighbors.

Scale\_factor Scalar; optional argument for re-scaling the distances.

isotropic Logical; indicates whether distances should be calculated separately for each

coordinate dimension (FALSE) or simultaneously for all coordinate dimensions (TRUE). isotropic = TRUE can only be used for two-dimensional coordinate

systems.

#### Value

Arrays with nearest neighbor distances in each coordinate direction.

#### **Examples**

```
# Generate some coordinates and neighbors
coords <- cbind(runif(100),runif(100))
nID <- determineNeighbors(coords, 10)
# Calculate distances
nsDist3d(coords, nID)</pre>
```

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nsgpModel

NIMBLE code for a generic nonstationary GP model

#### **Description**

This function sets up and compiles a nimble model for a general nonstationary Gaussian process.

#### Usage

```
nsgpModel(
  tau_model = "constant",
  sigma_model = "constant",
  Sigma_model = "constant",
  mu_model = "constant",
  likelihood = "fullGP",
  coords,
  data,
  constants = list(),
  monitorAllSampledNodes = TRUE,
  ...
)
```

#### **Arguments**

tau_model	Character; specifies the model to be used for the log(tau) process. Option	ns
	are "constant" (spatially-constant), "logLinReg" (log-linear regression), and	nd

"approxGP" (approximation to a Gaussian process).

sigma\_model Character; specifies the model to be used for the log(sigma) process. See tau\_model

for options.

Sigma\_model Character; specifies the model to be used for the Sigma anisotropy process. Op-

tions are "constant" (spatially-constant), "constantIso" (spatially-constant and isotropic), "covReg" (covariance regression), "compReg" (componentwise regression), "compRegIso" (isotropic componentwise regression), "npApproxGP" (nonparameteric regression via an approximation to a stationary Gaussian process), and "npApproxGPIso" (isotropic nonparameteric regression via an approximation to a stationary Gaussian process), and "npApproxGPIso" (isotropic nonparameteric regression via an approximation to a stationary Gaussian process), and "npApproxGPIso" (isotropic nonparameteric regression via an approximation to a stationary Gaussian process), and "npApproxGPIso" (isotropic nonparameteric regression via an approximation to a stationary Gaussian process), and "npApproxGPIso" (isotropic nonparameteric regression).

proximation to a stationary Gaussian process)

mu\_model Character; specifies the model to be used for the mu mean process. Options are

"constant" (spatially-constant), "linReg" (linear regression), and "zero" (a

fixed zero-mean).

likelihood Character; specifies the likelihood model. Options are "fullGP" (the exact

Gaussian process likelihood), "NNGP" (the nearest-neighbor GP for the response approximate likelihood), and "SGV" (the sparse general Vecchia approximate

likelihood).

coords N x d matrix of spatial coordinates.

data N-vector; observed vector of the spatial process of interest

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constants A list of constants required to build the model; depends on the specific parameter process models chosen.

monitorAllSampledNodes

Logical; indicates whether all sampled nodes should be stored (TRUE) or not (FALSE).

Additional arguments can be passed to the function; for example, as an alternative to the constants list, items can be passed directly via this argument.

#### Value

A nimbleCode object.

#### **Examples**

```
# Generate some data: stationary/isotropic
N <- 100
coords <- matrix(runif(2*N), ncol = 2)</pre>
alpha_vec <- rep(log(sqrt(1)), N) # Log process SD</pre>
delta_vec <- rep(log(sqrt(0.05)), N) # Log nugget SD</pre>
Sigma11_vec <- rep(0.4, N) # Kernel matrix element 1,1
Sigma22_vec <- rep(0.4, N) # Kernel matrix element 2,2
Sigma12_vec <- rep(0, N) # Kernel matrix element 1,2</pre>
mu_vec <- rep(0, N) # Mean</pre>
nu <- 0.5 # Smoothness
dist_list <- nsDist(coords)</pre>
Cor_mat <- nsCorr( dist1_sq = dist_list$dist1_sq, dist2_sq = dist_list$dist2_sq,</pre>
                    dist12 = dist_list$dist12, Sigma11 = Sigma11_vec,
                    Sigma22 = Sigma22_vec, Sigma12 = Sigma12_vec, nu = nu )
Cov_mat <- diag(exp(alpha_vec)) %*% Cor_mat %*% diag(exp(alpha_vec))</pre>
D_mat <- diag(exp(delta_vec)^2)</pre>
set.seed(110)
data <- as.numeric(mu_vec + t(chol(Cov_mat + D_mat)) %*% rnorm(N))</pre>
# Set up constants
constants <- list( nu = 0.5, Sigma_HP1 = 2)
# Defaults: tau_model = "constant", sigma_model = "constant", mu_model = "constant",
# and Sigma_model = "constant"
Rmodel <- nsgpModel(likelihood = "fullGP", constants = constants, coords = coords, data = data)
```

 ${\tt nsgpPredict}$ 

Posterior prediction for the NSGP

#### Description

nsgpPredict conducts posterior prediction for MCMC samples generated using nimble and nsgp-Model.

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#### Usage

```
nsgpPredict(
  model,
  samples,
  coords.predict,
  predict.process = TRUE,
  constants,
  seed = 0,
  ...
)
```

#### **Arguments**

model A NSGP nimble object; the output of nsgpModel.

samples A matrix of J rows, each is an MCMC sample of the parameters corresponding

to the specification in nsgpModel.

coords.predict M x d matrix of prediction coordinates.

predict.process

Logical; determines whether the prediction corresponds to the  $y(\cdot)$  process (TRUE)

or  $z(\cdot)$  (FALSE; this would likely only be used for, e.g., cross-validation).

constants An optional list of contants to use for prediction; alternatively, additional argu-

ments can be passed to the function via the ... argument.

seed An optional random seed argument for reproducibility.

. . . Additional arguments can be passed to the function; for example, as an alterna-

tive to the constants list, items can be passed directly via this argument.

## Value

The output of the function is a list with two elements: obs, a matrix of J posterior predictive samples for the N observed locations (only for likelihood = "SGV", which produces predictions for the observed locations by default; this element is NULL otherwise); and pred, a corresponding matrix of posterior predictive samples for the prediction locations. Ordering and neighbor selection for the prediction coordinates in the SGV likelihood are conducted internally, as with nsgpModel.

#### **Examples**

```
# Generate some data: stationary/isotropic
N <- 100
coords <- matrix(runif(2*N), ncol = 2)
alpha_vec <- rep(log(sqrt(1)), N) # Log process SD
delta_vec <- rep(log(sqrt(0.05)), N) # Log nugget SD
Sigma11_vec <- rep(0.4, N) # Kernel matrix element 1,1
Sigma22_vec <- rep(0.4, N) # Kernel matrix element 2,2
Sigma12_vec <- rep(0, N) # Kernel matrix element 1,2
mu_vec <- rep(0, N) # Mean
nu <- 0.5 # Smoothness
dist_list <- nsDist(coords)</pre>
```

orderCoordinatesMMD 21

```
Cor_mat <- nsCorr( dist1_sq = dist_list$dist1_sq, dist2_sq = dist_list$dist2_sq,</pre>
                    dist12 = dist_list$dist12, Sigma11 = Sigma11_vec,
                    Sigma22 = Sigma22_vec, Sigma12 = Sigma12_vec, nu = nu )
Cov_mat <- diag(exp(alpha_vec)) %*% Cor_mat %*% diag(exp(alpha_vec))</pre>
D_mat <- diag(exp(delta_vec)^2)</pre>
set.seed(110)
data <- as.numeric(mu_vec + t(chol(Cov_mat + D_mat)) %*% rnorm(N))</pre>
# Set up constants
constants <- list( nu = 0.5, Sigma\_HP1 = 2)
# Defaults: tau_model = "constant", sigma_model = "constant", mu_model = "constant",
# and Sigma_model = "constant"
Rmodel <- nsgpModel(likelihood = "fullGP", constants = constants, coords = coords, data = data)</pre>
conf <- configureMCMC(Rmodel)</pre>
Rmcmc <- buildMCMC(conf)</pre>
Cmodel <- compileNimble(Rmodel)</pre>
Cmcmc <- compileNimble(Rmcmc, project = Rmodel)</pre>
samples <- runMCMC(Cmcmc, niter = 200, nburnin = 100)</pre>
# Prediction
predCoords \leftarrow as.matrix(expand.grid(seq(0,1,1=10),seq(0,1,1=10)))
postpred <- nsgpPredict( model = Rmodel, samples = samples, coords.predict = predCoords )</pre>
```

orderCoordinatesMMD

Order coordinates according to a maximum-minimum distance criterion.

#### Description

orderCoordinatesMMD orders an array of (x,y) spatial coordinates according to the "maximum minimum distance" (MMD), as described in Guinness, 2018. (Points are selected to maximize their minimum distance to already- selected points).

#### Usage

```
orderCoordinatesMMD(coords, exact = FALSE)
```

#### **Arguments**

coords N x 2 array of N 2-dimensional (x,y) spatial coordinates.

exact Logical; FALSE uses a fast approximation to MMD ordering (and is almost al-

ways recommended), while TRUE uses exact MMD ordering but is infeasible for

large number of locations.

#### Value

A list of distances matrices, with the following components:

orderedCoords N x 2 matrix; contains the ordered spatial coordinates as coords. orderedIndicesNoNA

N-vector; contains the ordered indices with any NA values removed.

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#### **Examples**

```
coords <- cbind(runif(100), runif(100))
orderCoordinatesMMD(coords)</pre>
```

rmnorm\_nngp

Function for the evaluating the NNGP approximate density.

## Description

dmnorm\_nngp (and rmnorm\_nngp) calculate the approximate NNGP likelihood for a fixed set of parameters (i.e., A and D matrices). Finally, the distributions must be registered within nimble.

#### Usage

```
rmnorm_nngp(n, mean, AD, nID, N, k)
```

## **Arguments**

n	N-vector of data.
mean	N-vector with current values of the mean
AD	N x $(k+1)$ matrix; the first k columns are the 'A' matrix, and the last column is the 'D' vector.
nID	N x k matrix of neighbor indices.
N	Scalar; number of data measurements.
k	Scalar; number of nearest neighbors.

#### Value

The NNGP approximate density.

rmnorm\_sgv

Function for the evaluating the SGV approximate density.

## Description

dmnorm\_sgv (and rmnorm\_sgv) calculate the approximate SGV likelihood for a fixed set of parameters (i.e., the U matrix). Finally, the distributions must be registered within nimble.

#### Usage

```
rmnorm_sgv(n, mean, U, N, k)
```

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## Arguments

r	1	Vector of measurements
r	nean	Vector of mean valuees
Į	J	Matrix of size N x 3; representation of a sparse N x N Cholesky of the precision matrix. The first two columns contain row and column indices, respectively, and the last column is the nonzero elements of the matrix.
١	1	Number of measurements in x

k Number of neighbors for the SGV approximation.

#### Value

Not applicable.

R_sparse_chol	R_sparse_chol

## Description

R\_sparse\_chol

## Usage

```
R_{sparse\_chol(i, j, x, n)}
```

## Arguments

i	Vector of row indices.
j	Vector of column indices.

Vector of values in the matrix. Х

Length of the vector

```
R_sparse_crossprod
                         nimble\_sparse\_crossprod
```

## Description

```
nimble_sparse_crossprod
```

## Usage

```
R_{sparse\_crossprod(i, j, x, z, n, subset = -1, transp = 1)
```

24 R\_sparse\_tcrossprod

#### **Arguments**

<ul><li>j Vector of column indices.</li><li>x Vector of values in the matrix.</li></ul>	1	vector of row indices.
x Vector of values in the matrix.	j	Vector of column indices.
	X	Vector of values in the matrix.

z Vector to calculate the cross-product with.

n Length of the vector

subset Optional vector of rows to include in the calculation.

transp Optional indicator of using the transpose

R\_sparse\_solve

nimble\_sparse\_solve

#### **Description**

```
nimble_sparse_solve
```

#### Usage

```
R_sparse_solve(i, j, x, z)
```

#### **Arguments**

•	T 7 .	C	. 1.
7	Vector	of row	indices.
±	1 CC LCI	OIIOW	maices.

j Vector of column indices.

x Vector of values in the matrix.

z Vector to calculate the cross-product with.

R\_sparse\_tcrossprod

 $nimble\_sparse\_tcrossprod$ 

#### **Description**

```
nimble_sparse_tcrossprod
```

## Usage

```
R_sparse_tcrossprod(i, j, x, subset = -1)
```

#### **Arguments**

7	Vector	of row	indices.
1	VCCIOI	OLIUW	indices.

j Vector of column indices.

x Vector of values in the matrix.

subset Optional vector of rows to include in the calculation.

sgvSetup 25

sgvSetup	One-time setup wrapper function for the SGV approximation

#### Description

sgvSetup is a wrapper function that sets up the SGV approximation. Three objects are required: (1) ordering the locations, (2) identify nearest neighbors, and (3) determine the conditioning set. This function only needs to be run once per SGV analysis.

#### Usage

```
sgvSetup(
  coords,
  coords_pred = NULL,
  k = 15,
  seed = NULL,
  pred.seed = NULL,
  order_coords = TRUE
)
```

#### **Arguments**

coords Matrix of observed locations.

coords\_pred Optional matrix of prediction locations.

k Number of neighbors.

seed Setting the seed for reproducibility of the observed location ordering

pred. seed Setting the seed for reproducibility of the prediction ordering.

order\_coords Logical; should the coordinates be ordered.

#### Value

A list with the following components:

ord A vector of ordering position for the observed locations.

ord\_pred A vector of ordering position for the prediction locations (if coords\_pred is

provided).

ord\_all A concatenated vector of ord and ord\_pred.

coords\_ord A matrix of ordered locations (observed and prediction), included for conve-

nience.

nID\_ord A matrix of (ordered) neighbor indices.

condition\_on\_y\_ord

A matrix indicating whether the conditioning set for each (ordered) location is on the latent process (y, 1) or the observed values  $(z, \emptyset)$ .

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