## Package 'GeneralizedWendland'

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Type Package

Title Fully Parameterized Generalized Wendland Covariance Function

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**SystemRequirements** gsl (>= 2.7)

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LinkingTo Rcpp, RcppEigen, BH, Matrix

**Suggests** knitr, R.rsp, testthat (>= 3.0.0), mvtnorm, ggplot2, gridExtra, dplyr, microbenchmark

Description A fully parameterized Generalized Wendland covariance function for use in Gaus-

sian process models, as well as multiple methods for approximating it via covariance interpola-

tion. The available methods are linear interpolation, polynomial interpolation, and cubic spline interpolation.

Moreno Bevilacqua and Reinhard Fur-

rer and Tarik Faouzi and Emilio Porcu (2019) <url:<a href="https://projecteuclid.org/journalArticle/Download?urlId=10.1214%2F1AOS1652">https://projecteuclid.org/journalArticle/Download?urlId=10.1214%2F1AOS1652">https://projecteuclid.org/journalArticle/Download?urlId=10.1214%2F1AOS1652</a>>>.

Moreno Bevilacqua and Christian Caamaño-

Carrillo and Emilio Porcu (2022) <arXiv:2008.02904>.

Reinhard Furrer and Roman Flury and Florian Gerber (2022) <url:<a href="https://CRAN.R-project.org/package=spam">https://CRAN.R-project.org/package=spam">>>.

RcppModules Wendland

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GeneralizedWendland-package

Fully Parametrized Generalized Covariance Function for R

## **Description**

This package provides a fully parametrized generalized Wendland covariance function for use in geostatistical modeling, as well as various options for approximations and adjustments. In addition, the package comes with a modified process for parameter estimation, based on the spamimplementations, but compartmentalized using function factories.

## **Details**

The package requires the user to complete some initial steps before it can be used. Apart from the R dependencies, the user will need to manually install the GNU Scientific Library on their system and ensure that R can find the required libraries. On Windows systems, users can install devtools and then install gsl via MSYS2 > pacman.

### Author(s)

Thomas Caspar Fischer

## See Also

cov.wendland.

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choleskyFactory

Function Factory for Generating chol Function with unified arguments

## **Description**

A function factory which returns a function of the form function(Sigma) which performs a cholesky decomposition using an approach tailored to the type of input Sigma. Currently works for vectors, matrices, spam objects, and dgCMatrix objects from the **Matrix** package.

## Usage

```
choleskyFactory(chol.args = list(), Rstruct = NULL)
```

## **Arguments**

chol.args A list of optional settings for a cholesky function.

Rstruct A spam.chol.NgPeyton object which represents the sparsity structure of co-

variance matrix Sigma.

#### **Details**

The output of choleskyFactory is intended to replace calls to chol.default or chol.spam. The object type is determined during runtime, after which the appropriate function is called to obtain the cholesky decomposition. For spam objects, the function attempts to use update.spam.chol.NgPeyton if Rstruct is specified, and upon failure defaults to chol.spam. The result is then assigned in the execution environment of choleskyFactory, so that Rstruct will be defined in the next call.

## Value

A function of the form function(Sigma).

## Author(s)

Thomas Caspar Fischer

## References

Hadley Wickham (2015) *Advanced R*, CRC Press. Reinhard Furrer and Roman Flury and Florian Gerber (2022) spam: SPArse Matrix, R package version 2.8-0.

#### See Also

```
chol, chol.spam, update.spam.chol.NgPeyton
```

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## **Examples**

```
set.seed(1234)
locations <- data.frame(x = runif(10), y = runif(10))
theta <- c(0.5,1,1,0,0)
dmat <- as.matrix(dist(locations))
Sigma <- cov.wendland(dmat, theta)

cholFun <- choleskyFactory(chol.args = list())
cholD <- cholFun(Sigma)

cholFun <- choleskyFactory(chol.args = list(pivot = TRUE))
cholD_pivot <- cholFun(Sigma)

cholFun <- choleskyFactory(chol.args = list(pivot = "RCM"))
cholS_RCM <- cholFun(spam::as.spam(Sigma))</pre>
```

cov.askey

Askey covariance function

## **Description**

A covariance function of the form

$$\rho_{\beta,\kappa,\mu} = \begin{cases} \sigma + \theta & 0 \le r < \epsilon \\ (1 - r)^{\mu} & \epsilon \le r < 1 \\ 0 & 1 \le r \end{cases}$$

where  $r=h/\beta$ . This is equivalent to the generalized Wendland covariance with  $\kappa=0$ , but much more computationally efficient.

## Usage

```
cov.askey(h, theta, ..., cov.args = list())
```

## **Arguments**

h A numeric vector, matrix, or spam object storing distances.

theta Numeric vector  $\vec{\theta} = (\beta, \sigma, \mu, \theta)$  storing parameters.

... Other arguments.

cov.args Named list of arguments. See Details.

## **Details**

Using the list cov.args, users can provide the following arguments:

**cov.eps** (**default:** .Machine\$double.eps^0.5) The threshold distance  $\epsilon$  below which the function will return  $\sigma + \theta$ .

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## Value

Returns an object of the same type as input object h which stores the computed covariance values, i.e. a spam object if input h was also a spam object.

## Author(s)

Thomas Caspar Fischer

#### References

Moreno Bevilacqua and Tarik Faouzi and Reinhard Furrer and Emilio Porcu (2019) Estimation and prediction using generalized Wendland covariance functions under fixed domain asymptotics, *Annals of Statistics*, **47**(2), 828–856.

## See Also

cov.wendland

cov.wendland

Generalized Wendland Covariance Function

## **Description**

A fully parametrized generalized Wendland covariance function for use in geostatistical modeling, as well as multiple methods of obtaining computationally inexpensive approximations.

$$\rho_{\beta,\kappa,\mu} = \begin{cases} \sigma + \theta & 0 \le r < \epsilon \\ \frac{\sigma}{B(1+2\kappa,\mu)} \int_r^1 (u^2 - r^2)^{\kappa} (1-u)^{\mu-1} du & \epsilon \le r < 1 \\ 0 & 1 \le r \end{cases}$$

where  $r = h/\beta$ 

## Usage

```
cov.wendland(h, theta, ..., cov.args = list())
```

## **Arguments**

h A numeric vector, matrix, or spam object storing distances.

theta Numeric vector  $\vec{\theta} = (\beta, \sigma, \kappa, \mu, \theta)$  storing parameters.

... Other arguments.

cov.args Named list of arguments. See Details.

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## **Details**

Using the list cov.args, users can provide the following additional arguments:

numint.abstol (default: 1e-3) Absolute tolerance for numerical integration.

**numint.reltol** (**default:** 1e-3) Relative tolerance for numerical integration.

**numint.qag\_key** (**default:** 0) Method to use in QAG integration (Values 1 - 6)

**numint.subintervals** (**default:** 0) Number of subintervals to use in QAG/QAGS integration.

interp.method (default: 'none') Method to use for covariance interpolation. Valid methods are 'none', 'linear', 'polynomial', and 'cspline'.

interp.num\_support (default: 0) Number of support points to use for covariance interpolation.

**cov.reparameterize** (**default:** TRUE) Whether to apply the reparameterization  $\mu = \frac{1+d}{2} + \kappa + \nu$ , where  $\nu$  takes the place of  $\mu$  in input vector  $\vec{\theta}$ . This allows users to use box constraints in maximum likelihood estimation, as the covariance function is valid for  $\nu \in [0, \infty)$  rather than  $\mu \in [\frac{1+d}{2} + \kappa, \infty)$ .

**cov.eps** (**default:** .Machine\$double.eps^0.5) The threshold distance  $\epsilon$  below which the function will return  $\sigma + \theta$ .

**cov.d\_value** (**default:** 2) Dimensionality of space in which measurements were taken. This only takes effect if cov.reparameterize is TRUE.

#### Value

Returns an object of the same type as input object h which stores the computed covariance values, i.e. a spam object if input h was also a spam object.

## Author(s)

Thomas Caspar Fischer

#### References

Moreno Bevilacqua and Tarik Faouzi and Reinhard Furrer and Emilio Porcu (2019) Estimation and prediction using generalized Wendland covariance functions under fixed domain asymptotics, *Annals of Statistics*, **47**(2), 828–856.

## **Examples**

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covarianceFactory

*covarianceFactory* 

## **Description**

A function factory which sets up a covariance function.

## Usage

```
covarianceFactory(covariance, cov.args = list())
```

## **Arguments**

covariance A function which takes as input an object containing distances (h), a vector of

parameters (theta), and a list of optional settings (cov.args)

cov.args A list of optional settings for a covariance function.

## **Details**

covarianceFactory() is a function factory which takes as input an arbitrary covariance function and a list of additional arguments and returns a function with these arguments. The argument cov.args mainly serves to pass the relevant arguments to the covariance function, but also allows users to specify the following two arguments:

**cov.fixed\_range\_value** (**default:** NA) A constant value for the range parameter. Note that the code assumes that the first value of theta corresponds to the range parameter, as this notation is used in the **spam** package.

**cov.fixed\_nugget\_value** (**default:** NA) A constant value for the nugget parameter. Note that the code assumes that the last value of theta corresponds to the nugget parameter, as this notation is used in the **spam** package.

Note that if either of these arguments are specified, the corresponding entries should also be omitted in theta.

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## Value

A function of the form function(h, theta). This function is enclosed in the execution environment of choleskyFactory and hence has access to the arguments covariance and cov.args. The manufactured function returns the result of covariance(h = h, theta = theta, cov.args = cov.args).

## Author(s)

Thomas Caspar Fischer

## References

Wickham, H. (2015) Advanced R, CRC Press.

#### See Also

```
covmat and cov.wendland
```

## **Examples**

```
library(GeneralizedWendland)
library(spam)

hs <- seq(0, 1, 0.05)
covSph <- covarianceFactory(cov.sph)
covExp <- covarianceFactory(cov.exp)
covWend <- covarianceFactory(cov.wendland)

plot(0, type = "n", xlim = c(0, 1), ylim = c(0, 1))
lines(hs, covSph(hs, theta = c(0.5, 1, 0)))
lines(hs, covExp(hs, theta = c(0.5, 1, 0)), col = "red")
lines(hs, covWend(hs, theta = c(0.5, 1, 0.5, 0.5, 0)), col = "green")</pre>
```

factory-covDiag

Diagnostics For Arbitrary Covariance Functions

## **Description**

A suite of diagnostic tools. The functions described here provide the user with quick access to diagnostics for arbitrary target covariance functions and arbitrary reference covariance functions.

## Usage

```
covDiagFactory(target_covariance,
  diagnostic_funs = c("accumulated_error", "point_diagnostics"),
  reference_covariance = cov.askey, reference_cov.args = list())
accumulated_error(target_covFun, target_cov.theta, reference_covFun,
```

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```
reference_cov.theta, ..., absolute = TRUE, lower = 0, upper = 1,
subdivisions = 500L, abs.tol = .Machine$double.eps^0.5,
rel.tol = .Machine$double.eps^0.25)

point_diagnostics(target_covFun, target_cov.theta, reference_covFun,
    reference_cov.theta, ..., grid_resolution = 100)
```

## **Arguments**

diagnostic\_funs

A character vector for specifying which diagnostics to compute and return. Currently, accumulated\_error and point\_diagnostics are implemented. Note that the functions themselves are not intended to be called directly by the user.

reference\_covariance

Covariance function with formals function(h, theta, ..., cov.args)

reference\_covFun

Same as reference\_covariance, but implicitly assumes that the input was generated using covarianceFactory().

reference\_cov.args

List with additional arguments to be passed to reference\_covariance.

reference cov.theta

Numeric vector containing parameters for reference\_covariance.

target\_covariance

Covariance function with formals function(h, theta, ..., cov.args)

target\_cov.theta

Numeric vector containing parameters for target\_covariance.

target\_covFun Same as target\_covariance, but implicitly assumes that the input was generated

using covarianceFactory().

... Other arguments

grid\_resolution

Number of points n to evaluate the covariance function at.

absolute Logical value. Whether to return absolute value.

lower Lower boundary for accumulated error. Defaults to 0. Passed to integrate().

upper Upper boundary for accumulated error. Defaults to 1. Passed to integrate().

subdivisions The maximum number of subintervals. Passed to integrate().

abs.tol Absolute accuracy. Passed to integrate()
rel.tol Relative accuracy. Passed to integrate()

#### **Details**

The function manufactured by covDiagFactory has the form function(target\_theta\_list, target\_args\_list = list(), reference\_cov.theta = NULL, ...) and serves to iterate over a large variety of parameters.

**target\_theta\_list** List of named numeric vectors, each providing at least one or more values for a parameter.

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target\_args\_list (default = list()) List of named vectors, each providing at least one or more values for each argument to be provided to target\_covariance.

reference\_cov.theta (default = NULL) A numeric vector with parameters for the reference covariance. This is primarily intended to use when comparing different covariance functions, in which case the target covariance is compared to the reference with constant parameters.If this argument is left at default and the target and reference are identical, the parameters in target\_theta\_list will be used by both. Otherwise this will raise an exception.

#### Value

covDiagFactory() is a function factory which generates a function for computing diagnostics across a large variety of parameter values and additional arguments. The manufactured function has the form function(target\_theta\_list, target\_args\_list = list(), reference\_cov.theta = NULL, ... and returns a list of the same length as diagnostic\_funs, each entry storing a data.frame with the results returned by the associated diagnostic function.

## Available diagnostic functions

All diagnostic functions have in common that, apart from the required parameters kappa and mu, any remaining parameters are optional and captured using the . . . operator. Any unspecified arguments are left at default. The provided arguments are then turned into a grid using expand.grid, which is then iterated over to compute the requested diagnostic metrics. Note that there are some built-in checks which ensure that invalid configurations are dropped from the grid. For example, rows with interpolator = 'none' and a non-zero number of supports are dropped to prevent redundant computations.

**Accumulated Error:** The accumulated error corresponds to the area between the approximated and exact covariance curve.

**Point diagnostics:** This option returns error metrics across a user-defined number of points on the interval [0,1]. The metrics returned are "error", "absolute error", "maximum error", "target covariance value", and "reference covariance value".

#### Author(s)

Thomas Caspar Fischer

## See Also

cov.wendland

## **Examples**

```
interpolators <- c("linear", "cspline", "polynomial")
diagnostics <- c("accumulated_error", "point_diagnostics")

diagnosticFun <- covDiagFactory(cov.wendland, diagnostic_funs = diagnostics,
    reference_covariance = cov.wendland)
target_theta_list <- list(range = 0.5, sill = 1, kappa = c(0, 0.5, 1), mu = 0,</pre>
```

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```
nugget = 0)
target_args_list <- list(interp.method = interpolators, interp.num_support = 25)
wendland_comparison <- diagnosticFun(target_theta_list = target_theta_list,
    target_args_list = target_args_list)

diagnosticFun <- covDiagFactory(cov.wendland, diagnostic_funs = diagnostics,
    reference_covariance = cov.askey)
target_theta_list <- list(range = 0.5, sill = 1, kappa = 0, mu = 0.5, nugget = 0)
target_args_list <- list(interp.method = interpolators, interp.num_support = 25)
askey_comparison <- diagnosticFun(target_theta_list = target_theta_list,
    target_args_list = target_args_list, reference_cov.theta = c(0.5, 1, 0.5, 0))</pre>
```

factory-predict

Function factory for prediction generator

## **Description**

A function factory which generates a function for sampling from the predictive distribution

## Usage

```
predictionFactory(y, locs0, locs1, covariance, X0 = list2DF(nrow = nrow(locs0)),
  X1 = list2DF(nrow = nrow(locs1)), ..., cov.args = list(), chol.args = list(),
  use_spam = TRUE)
```

#### **Arguments**

у	Observed measurements.
locs0	Locations at which measurements were obtained.
locs1	Locations at which to predict.
covariance	Covariance function.
X0	Covariates. By default corresponds to an empty data.frame() with $nrow(locs0)$ rows.
X1	Covariates for new locations. By default corresponds to an empty data.frame() with nrow(locs1) rows.
	Additional arguments. Unused.
cov.args	Additional arguments for covariance function.
chol.args	Additional arguments for function used to compute cholesky decomposition.
use_spam	Logical value. If TRUE, use spam to compute predictions.

## Value

Returns a function of the form function(n, param), where n corresponds to the number of simulations to run, and param is a parameter vector as returned by optim.

## Author(s)

Thomas Caspar Fischer

## **Examples**

```
set.seed(23)
n <- 100
res <- c(20, 20)
locs <- data.frame(x = runif(n), y = runif(n))</pre>
locs_new \leftarrow expand.grid(x = seq(0, 1, length.out = res[1]),
                         y = seq(0, 1, length.out = res[2]))
range <- 0.3
dmat <- as.matrix(dist(locs))</pre>
theta <- c(range, 1, 1, 0, 0)
cov.args <- list()</pre>
chol.args <- list()</pre>
Sigma <- cov.wendland(h = dmat, theta = theta, cov.args = cov.args)</pre>
y <- c(spam::rmvnorm(n = 1, Sigma = Sigma))
predictionFun <- predictionFactory(y = y, locs0 = locs, locs1 = locs_new,</pre>
  covariance = cov.wendland, cov.args = cov.args, chol.args = chol.args,
  use\_spam = FALSE)
predictions <- predictionFun(n=10, param=theta)</pre>
image(x = seq(0, 1, length.out=res[1]),
      y = seq(0, 1, length.out=res[2]),
      z = matrix(apply(predictions,2,mean), res[1], res[2]),
      col = hcl.colors(9, "Blue-Red"),
      breaks = qnorm(seq(0.05, 0.95, 0.1)),
      xlab = "", ylab = "", xaxt = "n", yaxt = "n",
      useRaster = TRUE)
```

generalizedwendland-error

Simple errors defined by GeneralizedWendland package

## Description

An overview of the simpleError objects defined by the **GeneralizedWendland** package.

## **Error definitions**

update.spam.chol.error: "Updated covariance entries do not match length of original one."

Warning which is raised when update.spam.chol.NgPeyton fails because the length of the entries in the updated covariance matrix is not equal to the length of the original matrix. This usually indicates that the initial sparsity structure was too sparse for the given parameters.

wendland.insuffparam.error: "Too few parameters for Wendland." Insert description here

wendland.excessparam.error: "Too many parameters for Wendland. Did you supply fix range or nugget?"

Insert description here

covfun.notfunction.error: "Argument covariance must be a function." Insert description here

## Author(s)

Thomas Caspar Fischer

generalizedwendland-warning

Simple warnings defined by GeneralizedWendland package.

## **Description**

An overview of the simpleError objects defined by the **GeneralizedWendland** package.

## Warning definitions

update.spam.chol.warn: "Updated covariance entries do not match length of original one. Deleting stored Rstruct."

Warning which is raised when update.spam.chol.NgPeyton fails because the length of the entries in the updated covariance matrix is not equal to the length of the original matrix. This usually indicates that the initial sparsity structure was too sparse for the given parameters.

wendland.interp.redundantsupport.warn: "Argument interp.num\_support > 0 while using exact method. Set to 0." Insert description here.

wendland.interp.lowsupport.warn: "Argument interp.method!= 'none' with less than 3 support points. Forced to 'no Insert description here.

wendland.interp.unimplemented.warn: "Interpolator not implemented. Forcing exact method."

Insert description here.

## Author(s)

Thomas Caspar Fischer

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Function Factory for Generating mle Function with unified arguments

## Description

A factory function which returns a function of the form function(y, X = data.frame(), distmat, init\_parameters, theta\_llim, theta\_ulim) which can be called to compute the maximum likelihood estimates for a Kriging model.

## Usage

```
mleFactory(covariance, cov.args = list(), chol.args = list(),
  optim.args = list(), hessian = FALSE, optimParallel.args = list())
```

## **Arguments**

covariance	A function of the form function(h, theta,, cov.args = list()), where h is an object storing a distance matrix, theta is a numeric vector of parameters for the linear predictor and covariance function, and cov.args is a list of optional arguments for the covariance function.		
cov.args	A list of optional settings for a covariance function.		
chol.args	A list of optional settings for a cholesky function. <i>Note</i> : Valid input arguments change depending on whether the distance matrix provided to the output function is sparse. This may change in a future version.		
optim.args	A list of optional settings for optim. See ${\tt optim}$ for documentation of valid arguments.		
hessian	A logical value which specifies whether the hessian matrix is to be returned in the output. Is FALSE by default.		
optimParallel.args			
	A list of optional settings for optimParallel. See optimParallel for documentation of valid arguments.		

#### **Details**

The purpose of this function factory is to return an mle function with unified arguments. The returned function performs the same task as for example spam::mle(), but simplifies the process in two ways: The returned function detects whether the Gaussian process is a zero-mean process through the input argument X and whether methods from the **spam** package should be used based on the type of input argument distmat, and autonomously chooses appropriate methods to compute the neg2loglikelihood. Hence the user does not need to choose a specialized method themselves.

### Value

A function of the form function(y, X = data.frame(), distmat, beta0 = NULL, init\_parameters, theta\_llim, theta\_ulim) which returns the output of optim or optimParallel if optimParallel.args was specified.

neg2loglikDiagFactory

## Author(s)

Thomas Caspar Fischer

## References

Hadley Wickham (2015) Advanced R, CRC Press.

#### See Also

optim, optimParallel, covarianceFactory, choleskyFactory and optimFactory

## **Examples**

```
set.seed(57)
n <- 50
range <- 0.4
theta <- c(range, 1, 1, 0, 0)
locs <- data.frame(x = runif(n), y = runif(n))</pre>
dmat <- as.matrix(dist(locs))</pre>
Sigma <- cov.wendland(h = dmat, theta = theta)</pre>
y <- c(spam::rmvnorm(1, Sigma = Sigma))</pre>
init_parameters \langle c(0.7, 2, 0, 2, 2) \rangle
lower_constraints <- c(0.1, 0.1, 0, 0, 0)
upper_constraints <- c(sqrt(2), 2, 2, 2, 2)
mleFunction <- mleFactory(covariance = cov.wendland)</pre>
mle_result1 <- mleFunction(y = y, distmat = dmat,</pre>
                        init_parameters = init_parameters, theta_llim = lower_constraints,
                             theta_ulim = upper_constraints)
mleFunctionDM <- mleFactory(covariance = cov.wendland,</pre>
                              cov.args = list(fixed_range_value = range))
mle_result2 <- mleFunctionDM(y = y, X = data.frame(), distmat = dmat,</pre>
                               init_parameters = init_parameters[-1],
                               theta_llim = lower_constraints[-1],
                               theta_ulim = upper_constraints[-1])
```

neg2loglikDiagFactory Diagnostics for arbitrarily specified, likelihood-based Gaussian process models

## **Description**

A helper function for rapidly exploring the parameter space around the maximum likelihood estimate

## Usage

```
neg2loglikDiagFactory(y, X = data.frame(), distmat, covariance, ...)
```

## **Arguments**

у	Dependent variable
X	Optional design matrix with covariates
distmat	Distance matrix. Can be provided either as a dense matrix or spam object.
covariance	Covariance function.
	Other arguments to be passed on.

#### **Details**

theta\_list Named list of vectors with parameters to be passed to covariance.
cov.args\_list (default = list()) Named list of vectors with arguments to be passed to covariance
chol.args\_list (default = list()) Named list of vectors with arguments to be passed to choleskyFactory.

#### Value

Returns a function of the form function(theta\_list, cov.args\_list = list(), chol.args\_list = list()) which returns a data.frame containing the neg2loglikelihood at all permutations of the provided arguments.

## Note

The function manufactured by neg2loglikDiagFactory in principle also accepts covariance functions generated using covarianceFactory. However, the function is not yet compatible with the arguments fixed\_range\_value and fixed\_nugget\_value. For now, these should be left at default when using covarianceFactory.

#### Author(s)

Thomas Caspar Fischer

## **Examples**

```
set.seed(63)
n <- 50
range <- 0.7
theta <- c(range, 1, 1, 0, 0)

locs <- data.frame(x = runif(n), y = runif(n))
dmat <- as.matrix(dist(locs))
Sigma <- cov.wendland(h = dmat, theta = theta)
y <- c(spam::rmvnorm(1, Sigma = Sigma))

neg2loglikIterator <- neg2loglikDiagFactory(y = y, distmat = dmat, covariance = cov.wendland)</pre>
```

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```
theta_list <- list(range = 0.5, sill = 1, kappa = 0, mu = c(0, 0.25, 0.5),
  nugget = 0)
cov.args_list <- list(numint.abstol = c(1e-1, 1e-3, 1e-6), numint.reltol = c(1e-3))
results <- neg2loglikIterator(theta_list, cov.args_list = cov.args_list)</pre>
```

neg2loglikFactory Function Factory for neg2loglikelihood with Unified Input Arguments

## **Description**

A function factory which generates a function of the form function(parameters) which returns the neg2loglikelihood.

## Usage

```
neg2loglikFactory(y, X, distmat, covariance = NULL, cov.args = list(),
  chol.args = list(), Rstruct = NULL, covarianceFunction = NULL,
  choleskyFunction = NULL)
```

## **Arguments**

Numeric vector. Dependent variable. У Χ Optional data.frame containing covariates. distmat Distance matrix, either a numeric matrix or a spam object. A function which takes as input an object containing distances (h), a vector of covariance parameters (theta), and a list of optional settings (cov.args). A list of optional settings for a covariance function. cov.args chol.args A list of optional settings for a cholesky function. Rstruct A 'spam.chol.NgPeyton' object which represents the sparsity structure. covarianceFunction A function returned by covarianceFactory(). choleskyFunction A function returned by choleskyFactory().

#### Details

This function factory returns a function of the form function(parameters) which computes the neg2loglikelihood for given input parameters. The purpose of this is to reduce the number of arguments that need to be specified by the user in a call to optim, or optimParallel. Furthermore, the function detects whether the input distmat is a spam object, and autonomously selects the appropriate method for computing the neg2loglikelihood.

The function is intended to be called from within mleFactory, but is also exported by NAMES-PACE for users wishing to make use of the function. There are two distinct strategies available for using the function.

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**Option 1**: the user may specify covariance, cov.args, chol.args, and Rstruct in the call. This syntax is more in line with the corresponding functions found in the **spam** package, yet still allows passing arguments for customizing the behaviour of the cholesky decomposition.

**Option 2**: the user may instead specify covarianceFunction and choleskyFunction, obtained from calls to covarianceFactory and choleskyFactory, respectively.

In both cases, the arguments y, X, and distmat are required input. Note that the two options are equivalent, apart from the second option allowing for more concise code.

#### Value

Returns function of the form function(parameters).

## Author(s)

Thomas Caspar Fischer

#### References

Hadley Wickham (2015) Advanced R, CRC Press.

#### See Also

covarianceFactory and choleskyFactory

## **Examples**

```
set.seed(63)
n <- 50
range <- 0.7
theta <- c(range, 1, 1, 0, 0)
locs <- data.frame(x = runif(n), y = runif(n))</pre>
dmat <- as.matrix(dist(locs))</pre>
Sigma <- cov.wendland(h = dmat, theta = theta)</pre>
y <- c(spam::rmvnorm(1, Sigma = Sigma))</pre>
X <- data.frame()</pre>
neg2loglikFun <- neg2loglikFactory(y = y, X = X, distmat = dmat,</pre>
  covariance = cov.wendland, cov.args = list(), chol.args = list())
result1 <- neg2loglikFun(theta)</pre>
covarianceFun <- covarianceFactory(cov.wendland, cov.args = list())</pre>
choleskyFun <- choleskyFactory(chol.args = list())</pre>
neg2loglikFun <- neg2loglikFactory(y = y, X = X, distmat = dmat,</pre>
  covarianceFunction = covarianceFun, choleskyFunction = choleskyFun)
result2 <- neg2loglikFun(theta)</pre>
```

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optimFactory

Function Factory for Optimization function with Unified Arguments

## **Description**

A function factory which returns a function with unified input arguments, and provides compatibility with the package **optimParallel**.

## Usage

```
optimFactory(optim.args = list(), hessian = FALSE, optimParallel.args = list())
```

## Arguments

optim.args A named list of optional settings for optim. See optim for documentation of

valid arguments.

hessian A logical which specifies whether the hessian matrix is to be returned with the

output.

optimParallel.args

A named list which is passed to optimParallel from the optimParallel pack-

age. See details.

## **Details**

The function factory optimFactory() returns a function of the form function(par, fn, gr = NULL, ..., lower, upper). It is intended to replace calls to optim or optimParallel by wrapping both functions. By default, it returns a function that corresponds to optim with default arguments.

To use optimParallel, users may specify the following arguments in optimParallel.args:

num\_cores (default = NULL) The number of cores to use during numerical optimization. Is NULL
 by default, which corresponds to using stats::optim. When num\_cores is a numeric value,
 the actual number of cores is set to min(detectCores()-1, num\_cores) to avoid accidentally
 overloading the user's system.

**forward (default =** FALSE) A logical value which controls whether optimParallel should use central difference approximation of the gradient (FALSE) or forward difference approximation (TRUE).

**loginfo** (**default** = FALSE) A logical value which controls whether optimParallel should return additional information about the optimization process. See optimParallel.

#### Value

A function of the form function(par, fn, gr = NULL, ..., lower, upper) which returns the output obtained from calls to optim or optimParallel

## Author(s)

Thomas Caspar Fischer

## References

Hadley Wickham (2015) *Advanced R*, CRC Press. Florian Gerber and Reinhard Furrer (2019) optimParallel: An R package providing a parallel version of the L-BFGS-B optimization method, *The R Journal*, **11**(1), 352–358

#### See Also

```
optim and optimParallel
```

## **Examples**

```
library(GeneralizedWendland)
library(optimParallel)
set.seed(43)
n <- 50
range <- 0.4
dist_max <- 2
theta <- c(range, 1, 1, 0, 0)
locs <- data.frame(x = runif(n, 0, sqrt(dist_max)),</pre>
                   y = runif(n, 0, sqrt(dist_max)))
dmat <- spam::nearest.dist(locs, locs, delta = dist_max)</pre>
Sigma <- cov.wendland(h = dmat, theta = theta)
y <- c(spam::rmvnorm(1, Sigma = Sigma))
init_parameters <- c(0.7, 2, 0, 2, 2)
lower_constraints <- c(0.1, 0.1, 0, 0, 0)
upper_constraints <- c(sqrt(2), 2, 2, 2, 2)
mleFunction <- mleFactory(covariance = cov.wendland)</pre>
(mle_result <- mleFunction(y = y, distmat = dmat, init_parameters = init_parameters,</pre>
                        theta_llim = lower_constraints, theta_ulim = upper_constraints))
mleFunctionPar <- mleFactory(covariance = cov.wendland, optimParallel.args = list(num_cores = 2))</pre>
(mle_result_par <- mleFunctionPar(y = y, distmat = dmat, init_parameters = init_parameters,</pre>
                        theta_llim = lower_constraints, theta_ulim = upper_constraints))
```

Rcpp\_Wendland-class Class "Rcpp\_Wendland"

## Description

Rcpp class which serves as an interface to the C++ implementation of the generalized Wendland covariance function.

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#### **Details**

Parts of the covariance function require C and C++ dependencies. This Rcpp class serves as an interface to these dependencies.

#### Methods

## **Constructor:**

Constructor wend <- new("Rcpp\_Wendland"): Creates an instance of the Rcpp\_Wendland class.

## **Get/Set methods:**

**setParameters** wend\$setParameters(range, sill, kappa, mu, nugget): Set Parameters **setEpsTol** wend\$setEpsTol(eps): set numeric precision.

## **Integration options:**

setIntegratorQNG wend\$setIntegrator(abstol, reltol, intervals=0, qag\_key=0)

## **Interpolation options:**

setInterpolator wend\$setInterpolatorLinear(num\_points, interp\_type=0)

## **Computation:**

compute wend\$compute(d): Compute for single value.

computeVector wend\$computeVector(d): Compute for numeric vector.

computeMatrix wend\$computeMatrix(d): Compute for numeric matrix.

computeMSparse wend\$computeMSparse(d): Compute for dgCMatrix from Matrix.

computeSpam wend\$computeSpam(index, values): Compute for spam object, turned into
triplet form using spam::triplet.

## Author(s)

Thomas Caspar Fischer

#### References

Dirk Eddelbuettel (2013) Seamless R and C++ Integration with Rcpp. Springer, New York

## See Also

cov.wendland

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