Package 'rlibkriging'

September 25, 2026

Type Package

Title Kriging Models using the 'libKriging' Library

Version 1.2-3

Date 2026-09-24

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Description Interface to 'libKriging' 'C++' library <https://github.com/libKriging> that should provide most standard Kriging / Gaussian process regression features
(like in 'DiceKriging', 'kergp' or 'RobustGaSP' packages).
'libKriging' relies on Armadillo linear algebra library (Apache 2 license) by Conrad Sanderson, 'lbfgsb_cpp' is a 'C++' port around by Pascal Have of 'lbfgsb' library (BSD-3 license) by Ciyou Zhu, Richard Byrd, Jorge Nocedal and Jose Luis Morales used for hyperparameters optimization.

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Encoding UTF-8

LinkingTo Rcpp, RcppArmadillo

Depends R (>= 4.2)

Imports Rcpp (>= 1.0.12), methods, utils, DiceKriging

Suggests testthat, foreach, roxygen2, RobustGaSP

SystemRequirements GNU make, cmake (>= 3.2.0), gcc

URL https://github.com/libKriging

Config/roxygen2/version 8.1.0

NeedsCompilation yes

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Repository CRAN

Date/Publication 2026-09-25 07:20:10 UTC

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`activation` *Get activation function name*

Description

Get activation function name

Usage

```
activation(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

`activation.MLPKriging` *Get activation function for an MLPKriging model*

Description

Get activation function for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
activation(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

as.km *Coerce an Object into a* km *Object*

Description

Coerce an object into an object with S4 class "km" from the **DiceKriging** package.

Usage

```
as.km(x, ...)
```

Arguments

x	Object to be coerced.
...	Further arguments for methods.

Details

Such a coercion is typically used to compare the performance of the methods implemented in the current **rlibkriging** package to those which are available in the **DiceKriging** package.

Value

An object with S4 class "km".

as.km.Kriging *Coerce a* Kriging *object into the* "km" *class of the* **DiceKriging** *package.*

Description

Coerce a Kriging object into the "km" class of the **DiceKriging** package.

Usage

```
## S3 method for class 'Kriging'
as.km(x, .call = NULL, ...)
```

Arguments

x	An object with S3 class "Kriging".
.call	Force the call slot to be filled in the returned km object.
...	Not used.

Value

An object of having the S4 class "KM" which extends the "km" class of the **DiceKriging** package and contains an extra Kriging slot.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, "matern3_2")
print(k)

k_km <- as.km(k)
print(k_km)
```

---

as.list.Kriging *Coerce a* Kriging *Object into a List*

Description

Coerce a Kriging Object into a List

Usage

```
## S3 method for class 'Kriging'
as.list(x, ...)
```

Arguments

x	An object with class "Kriging".
...	Ignored

Value

A list with its elements copying the content of the Kriging object fields: kernel, optim, objective, theta (vector of ranges), sigma2 (variance), X, centerX, scaleX, y, centerY, scaleY, regmodel, F, T, M, z, beta.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x ) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2")

l <- as.list(k)
cat(paste0(names(l), " =" , l, collapse = "\n"))
```

---

beta *Get trend coefficients beta*

Description

Get trend coefficients beta

Usage

```
beta(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

---

beta.MLPKriging *Get trend coefficients beta for an MLPKriging model*

Description

Get trend coefficients beta for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
beta(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

beta.WarpKriging *Get trend coefficients beta for a WarpKriging model*

Description

Get trend coefficients beta for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
beta(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

centerX *Get input centering vector*

Description

Get input centering vector

Usage

```
centerX(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

centerX.MLPKriging *Get input centering vector for an MLPKriging model*

Description

Get input centering vector for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
centerX(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

centerX.WarpKriging *Get input centering vector for a WarpKriging model*

Description

Get input centering vector for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
centerX(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

centerY *Get output centering value*

Description

Get output centering value

Usage

```
centerY(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

centerY.MLPKriging *Get output centering value for an MLPKriging model*

Description

Get output centering value for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
centerY(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

centerY.WarpKriging *Get output centering value for a WarpKriging model*

Description

Get output centering value for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
centerY(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

classKriging *Shortcut to provide functions to the S3 class "Kriging"*

Description

Shortcut to provide functions to the S3 class "Kriging"

Usage

```
classKriging(nk)
```

Arguments

nk	A pointer to a C++ object of class "Kriging"

Value

An object of class "Kriging" with methods to access and manipulate the data

classMLPKriging *Shortcut to provide functions to the S3 class "MLPKriging"*

Description

Shortcut to provide functions to the S3 class "MLPKriging"

Usage

```
classMLPKriging(obj)
```

Arguments

obj	A list with a ptr element pointing to a C++ MLPKriging object

Value

An object of class "MLPKriging" with methods accessible via $

classNestedKriging *Shortcut to provide functions to the S3 class "NestedKriging"*

Description

Shortcut to provide functions to the S3 class "NestedKriging"

Usage

```
classNestedKriging(nk)
```

Arguments

nk	A pointer to a C++ object of class "NestedKriging"

Value

An object of class "NestedKriging" with methods to access and manipulate the data

classWarpKriging *Shortcut to provide functions to the S3 class "WarpKriging"*

Description

Shortcut to provide functions to the S3 class "WarpKriging"

Usage

```
classWarpKriging(obj)
```

Arguments

obj	A list with a ptr element pointing to a C++ WarpKriging object

Value

An object of class "WarpKriging" with methods accessible via $

copy *Duplicate object.*

Description

Duplicate a model given in object.

Usage

```
copy(object, ...)
```

Arguments

object	An object representing a fitted model.
...	Ignored.

Value

The copied object.

copy.Kriging *Duplicate a Kriging Model*

Description

Duplicate a Kriging Model

Usage

```
## S3 method for class 'Kriging'
copy(object, ...)
```

Arguments

object	An S3 Kriging object.
...	Not used.

Value

The copy of object.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective="LMP")
print(k)

print(copy(k))
```

copy.MLPKriging *Deep copy of MLPKriging model*

Description

Deep copy of MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
copy(object, ...)
```

Arguments

object	MLPKriging object
...	ignored

Value

a new independent MLPKriging object

`copy.WarpKriging` *Deep copy of WarpKriging model*

Description

Deep copy of WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
copy(object, ...)
```

Arguments

object	WarpKriging object
...	ignored

Value

a new independent WarpKriging object

covMat *covariance function*

Description

Compute the covariance matrix of a model given in `object`, between given set of points.

Usage

```
covMat(object, ...)
```

Arguments

`object`	An object representing a fitted model.
`...`	Further arguments of function (eg. points, range).

Value

The covariance matrix.

covMat.Kriging *Compute Covariance Matrix of Kriging Model*

Description

Compute Covariance Matrix of Kriging Model

Usage

```
## S3 method for class 'Kriging'
covMat(object, x1, x2, ...)
```

Arguments

`object`	An S3 Kriging object.
`x1`	Numeric matrix of input points.
`x2`	Numeric matrix of input points.
`...`	Not used.

Value

A matrix of the covariance matrix of the Kriging model.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "gauss")

x1 = runif(10)
x2 = runif(10)

covMat(k, x1, x2)
```

---

covMat.WarpKriging *Covariance matrix between two sets of points (warped kernel)*

Description

Covariance matrix between two sets of points (warped kernel)

Usage

```
## S3 method for class 'WarpKriging'
covMat(object, X1, X2, ...)
```

Arguments

object	A WarpKriging model object.
X1	numeric matrix (n1 x d) of input points.
X2	numeric matrix (n2 x d) of input points.
...	Unused.

Value

the n1 x n2 covariance matrix $\sigma^2 k(\Phi(X1), \Phi(X2))$.

`feature_dim` *Get feature dimensionality (d_out)*

Description

Get feature dimensionality (d_out)

Usage

```
feature_dim(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

`feature_dim.MLPKriging` *Get feature dimensionality for an MLPKriging model*

Description

Get feature dimensionality for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
feature_dim(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

feature_dim.WarpKriging *Get feature dimensionality of warped space*

Description

Get feature dimensionality of warped space

Usage

```
## S3 method for class 'WarpKriging'
feature_dim(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

fit *Fit model on data.*

Description

Fit a model given in object.

Usage

```
fit(object, ...)
```

Arguments

object	An object representing a fitted model.
...	Further arguments of function

Value

No return value. Kriging object argument is modified.

`fit.Kriging` *Fit* `Kriging` *object on given data.*

Description

The hyper-parameters (variance and vector of correlation ranges) are estimated thanks to the optimization of a criterion given by `objective`, using the method given in `optim`.

Usage

```
## S3 method for class 'Kriging'
fit(
  object,
  y,
  X,
  regmodel = c("constant", "linear", "interactive", "quadratic", "none"),
  normalize = FALSE,
  optim = c("BFGS", "none"),
  objective = c("LL", "LOO", "LMP"),
  parameters = NULL,
  noise = NULL,
  ...
)
```

Arguments

`object`	S3 Kriging object.
`y`	Numeric vector of response values.
`X`	Numeric matrix of input design.
`regmodel`	Universal Kriging linear trend: `"constant"`, `"linear"`, `"interactive"`, `"quadratic"`.
`normalize`	Logical. If `TRUE` both the input matrix `X` and the response `y` in normalized to take values in the interval $[0, 1]$.
`optim`	Character giving the Optimization method used to fit hyper-parameters. Possible values are: `"BFGS"` and `"none"`, the later simply keeping the values given in `parameters`. The method `"BFGS"` uses the gradient of the objective (note that `"BFGS10"` means 10 multi-start of BFGS).
`objective`	Character giving the objective function to optimize. Possible values are: `"LL"` for the Log-Likelihood, `"LOO"` for the Leave-One-Out sum of squares, `"LMP"` for the Log-Marginal Posterior, `"LLVecchia"` or `"LLVecchia(m)"` for the Vecchia approximated log-likelihood (see `Kriging`), and `"LLNystrom"` or `"LLNystrom(k)"` for the Nystrom approximated log-likelihood (see `Kriging`).
`parameters`	Initial values for the hyper-parameters. When provided this must be named list with elements `"sigma2"` and `"theta"` containing the initial value(s) for the variance and for the range parameters. If `theta` is a matrix with more than one row, each row is used as a starting point for optimization.

noise	Either a numeric vector of per-observation noise variances, or "nugget" to estimate a homogeneous nugget, or NULL (default) for noise-free interpolation.
...	Ignored.

Value

No return value. Kriging object argument is modified.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
plot(f)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)
points(X, y, col = "blue", pch = 16)

k <- Kriging("matern3_2")
print(k)

fit(k,y,X)
print(k)
```

---

fit.MLPKriging *Fit an MLPKriging model to data*

Description

(Re-)fit an already-constructed MLPKriging object on new data. The MLP architecture and kernel are kept from construction.

Usage

```
## S3 method for class 'MLPKriging'
fit(
  object,
  y,
  X,
  regmodel = "constant",
  normalize = FALSE,
  optim = "BFGS+Adam",
  objective = "LL",
  parameters = NULL,
  ...
)
```

Arguments

object	MLPKriging object
y	numeric vector of observations (n)
X	numeric matrix of inputs (n x d)
regmodel	trend: "constant", "linear", "quadratic"
normalize	logical; normalise inputs?
optim	optimiser
objective	"LL" (log-likelihood)
parameters	optional named list of tuning parameters
...	ignored

Value

No return value. MLPKriging object argument is modified.

---

fit.WarpKriging *Fit a WarpKriging model to data*

Description

(Re-)fit an already-constructed WarpKriging object on new data. The warping specification and kernel are kept from construction.

Usage

```
## S3 method for class 'WarpKriging'
fit(
  object,
  y,
  X,
  regmodel = "constant",
  normalize = FALSE,
  optim = "BFGS+Adam",
  objective = "LL",
  parameters = NULL,
  noise = NULL,
  ...
)
```

Arguments

object	WarpKriging object (created with the constructor or an empty-kernel call)
y	numeric vector of observations (n)
X	numeric matrix of inputs (n x d)
regmodel	trend: "constant", "linear", "quadratic"
normalize	logical; normalise continuous inputs?
optim	optimiser; "none" keeps the values from parameters
objective	"LL" (log-likelihood)
parameters	optional named list of initial hyper-parameter values (theta, warp_params, noise) and/or optimiser knobs (adam_lr, max_iter_adam, max_iter_bfgs). See WarpKriging.
noise	numeric vector of per-observation noise variances (length n), or NULL (default) for noise-free interpolation.
...	ignored

Value

No return value. WarpKriging object argument is modified.

F_ *Get trend matrix F*

Description

Get trend matrix F

Usage

```
F_(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

F_.MLPKriging *Get trend matrix F for an MLPKriging model*

Description

Get trend matrix F for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
F_(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

F_.WarpKriging *Get trend matrix F for a WarpKriging model*

Description

Get trend matrix F for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
F_(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

`hidden_dims` *Get hidden layer sizes*

Description

Get hidden layer sizes

Usage

```
hidden_dims(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

`hidden_dims.MLPKriging` *Get hidden layer sizes for an MLPKriging model*

Description

Get hidden layer sizes for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
hidden_dims(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

is_fitted *Check if the model has been fitted*

Description

Check if the model has been fitted

Usage

```
is_fitted(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

is_fitted.MLPKriging *Check whether an MLPKriging model is fitted*

Description

Check whether an MLPKriging model is fitted

Usage

```
## S3 method for class 'MLPKriging'
is_fitted(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

is_fitted.WarpKriging *Check whether a WarpKriging model is fitted*

Description

Check whether a WarpKriging model is fitted

Usage

```
## S3 method for class 'WarpKriging'
is_fitted(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

kernel *Get kernel name*

Description

Get kernel name

Usage

```
kernel(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

Value

Character scalar naming the covariance kernel.

kernel.WarpKriging *Get kernel name*

Description

Get kernel name

Usage

```
## S3 method for class 'WarpKriging'
kernel(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

KM *Create an* KM *Object*

Description

Create an object of S4 class "KM" similar to a km object in the **DiceKriging** package.

Usage

```
KM(
  formula = ~1,
  design,
  response,
  covtype = c("matern5_2", "gauss", "matern3_2", "exp"),
  coef.trend = NULL,
  coef.cov = NULL,
  coef.var = NULL,
  nugget = NULL,
  nugget.estim = FALSE,
  noise.var = NULL,
  estim.method = c("MLE", "LOO"),
  penalty = NULL,
  optim.method = "BFGS",
  lower = NULL,
  upper = NULL,
  parinit = NULL,
  multistart = 1,
  control = NULL,
```

```
  gr = TRUE,
  iso = FALSE,
  scaling = FALSE,
  knots = NULL,
  kernel = NULL,
  ...
)
```

Arguments

formula	R formula object to setup the linear trend in Universal Kriging. Supports ~ 1, ~. and ~ .^2.
design	Data frame. The design of experiments.
response	Vector of output values.
covtype	Covariance structure. For now all the kernels are tensor product kernels.
coef.trend	Optional value for a fixed vector of trend coefficients. If given, no optimization is done.
coef.cov	Optional value for a fixed correlation range value. If given, no optimization is done.
coef.var	Optional value for a fixed variance. If given, no optimization is done.
nugget	Ignored (kept for DiceKriging API compatibility).
nugget.estim	Logical. If TRUE, fit a nugget effect.
noise.var	Numeric vector of known per-point noise variances.
estim.method	Estimation criterion. "MLE" for Maximum-Likelihood or "LOO" for Leave-One-Out cross-validation.
penalty	Not implemented yet.
optim.method	Optimization algorithm used in the optimization of the objective given in estim.method. Supports "BFGS".
lower, upper	Not implemented yet.
parinit	Initial values for the correlation ranges which will be optimized using optim.method.
multistart, control, gr, iso	Not implemented yet.
scaling, knots, kernel	Not implemented yet.
...	Ignored.

Details

The class "KM" extends the "km" class of the **DiceKriging** package, hence has all slots of "km". It also has an extra slot "Kriging" slot which contains a copy of the original object.

Value

A KM object. See **Details**.

Author(s)

Yann Richet <yann.richet@asnr.fr>

See Also

km in the **DiceKriging** package for more details on the slots.

Examples

```
# a 16-points factorial design, and the corresponding response
d <- 2; n <- 16
design.fact <- as.matrix(expand.grid(x1 = seq(0, 1, length = 4),
                                     x2 = seq(0, 1, length = 4)))
y <- apply(design.fact, 1, DiceKriging::branin)

# Using `km` from DiceKriging and a similar `KM` object
# kriging model 1 : matern5_2 covariance structure, no trend, no nugget effect
km1 <- DiceKriging::km(design = design.fact, response = y, covtype = "gauss",
                       parinit = c(.5, 1), control = list(trace = FALSE))
KM1 <- KM(design = design.fact, response = y, covtype = "gauss",
          parinit = c(.5, 1))
```

KM-class *S4 class for Kriging Models Extending the "km" Class*

Description

This class is intended to be used either by using its own dedicated S4 methods or by using the S4 methods inherited from the "km" class of the **libKriging** package.

Slots

`d,n,X,y,p,F` Number of (numeric) inputs, number of observations, design matrix, response vector, number of trend variables, trend matrix.

`trend.formula,trend.coef` Formula used for the trend, vector $\hat{\boldsymbol{\beta}}$ of estimated (or fixed) trend coefficients with length p.

`covariance` A S4 object with class "covTensorProduct" representing a covariance kernel.

`noise.flag,noise.var` Logical flag and numeric value for an optional noise term.

`known.param` A character code indicating what parameters are known.

`lower,upper` Bounds on the correlation range parameters.

`method,penalty,optim.method,control,gr,parinit` Objects defining the estimation criterion, the optimization.

`T,M,z` Auxiliary variables (matrices and vectors) that can be used in several computations.

`case` The possible concentration (a.k.a. profiling) of the likelihood.

`param.estim` Logical. Is an estimation used?

`Kriging` A copy of the `Kriging` object used to create the current `KM` object.

Author(s)

Yann Richet <yann.richet@asnr.fr>

See Also

km-class in the **DiceKriging** package. The creator KM.

`Kriging` *Create an object with S3 class* `"Kriging"` *using the* **libKriging** *library.*

Description

The hyper-parameters (variance and vector of correlation ranges) are estimated thanks to the optimization of a criterion given by `objective`, using the method given in `optim`.

Usage

```
Kriging(
  y = NULL,
  X = NULL,
  kernel = NULL,
  regmodel = c("constant", "linear", "interactive", "quadratic", "none"),
  normalize = FALSE,
  optim = c("BFGS", "none"),
  objective = c("LL", "LOO", "LMP"),
  parameters = NULL,
  noise = NULL
)
```

Arguments

`y`	Numeric vector of response values.
`X`	Numeric matrix of input design.
`kernel`	Character defining the covariance model: `"exp"`, `"gauss"`, `"matern3_2"`, `"matern5_2"`.
`regmodel`	Universal Kriging linear trend: `"constant"`, `"linear"`, `"interactive"`, `"quadratic"`.
`normalize`	Logical. If `TRUE` both the input matrix `X` and the response `y` in normalized to take values in the interval $[0, 1]$.
`optim`	Character giving the Optimization method used to fit hyper-parameters. Possible values are: `"BFGS"` and `"none"`, the later simply keeping the values given in `parameters`. The method `"BFGS"` uses the gradient of the objective (note that `"BFGS10"` means 10 multi-start of BFGS).

objective — Character giving the objective function to optimize. Possible values are: "LL" for the Log-Likelihood, "LOO" for the Leave-One-Out sum of squares, "LMP" for the Log-Marginal Posterior, "LLVecchia" or "LLVecchia(m)" for the Vecchia approximated log-likelihood with m conditioning neighbors (default 30): each evaluation costs O(n m^3) instead of O(n^3), recommended for large designs in low dimension; and "LLNystrom" or "LLNystrom(k)" for the Nystrom (global low-rank) approximated log-likelihood with rank k (default 50): each evaluation costs O(n k^2) instead of O(n^3), also recommended for large designs.

parameters — Initial values for the hyper-parameters. When provided this must be named list with elements "sigma2" and "theta" containing the initial value(s) for the variance and for the range parameters. If theta is a matrix with more than one row, each row is used as a starting point for optimization.

noise — Either a numeric vector of per-observation noise variances, or "nugget" to estimate a homogeneous nugget, or NULL (default) for noise-free interpolation.

Value

An object with S3 class "Kriging". Should be used with its predict, simulate, update methods.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)
## fit and print
k <- Kriging(y, X, kernel = "matern3_2")
print(k)

x <- as.matrix(seq(from = 0, to = 1, length.out = 101))
p <- predict(k, x = x, return_stdev = TRUE, return_cov = FALSE)

plot(f)
points(X, y)
lines(x, p$mean, col = "blue")
polygon(c(x, rev(x)), c(p$mean - 2 * p$stdev, rev(p$mean + 2 * p$stdev)),
border = NA, col = rgb(0, 0, 1, 0.2))

s <- simulate(k, nsim = 10, seed = 123, x = x)

matlines(x, s, col = rgb(0, 0, 1, 0.2), type = "l", lty = 1)
```

leaveOneOut *Compute Leave-One-Out*

Description

Compute the leave-One-Out error of a model given in `object`.

Usage

```
leaveOneOut(object, ...)
```

Arguments

`object`	An object representing a fitted model.
`...`	Ignored.

Value

The Leave-One-Out sum of squares.

leaveOneOut.Kriging *Get leaveOneOut of Kriging Model*

Description

Get leaveOneOut of Kriging Model

Usage

```
## S3 method for class 'Kriging'
leaveOneOut(object, ...)
```

Arguments

`object`	An S3 Kriging object.
`...`	Not used.

Value

The leaveOneOut computed for fitted $\boldsymbol{theta}$.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective="LOO")
print(k)

leaveOneOut(k)
```

---

leaveOneOutFun *Leave-One-Out function*

Description

Compute the leave-One-Out error of a model given in `object`, at a different value of the parameters.

Usage

```
leaveOneOutFun(object, ...)
```

Arguments

`object`	An object representing a fitted model.
`...`	Further arguments of function (eg. range).

Value

The Leave-One-Out sum of squares.

---

leaveOneOutFun.Kriging *Compute Leave-One-Out (LOO) error for an object with S3 class "Kriging" representing a kriging model.*

Description

The returned value is the sum of squares $\sum_{i=1}^{n}[y_i - \hat{y}_{i,(-i)}]^2$ where $\hat{y}_{i,(-i)}$ is the prediction of y_i based on the the observations y_j with $j \neq i$.

Usage

```
## S3 method for class 'Kriging'
leaveOneOutFun(object, theta, return_grad = FALSE, bench = FALSE, ...)
```

Arguments

object	A Kriging object.
theta	A numeric vector of range parameters at which the LOO will be evaluated.
return_grad	Logical. Should the gradient (w.r.t. theta) be returned?
bench	Logical. Should the function display benchmarking output
...	Not used.

Value

The leave-One-Out value computed for the given vector $\boldsymbol{\theta}$ of correlation ranges.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective = "LOO", optim="BFGS")
print(k)

loo <-  function(theta) leaveOneOutFun(k, theta)$leaveOneOut
t <-  seq(from = 0.001, to = 2, length.out = 101)
plot(t, loo(t), type = "l")
abline(v = k$theta(), col = "blue")
```

---

leaveOneOutVec *Leave-One-Out vector*

Description

Compute the leave-One-Out vector error of a model given in object, at a different value of the parameters.

Usage

```
leaveOneOutVec(object, ...)
```

Arguments

object	An object representing a fitted model.
...	Further arguments of function (eg. range).

Value

The Leave-One-Out errors (mean and stdev) for each conditional point.

`leaveOneOutVec.Kriging` *Compute Leave-One-Out (LOO) vector error for an object with S3 class* "Kriging" *representing a kriging model.*

Description

The returned value is the mean and stdev of $\hat{y}_{i,(-i)}$, the prediction of y_i based on the the observations y_j with $j \neq i$.

Usage

```
## S3 method for class 'Kriging'
leaveOneOutVec(object, theta, ...)
```

Arguments

`object`	A `Kriging` object.
`theta`	A numeric vector of range parameters at which the LOO will be evaluated.
`...`	Not used.

Value

The leave-One-Out vector computed for the given vector $\boldsymbol{\theta}$ of correlation ranges.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(c(0.0, 0.25, 0.5, 0.75, 1.0))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2")
print(k)

x <- as.matrix(seq(0, 1, , 101))
p <- predict(k, x, TRUE, FALSE)

plot(f)
points(X, y)
lines(x, p$mean, col = 'blue')
```

```
polygon(c(x, rev(x)), c(p$mean - 2 * p$stdev, rev(p$mean + 2 * p$stdev)),
        border = NA, col = rgb(0, 0, 1, 0.2))

# Compute leave-one-out (no range re-estimate) on 2nd point
X_no2 = X[-2,,drop=FALSE]
y_no2 = f(X_no2)
k_no2 = Kriging(y_no2, X_no2, "matern3_2", optim = "none", parameters = list(theta = k$theta()))
print(k_no2)

p_no2 <- predict(k_no2, x, TRUE, FALSE)
lines(x, p_no2$mean, col = 'red')
polygon(c(x, rev(x)), c(p_no2$mean - 2 * p_no2$stdev, rev(p_no2$mean + 2 * p_no2$stdev)),
        border = NA, col = rgb(1, 0, 0, 0.2))

# Use leaveOneOutVec to get the same
loov = k$leaveOneOutVec(matrix(k$theta()))
points(X[2],loov$mean[2],col='red')
lines(rep(X[2],2),loov$mean[2]+2*c(-loov$stdev[2],loov$stdev[2]),col='red')
```

`load` *Load any Kriging Model from a file storage. Back to base::load if not a Kriging object.*

Description

Load any Kriging Model from a file storage. Back to base::load if not a Kriging object.

Usage

```
load(filename, ...)
```

Arguments

`filename`	A file holding any Kriging object.
`...`	Arguments used by base::load.

Value

The loaded "*"Kriging object, or nothing if base::load is used (update parent environment).

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective="LMP")
print(k)

outfile = tempfile("k.json")
save(k,outfile)

print(load(outfile))
```

`load.Kriging` *Load a Kriging Model from a file storage*

Description

Load a Kriging Model from a file storage

Usage

```
load.Kriging(filename, ...)
```

Arguments

`filename`	File name to load from.
`...`	Not used.

Value

The loaded Kriging object.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective="LMP")
print(k)

outfile = tempfile("k.json")
```

```
save(k,outfile)

print(load.Kriging(outfile))
unlink(outfile)
```

`load.MLPKriging` *Load an MLPKriging model from file*

Description

Load an MLPKriging model from file

Usage

```
## S3 method for class 'MLPKriging'
load(filename, ...)
```

Arguments

`filename`	path to saved file
`...`	ignored

Value

MLPKriging object

`load.WarpKriging` *Load a WarpKriging model from file*

Description

Load a WarpKriging model from file

Usage

```
## S3 method for class 'WarpKriging'
load(filename, ...)
```

Arguments

`filename`	path to saved file
`...`	ignored

Value

WarpKriging object

logLikelihood *Compute Log-Likelihood*

Description

Compute the log-Likelihood of a model given in `object`.

Usage

```
logLikelihood(object, ...)
```

Arguments

`object`	An object representing a fitted model.
`...`	Ignored.

Value

The log-likelihood.

logLikelihood.Kriging *Get Log-Likelihood of Kriging Model*

Description

Get Log-Likelihood of Kriging Model

Usage

```
## S3 method for class 'Kriging'
logLikelihood(object, ...)
```

Arguments

`object`	An S3 Kriging object.
`...`	Not used.

Value

The log-Likelihood computed for fitted $\boldsymbol{theta}$.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective="LL")
print(k)

logLikelihood(k)
```

---

logLikelihood.WarpKriging *Log-likelihood of the fitted model*

Description

Log-likelihood of the fitted model

Usage

```
## S3 method for class 'WarpKriging'
logLikelihood(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

---

logLikelihoodFun *Log-Likelihood function*

Description

Compute the log-Likelihood of a model given in `object`, at a different value of the parameters.

Usage

```
logLikelihoodFun(object, ...)
```

Arguments

object	An object representing a fitted model.
...	Further arguments of function (eg. range).

Value

The log-likelihood.

logLikelihoodFun.Kriging *Compute Log-Likelihood of Kriging Model*

Description

Compute Log-Likelihood of Kriging Model

Usage

```
## S3 method for class 'Kriging'
logLikelihoodFun(
  object,
  theta,
  return_grad = FALSE,
  return_hess = FALSE,
  bench = FALSE,
  ...
)
```

Arguments

object	An S3 Kriging object.
theta	A numeric vector of (positive) range parameters at which the log-likelihood will be evaluated.
return_grad	Logical. Should the function return the gradient?
return_hess	Logical. Should the function return Hessian?
bench	Logical. Should the function display benchmarking output?
...	Not used.

Value

The log-Likelihood computed for given $\boldsymbol{theta}$.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2")
```

```
print(k)

ll <- function(theta) logLikelihoodFun(k, theta)$logLikelihood

t <- seq(from = 0.001, to = 2, length.out = 101)
plot(t, ll(t), type = 'l')
abline(v = k$theta(), col = "blue")
```

`logLikelihoodFun.MLPKriging` *Evaluate log-likelihood at given GP theta*

Description

Evaluate log-likelihood at given GP theta

Usage

```
## S3 method for class 'MLPKriging'
logLikelihoodFun(object, theta, return_grad = FALSE, return_hess = FALSE, ...)
```

Arguments

`object`	MLPKriging object
`theta`	range parameter vector
`return_grad`	return gradient?
`return_hess`	return hessian?
`...`	ignored

`logLikelihoodFun.WarpKriging` *Evaluate log-likelihood at given theta*

Description

Evaluate log-likelihood at given theta

Usage

```
## S3 method for class 'WarpKriging'
logLikelihoodFun(object, theta, return_grad = FALSE, return_hess = FALSE, ...)
```

Arguments

object	WarpKriging object
theta	range parameter vector
return_grad	return gradient?
return_hess	return hessian?
...	ignored

Value

list with logLikelihood and optionally gradient, hessian

---

logMargPost *Compute log-Marginal Posterior*

Description

Compute the log-Marginal Posterior of a model given in object.

Usage

```
logMargPost(object, ...)
```

Arguments

object	An object representing a fitted model.
...	Ignored.

Value

The log-marginal posterior.

---

logMargPost.Kriging *Get logMargPost of Kriging Model*

Description

Get logMargPost of Kriging Model

Usage

```
## S3 method for class 'Kriging'
logMargPost(object, ...)
```

Arguments

object	An S3 Kriging object.
...	Not used.

Value

The logMargPost computed for fitted $\boldsymbol{theta}$.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective="LMP")
print(k)

logMargPost(k)
```

---

logMargPostFun *log-Marginal Posterior function*

Description

Compute the log-Marginal Posterior of a model given in object, at a different value of the parameters.

Usage

```
logMargPostFun(object, ...)
```

Arguments

object	An object representing a fitted model.
...	Further arguments of function (eg. range).

Value

The log-marginal posterior.

logMargPostFun.Kriging *Compute the log-marginal posterior of a kriging model, using the prior XXXY.*

Description

Compute the log-marginal posterior of a kriging model, using the prior XXXY.

Usage

```
## S3 method for class 'Kriging'
logMargPostFun(object, theta, return_grad = FALSE, bench = FALSE, ...)
```

Arguments

object	S3 Kriging object.
theta	Numeric vector of correlation range parameters at which the function is to be evaluated.
return_grad	Logical. Should the function return the gradient (w.r.t theta)?
bench	Logical. Should the function display benchmarking output?
...	Not used.

Value

The value of the log-marginal posterior computed for the given vector theta.

Author(s)

Yann Richet <yann.richet@asnr.fr>

References

XXXY A reference describing the model (prior, ...)

See Also

rgasp in the RobustGaSP package.

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, "matern3_2", objective="LMP")
```

```
print(k)

lmp <- function(theta) logMargPostFun(k, theta)$logMargPost

t <- seq(from = 0.01, to = 2, length.out = 101)
plot(t, lmp(t), type = "l")
abline(v = k$theta(), col = "blue")
```

`M` *Get whitened trend matrix M*

Description

Get whitened trend matrix M

Usage

```
M(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

`M.MLPKriging` *Get whitened trend matrix M for an MLPKriging model*

Description

Get whitened trend matrix M for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
M(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

M.WarpKriging *Get whitened trend matrix M for a WarpKriging model*

Description

Get whitened trend matrix M for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
M(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

MLPKriging *Create an MLPKriging model (Deep Kernel Learning)*

Description

Kriging with a joint multi-layer perceptron applied to all inputs before the GP kernel is evaluated. The MLP weights, GP range parameters, variance and trend are jointly fitted by maximising the concentrated log-likelihood.

Usage

```
MLPKriging(
  y,
  X,
  hidden_dims,
  d_out = 2,
  activation = "selu",
  kernel = "gauss",
  regmodel = "constant",
  normalize = FALSE,
  optim = "BFGS+Adam",
  objective = "LL",
  parameters = NULL
)
```

Arguments

`y`	numeric vector of observations (n)
`X`	numeric matrix of inputs (n x d)
`hidden_dims`	integer vector of hidden layer sizes, e.g. `c(32, 16)`
`d_out`	output feature dimensionality (default 2)
`activation`	activation function: "relu", "selu", "tanh", "sigmoid", "elu"
`kernel`	covariance kernel: "gauss", "matern3_2", "matern5_2", "exp"
`regmodel`	trend: "constant", "linear", "quadratic"
`normalize`	logical; normalise inputs?
`optim`	optimiser (default "BFGS+Adam")
`objective`	"LL" (log-likelihood)
`parameters`	optional named list of tuning parameters, e.g. `list(max_iter_adam = "300", adam_lr = "0.001", max_iter_bfgs = "50")`

Value

An S3 object of class "MLPKriging".

Examples

```
X <- as.matrix(seq(0.01, 0.99, length.out = 10))
f <- function(x) 1 - 1/2 * (sin(12*x)/(1+x) + 2*cos(7*x)*x^5 + 0.7)
y <- f(X)
k <- MLPKriging(y, X, hidden_dims = c(16, 8), d_out = 2,
                activation = "selu", kernel = "gauss")
print(k)
```

`NestedKriging` *Create an object with S3 class "NestedKriging" using the* **libKriging** *library.*

Description

Divide-and-conquer Kriging for large designs: the data are partitioned in `nb_groups` groups, one `Kriging` submodel is fitted per group (then all share a common prior), and predictions are aggregated.

Usage

```
NestedKriging(
  y = NULL,
  X = NULL,
  kernel = NULL,
  nb_groups = NULL,
  aggregation = "NK",
  partition = "kmeans",
  seed = 123,
  regmodel = "constant",
  optim = "BFGS",
  objective = "LL",
  parameters = NULL,
  warping = NULL
)
```

Arguments

y	Numeric vector of response values.
X	Numeric matrix of input design.
kernel	Character defining the covariance model: "exp", "gauss", "matern3_2", "matern5_2".
nb_groups	Number of submodels (each of size ~ nrow(X)/nb_groups).
aggregation	Character: "NK" (optimal nested-kriging aggregation of Rulliere et al. 2018, default), "PoE", "gPoE", "BCM" or "rBCM".
partition	Character: "kmeans" (default) or "random".
seed	Integer seed for the partition.
regmodel	Linear trend; "NK" aggregation requires "constant".
optim	Character, hyper-parameter optimization method of the submodels: "BFGS" or "none".
objective	Character: "LL" (default), "LOO", "LMP", or "LLVecchia(m)" — the common prior is then estimated by one global Vecchia fit (O(n m^3), cross-group information).
parameters	Initial or fixed values for the hyper-parameters (named list with "sigma2", "theta", "beta").
warping	Optional character vector of per-dimension warp specs (see WarpKriging); submodels are then WarpKriging.

Value

An object with S3 class "NestedKriging", to be used with its predict method.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(X) apply(X, 1, function(x) sin(3 * x[1]) + cos(5 * x[2]))
set.seed(123)
X <- matrix(runif(2 * 400), ncol = 2)
y <- f(X)
k <- NestedKriging(y, X, kernel = "matern5_2", nb_groups = 8)
x <- matrix(runif(2 * 100), ncol = 2)
p <- predict(k, x)
```

`noise` *Get per-observation noise variances*

Description

Get per-observation noise variances

Usage

```
noise(object, ...)
```

Arguments

`object`	A WarpKriging model object.
`...`	Unused.

Value

numeric vector of per-observation noise variances, or a length-0 vector when the model was fitted noise-free.

`noise.WarpKriging` *Get per-observation noise variances for a WarpKriging model*

Description

Get per-observation noise variances for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
noise(object, ...)
```

Arguments

`object`	A WarpKriging model object.
`...`	Unused.

NoiseKM *Create a KM object with heteroscedastic noise (deprecated)*

Description

This is a thin compatibility wrapper. Use `KM(noise.var = ...)` directly instead.

Usage

```
NoiseKM(..., noise.var)
```

Arguments

`...`	Arguments passed to `KM`.
`noise.var`	Numeric vector of known per-point noise variances.

Value

A `KM` object. See `KM`.

normalize *Get normalize flag*

Description

Get normalize flag

Usage

```
normalize(object, ...)
```

Arguments

`object`	A Kriging/MLPKriging/WarpKriging model object.
`...`	Unused.

normalize.MLPKriging *Get normalize flag for an MLPKriging model*

Description

Get normalize flag for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
normalize(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

normalize.WarpKriging *Get normalize flag for a WarpKriging model*

Description

Get normalize flag for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
normalize(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

NuggetKM *Create a KM object with nugget effect (deprecated)*

Description

This is a thin compatibility wrapper. Use `KM(nugget.estim = TRUE)` directly instead.

Usage

```
NuggetKM(...)
```

Arguments

`...`	Arguments passed to `KM`.

Value

A `KM` object. See `KM`.

predict,KM-method *Prediction Method for a* `KM` *Object*

Description

Compute predictions for the response at new given input points. These conditional mean, the conditional standard deviation and confidence limits at the 95% level. Optionnally the conditional covariance can be returned as well.

Usage

```
## S4 method for signature 'KM'
predict(
  object,
  newdata,
  type = "UK",
  se.compute = TRUE,
  cov.compute = FALSE,
  light.return = TRUE,
  bias.correct = FALSE,
  checkNames = FALSE,
  ...
)
```

Arguments

object	KM object.
newdata	Matrix of "new" input points where to perform prediction.
type	character giving the kriging type. For now only "UK" is possible.
se.compute	Logical. Should the standard error be computed?
cov.compute	Logical. Should the covariance matrix between newdata points be computed?
light.return	Logical. If TRUE, no auxiliary results will be returned (such as the Cholesky root of the correlation matrix).
bias.correct	Logical. If TRUE the UK variance and covariance are .
checkNames	Logical to check the consistency of the column names between the design stored in object@X and the new one given newdata.
...	Ignored.

Details

Without a dedicated predict method for the class "KM", this method would have been inherited from the "km" class. The dedicated method is expected to run faster. A comparison can be made by coercing a KM object to a km object with as.km before calling predict.

Value

A named list. The elements are the conditional mean and standard deviation (mean and sd), the predicted trend (trend) and the confidence limits (lower95 and upper95). Optionnally, the conditional covariance matrix is returned in cov.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
## a 16-points factorial design, and the corresponding response
d <- 2; n <- 16
design.fact <- expand.grid(x1 = seq(0, 1, length = 4), x2 = seq(0, 1, length = 4))
y <- apply(design.fact, 1, DiceKriging::branin)

## library(DiceKriging)
## kriging model 1 : matern5_2 covariance structure, no trend, no nugget
## m1 <- km(design = design.fact, response = y, covtype = "gauss",
##          parinit = c(.5, 1), control = list(trace = FALSE))
KM1 <- KM(design = design.fact, response = y, covtype = "gauss",
              parinit = c(.5, 1))
Pred <- predict(KM1, newdata = matrix(.5,ncol = 2), type = "UK",
               checkNames = FALSE, light.return = TRUE)
```

predict.Kriging *Predict from a* Kriging *object.*

Description

Given "new" input points, the method compute the expectation, variance and (optionnally) the covariance of the corresponding stochastic process, conditional on the values at the input points used when fitting the model.

Usage

```
## S3 method for class 'Kriging'
predict(
  object,
  x,
  return_stdev = TRUE,
  return_cov = FALSE,
  return_deriv = FALSE,
  ...
)
```

Arguments

object	S3 Kriging object.
x	Input points where the prediction must be computed.
return_stdev	Logical. If TRUE the standard deviation is returned.
return_cov	Logical. If TRUE the covariance matrix of the predictions is returned.
return_deriv	Logical. If TRUE the derivatives of mean and sd of the predictions are returned.
...	Ignored.

Value

A list containing the element mean and possibly stdev and cov.

Note

The names of the formal arguments differ from those of the predict methods for the S4 classes "km" and "KM". The formal x corresponds to newdata, stdev corresponds to se.compute and cov to cov.compute. These names are chosen **Python** and **Octave** interfaces to **libKriging**.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
plot(f)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)
points(X, y, col = "blue", pch = 16)

k <- Kriging(y, X, "matern3_2")

x <-seq(from = 0, to = 1, length.out = 101)
p <- predict(k, x)

lines(x, p$mean, col = "blue")
polygon(c(x, rev(x)), c(p$mean - 2 * p$stdev, rev(p$mean + 2 * p$stdev)),
 border = NA, col = rgb(0, 0, 1, 0.2))
```

`predict.MLPKriging` *Predict with an MLPKriging model*

Description

Predict with an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
predict(
  object,
  x,
  return_stdev = TRUE,
  return_cov = FALSE,
  return_deriv = FALSE,
  ...
)
```

Arguments

`object`	MLPKriging object
`x`	prediction matrix (m x d)
`return_stdev`	return standard deviations?
`return_cov`	return full covariance?
`return_deriv`	return derivatives of mean and stdev wrt x?
`...`	ignored

Value

list with `mean`, optionally `stdev`, `cov`, `mean_deriv`, `stdev_deriv`

predict.NestedKriging *Predict from a* NestedKriging *object.*

Description

Predict from a NestedKriging object.

Usage

```
## S3 method for class 'NestedKriging'
predict(object, x, return_stdev = TRUE, ...)
```

Arguments

object	S3 NestedKriging object.
x	Input points (matrix) where to predict.
return_stdev	Logical, return standard deviation (default TRUE).
...	Ignored.

Value

A list with elements mean and (optionally) stdev.

predict.WarpKriging *Predict with a WarpKriging model*

Description

Predict with a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
predict(
  object,
  x,
  return_stdev = TRUE,
  return_cov = FALSE,
  return_deriv = FALSE,
  ...
)
```

Arguments

object	WarpKriging object
x	prediction matrix (m x d)
return_stdev	return standard deviations?
return_cov	return full covariance?
return_deriv	return derivatives of mean and stdev wrt x?
...	ignored

Value

list with mean, optionally stdev, cov, mean_deriv, stdev_deriv

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
X <- as.matrix(seq(0.05, 0.95, length.out = 10))
y <- f(X)

wk <- WarpKriging(y, X, warping = "kumaraswamy", kernel = "gauss", optim = "BFGS")
x <- as.matrix(seq(0, 1, length.out = 101))
p <- wk$predict(x, return_stdev = TRUE)

plot(f)
points(X, y, col = "blue", pch = 16)
lines(x, p$mean, col = "blue")
polygon(c(x, rev(x)), c(p$mean - 2 * p$stdev, rev(p$mean + 2 * p$stdev)),
        border = NA, col = rgb(0, 0, 1, 0.2))
```

---

print.Kriging *Print the content of a* Kriging *object.*

Description

Print the content of a Kriging object.

Usage

```
## S3 method for class 'Kriging'
print(x, ...)
```

Arguments

x	A (S3) Kriging Object.
...	Ignored.

Value

String of printed object.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, "matern3_2")

print(k)
## same thing
k
```

---

print.NestedKriging *Print a* NestedKriging *object.*

Description

Print a NestedKriging object.

Usage

```
## S3 method for class 'NestedKriging'
print(x, ...)
```

Arguments

x	S3 NestedKriging object.
...	Ignored.

regmodel *Get regression model type*

Description

Get regression model type

Usage

```
regmodel(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

regmodel.MLPKriging *Get regression model type for an MLPKriging model*

Description

Get regression model type for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
regmodel(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

regmodel.WarpKriging *Get regression model type for a WarpKriging model*

Description

Get regression model type for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
regmodel(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

save *Save a Kriging Model inside a file. Back to base::save if argument is not a Kriging object.*

Description

Save a Kriging Model inside a file. Back to base::save if argument is not a Kriging object.

Usage

```
save(object = NULL, filename = NULL, ...)
```

Arguments

object	An object representing a model.
filename	A file to save the object.
...	Arguments used by base::save.

Author(s)

Yann Richet <yann.richet@asnr.fr>

save.Kriging *Save a Kriging Model to a file storage*

Description

Save a Kriging Model to a file storage

Usage

```
## S3 method for class 'Kriging'
save(object, filename, ...)
```

Arguments

object	An S3 Kriging object.
filename	File name to save in.
...	Not used.

Value

The loaded Kriging object.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)

k <- Kriging(y, X, kernel = "matern3_2", objective="LMP")
print(k)

outfile = tempfile("k.json")
save(k,outfile)
unlink(outfile)
```

save.MLPKriging *Save an MLPKriging model to file*

Description

Save an MLPKriging model to file

Usage

```
## S3 method for class 'MLPKriging'
save(object, filename, ...)
```

Arguments

object	MLPKriging object
filename	path to save file
...	ignored

save.WarpKriging *Save a WarpKriging model to file*

Description

Save a WarpKriging model to file

Usage

```
## S3 method for class 'WarpKriging'
save(object, filename, ...)
```

Arguments

object	WarpKriging object
filename	path to save file
...	ignored

scaleX *Get input scaling vector*

Description

Get input scaling vector

Usage

```
scaleX(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

scaleX.MLPKriging *Get input scaling vector for an MLPKriging model*

Description

Get input scaling vector for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
scaleX(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

scaleX.WarpKriging *Get input scaling vector for a WarpKriging model*

Description

Get input scaling vector for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
scaleX(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

scaleY *Get output scaling value*

Description

Get output scaling value

Usage

```
scaleY(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

scaleY.MLPKriging *Get output scaling value for an MLPKriging model*

Description

Get output scaling value for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
scaleY(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

scaleY.WarpKriging *Get output scaling value for a WarpKriging model*

Description

Get output scaling value for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
scaleY(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

sigma2 *Get process variance*

Description

Get process variance

Usage

```
sigma2(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

Value

Numeric process variance estimate.

sigma2.WarpKriging *Get process variance (concentrated MLE)*

Description

Get process variance (concentrated MLE)

Usage

```
## S3 method for class 'WarpKriging'
sigma2(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

simulate,KM-method *Simulation from a* KM *Object*

Description

The simulate method is used to simulate paths from the kriging model described in object.

Usage

```
## S4 method for signature 'KM'
simulate(
  object,
  nsim = 1,
  seed = NULL,
  newdata,
  cond = TRUE,
  nugget.sim = 0,
  checkNames = FALSE,
  ...
)
```

Arguments

object	A KM object.
nsim	Integer: number of response vectors to simulate.
seed	Random seed.
newdata	Numeric matrix with it rows giving the points where the simulation is to be performed.
cond	Logical telling wether the simulation is conditional or not. Only TRUE is accepted for now.
nugget.sim	Numeric. A postive nugget effect used to avoid numerical instability.
checkNames	Check consistency between the design data X within object and newdata. The default is FALSE. XXXY Not used!!!
...	Ignored.

Details

Without a dedicated simulate method for the class "KM", this method would have been inherited from the "km" class. The dedicated method is expected to run faster. A comparison can be made by coercing a KM object to a km object with as.km before calling simulate.

Value

A numeric matrix with nrow(newdata) rows and nsim columns containing as its columns the simulated paths at the input points given in newdata.

XXX method simulate KM

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <-  function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
plot(f)
set.seed(123)
X <- as.matrix(runif(5))
y <- f(X)
points(X, y, col = 'blue')
k <- KM(design = X, response = y, covtype = "gauss")
x <- seq(from = 0, to = 1, length.out = 101)
s_x <- simulate(k, nsim = 3, newdata = x)
lines(x, s_x[ , 1], col = 'blue')
lines(x, s_x[ , 2], col = 'blue')
lines(x, s_x[ , 3], col = 'blue')
```

---

simulate.Kriging *Simulation from a* Kriging *model object.*

Description

This method draws paths of the stochastic process at new input points conditional on the values at the input points used in the fit.

Usage

```
## S3 method for class 'Kriging'
simulate(
  object,
  nsim = 1,
  seed = 123,
  x,
  with_noise = NULL,
  will_update = FALSE,
  ...
)
```

Arguments

object	S3 Kriging object.
nsim	Number of simulations to perform.
seed	Random seed used.
x	Points in model input space where to simulate.

with_noise	Logical or numeric specification controlling whether observation noise is included in the simulated paths. Use TRUE to include fitted noise when available, FALSE to exclude nugget noise, or NULL for the default behaviour.
will_update	Set to TRUE if you plan to call update_simulate() later.
...	Ignored.

Value

a matrix with nrow(x) rows and nsim columns containing the simulated paths at the inputs points given in x.

Note

The names of the formal arguments differ from those of the simulate methods for the S4 classes "km" and "KM". The formal x corresponds to newdata. These names are chosen **Python** and **Octave** interfaces to **libKriging**.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
plot(f)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)
points(X, y, col = "blue")

k <- Kriging(y, X, kernel = "matern3_2")

x <- seq(from = 0, to = 1, length.out = 101)
s <- simulate(k, nsim = 3, x = x)

lines(x, s[ , 1], col = "blue")
lines(x, s[ , 2], col = "blue")
lines(x, s[ , 3], col = "blue")
```

---

simulate.MLPKriging *Simulate from an MLPKriging model*

Description

Simulate from an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
simulate(object, nsim = 1, seed = 123, x, will_update = FALSE, ...)
```

Arguments

object	MLPKriging object
nsim	number of simulations
seed	random seed
x	simulation matrix (m x d)
will_update	logical; if TRUE keep the internal state for a subsequent update_simulate() call.
...	ignored

Value

matrix (m x nsim)

---

simulate.WarpKriging *Simulate from a WarpKriging model*

Description

Simulate from a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
simulate(object, nsim = 1, seed = 123, x, will_update = FALSE, ...)
```

Arguments

object	WarpKriging object
nsim	number of simulations
seed	random seed
x	simulation matrix (m x d)
will_update	logical; if TRUE, cache data for update_simulate
...	ignored

Value

matrix (m x nsim)

`subsetOfData` *Subset-of-data pre-fit reduction.*

Description

Selects a subset of `n_max` rows from a design `X`, meant to be used as a cheap pre-fit reduction for large designs: fit on `X[idx, ]`/`y[idx]` instead of the full data. Unlike Vecchia/Nystrom (which still use every point), this discards `n - n_max` points outright, in exchange for an ordinary exact fit on the reduced design.

Usage

```
subsetOfData(X, n_max, method = "kmeans", seed = 123)
```

Arguments

`X`	n x d design matrix.
`n_max`	Target subset size; if `n_max >= nrow(X)`, returns all indices (no-op).
`method`	`"kmeans"` (default): `n_max` k-means centroids on `X`, each replaced by its nearest actual data point, so the subset always consists of real observations; falls back to `"random"` if k-means degenerates. `"random"`: uniform subsample without replacement.
`seed`	RNG seed (k-means initialization and/or random fallback).

Value

Sorted 1-based row-indices into `X` (and the matching `y`) to keep.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
X <- matrix(runif(200), ncol = 2)
idx <- subsetOfData(X, 20)
Xr <- X[idx, ]
```

theta *Get GP range parameters*

Description

Get GP range parameters

Usage

```
theta(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

Value

Numeric vector of range parameters.

theta.WarpKriging *Get GP range parameters*

Description

Get GP range parameters

Usage

```
## S3 method for class 'WarpKriging'
theta(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

T_ *Get Cholesky factor T*

Description

Get Cholesky factor T

Usage

```
T_(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

T_.MLPKriging *Get Cholesky factor T for an MLPKriging model*

Description

Get Cholesky factor T for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
T_(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

T_.WarpKriging *Get Cholesky factor T for a WarpKriging model*

Description

Get Cholesky factor T for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
T_(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

update,KM-method *Update a* KM *Object with New Points*

Description

The update method is used when new observations are added to a fitted kriging model. Rather than fitting the model from scratch with the updated observations added, the results of the fit as stored in object are used to achieve some savings.

Usage

```
## S4 method for signature 'KM'
update(
  object,
  newX,
  newy,
  newX.alreadyExist = FALSE,
  cov.reestim = TRUE,
  trend.reestim = cov.reestim,
  nugget.reestim = FALSE,
  newnoise.var = NULL,
  kmcontrol = NULL,
  newF = NULL,
  ...
)
```

Arguments

object	A KM object.
newX	A numeric matrix containing the new design points. It must have object@d columns in correspondence with those of the design matrix used to fit the model which is stored as object@X.
newy	A numeric vector of new response values, in correspondence with the rows of newX.
newX.alreadyExist	Logical. If TRUE, newX can contain some input points that are already in object@X.
cov.reestim	Logical. If TRUE, the vector theta of correlation ranges will be re-estimated using the new observations as well as the observations already used when fitting object. Only TRUE can be used for now.
trend.reestim	Logical. If TRUE the vector beta of trend coefficients will be re-estimated using all the observations. Only TRUE can be used for now.
nugget.reestim	Logical. If TRUE the nugget effect will be re-estimated using all the observations. Only FALSE can be used for now.
newnoise.var	Optional variance of an additional noise on the new response.
kmcontrol	A list of options to tune the fit. Not available yet.
newF	New trend matrix. XXXY?
...	Ignored.

Details

Without a dedicated update method for the class "KM", this would have been inherited from the class "km". The dedicated method is expected to run faster. A comparison can be made by coercing a KM object to a km object with as.km before calling update.

Value

The updated KM object.

Author(s)

Yann Richet <yann.richet@asnr.fr>

See Also

as.km to coerce a KM object to the class "km".

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
plot(f)
set.seed(123)
X <- as.matrix(runif(5))
y <- f(X)
```

```
points(X, y, col = "blue")
KMobj <- KM(design = X, response = y,covtype = "gauss")
x <-  seq(from = 0, to = 1, length.out = 101)
p_x <- predict(KMobj, x)
lines(x, p_x$mean, col = "blue")
lines(x, p_x$lower95, col = "blue")
lines(x, p_x$upper95, col = "blue")
newX <- as.matrix(runif(3))
newy <- f(newX)
points(newX, newy, col = "red")

## replace the object by its udated version
KMobj <- update(KMobj, newX=newX, newy=newy)

x <- seq(from = 0, to = 1, length.out = 101)
p2_x <- predict(KMobj, x)
lines(x, p2_x$mean, col = "red")
lines(x, p2_x$lower95, col = "red")
lines(x, p2_x$upper95, col = "red")
```

`update.Kriging` *Update a* `Kriging` *model object with new points*

Description

Update a `Kriging` model object with new points

Usage

```
## S3 method for class 'Kriging'
update(object, y_u, ..., X_u = NULL, noise_u = NULL, refit = TRUE)
```

Arguments

`object`	S3 Kriging object.
`y_u`	Numeric vector of new responses (output).
`...`	Ignored.
`X_u`	Numeric matrix of new input points.
`noise_u`	Optional numeric vector of observation noise variances attached to `y_u`.
`refit`	Logical. If `TRUE` the model is refitted (default is `TRUE`).

Value

No return value. Kriging object argument is modified.

Caution

The method *does not return the updated object*, but instead changes the content of `object`. This behaviour is quite unusual in R and differs from the behaviour of `update.km` in **DiceKriging** and the `update` method for class `KM`.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1- 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x)*x^5 + 0.7)
plot(f)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)
points(X, y, col = "blue")

k <- Kriging(y, X, "matern3_2")

x <- seq(from = 0, to = 1, length.out = 101)
p <- predict(k, x)
lines(x, p$mean, col = "blue")
polygon(c(x, rev(x)), c(p$mean - 2 * p$stdev, rev(p$mean + 2 * p$stdev)),
 border = NA, col = rgb(0, 0, 1, 0.2))

X_u <- as.matrix(runif(3))
y_u <- f(X_u)
points(X_u, y_u, col = "red")

## change the content of the object 'k'
update(k, y_u, X_u)

## include design points to see interpolation
x <- sort(c(X,X_u,seq(from = 0, to = 1, length.out = 101)))
p2 <- predict(k, x)
lines(x, p2$mean, col = "red")
polygon(c(x, rev(x)), c(p2$mean - 2 * p2$stdev, rev(p2$mean + 2 * p2$stdev)),
 border = NA, col = rgb(1, 0, 0, 0.2))
```

---

update.MLPKriging *Update an MLPKriging model with new observations*

Description

Update an MLPKriging model with new observations

Usage

```
## S3 method for class 'MLPKriging'
update(object, y_u, X_u, refit = TRUE, ...)
```

Arguments

object	MLPKriging object
y_u	new observations
X_u	new input matrix
refit	Logical. If TRUE the model is refitted (default is TRUE).
...	ignored

---

update.WarpKriging *Update a WarpKriging model with new observations*

Description

Update a WarpKriging model with new observations

Usage

```
## S3 method for class 'WarpKriging'
update(object, y_u, X_u, refit = TRUE, noise_u = NULL, ...)
```

Arguments

object	WarpKriging object
y_u	new observations
X_u	new input matrix
refit	logical; if TRUE (default), re-optimise hyperparameters. Set to FALSE for a fast incremental Cholesky update that keeps all hyper-parameters (and warping parameters) fixed.
noise_u	optional numeric vector of per-observation noise variances for the update points (length nrow(X_u)). Required when the model was fitted with noise; must be omitted otherwise.
...	ignored

update_simulate *Update simulation of model on data.*

Description

Update previous simulate of a model given in `object`.

Usage

```
update_simulate(object, ...)
```

Arguments

`object`	An object representing a fitted model.
`...`	Further arguments of function

Value

Updated simulation of model output.

update_simulate.Kriging *Update previous simulation of a* `Kriging` *model object.*

Description

This method draws paths of the stochastic process conditional on the values at the input points used in the fit, plus the new input points and their values given as argument (knonw as 'update' points).

Usage

```
## S3 method for class 'Kriging'
update_simulate(object, y_u, ..., X_u = NULL, noise_u = NULL)
```

Arguments

`object`	S3 Kriging object.
`y_u`	Numeric vector of new responses (output).
`...`	Ignored.
`X_u`	Numeric matrix of new input points.
`noise_u`	Optional numeric vector of observation noise variances attached to `y_u`.

Value

a matrix with `nrow(x)` rows and `nsim` columns containing the simulated paths at the inputs points given in `x`.

Author(s)

Yann Richet <yann.richet@asnr.fr>

Examples

```
f <- function(x) 1 - 1 / 2 * (sin(12 * x) / (1 + x) + 2 * cos(7 * x) * x^5 + 0.7)
plot(f)
set.seed(123)
X <- as.matrix(runif(10))
y <- f(X)
points(X, y, col = "blue")

k <- Kriging(y, X, kernel = "matern3_2")

x <- seq(from = 0, to = 1, length.out = 101)
s <- k$simulate(nsim = 3, x = x, will_update = TRUE)

lines(x, s[ , 1], col = "blue")
lines(x, s[ , 2], col = "blue")
lines(x, s[ , 3], col = "blue")

X_u <- as.matrix(runif(3))
y_u <- f(X_u)
points(X_u, y_u, col = "red")

su <- k$update_simulate(y_u, X_u)

lines(x, su[ , 1], col = "blue", lty=2)
lines(x, su[ , 2], col = "blue", lty=2)
lines(x, su[ , 3], col = "blue", lty=2)
```

---

update_simulate.MLPKriging

Update simulated paths with new observations (FOXY algorithm)

Description

Update simulated paths with new observations (FOXY algorithm)

Usage

```
## S3 method for class 'MLPKriging'
update_simulate(object, y_u, X_u, ...)
```

Arguments

object	MLPKriging object (must have called simulate with will_update=TRUE)
y_u	new observations
X_u	new input matrix
...	ignored

Value

matrix (m x nsim) of updated simulated paths

---

update_simulate.WarpKriging

Update simulated paths with new observations (FOXY algorithm)

Description

Update simulated paths with new observations (FOXY algorithm)

Usage

```
## S3 method for class 'WarpKriging'
update_simulate(object, y_u, X_u, noise_u = NULL, ...)
```

Arguments

object	WarpKriging object (must have called simulate with will_update=TRUE)
y_u	new observations
X_u	new input matrix
noise_u	optional numeric vector of per-observation noise variances for the update points (length nrow(X_u)); required when the model was fitted with noise.
...	ignored

Value

matrix (m x nsim) of updated simulated paths

warping *Get warping specifications as strings*

Description

Get warping specifications as strings

Usage

```
warping(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

warping.WarpKriging *Get warping specification for a WarpKriging model*

Description

Get warping specification for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
warping(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

`WarpKriging` *Create a WarpKriging model*

Description

Kriging with per-variable input warping. Each input dimension is independently transformed before the GP kernel is evaluated. Supports continuous, categorical, ordinal variables and joint deep kernel learning.

Usage

```
WarpKriging(
  y,
  X,
  warping,
  kernel = "gauss",
  regmodel = "constant",
  normalize = FALSE,
  optim = "BFGS+Adam",
  objective = "LL",
  parameters = NULL,
  noise = NULL
)
```

Arguments

`y`	numeric vector of observations (n)
`X`	numeric matrix of inputs (n x d)
`warping`	character vector of warp specifications, one per column of X. Use `warp_*()` helpers or plain strings: `"none"`, `"affine"`, `"boxcox"`, `"kumaraswamy"`, `"neural_mono(8)"`, `"mlp(16:8,2,selu)"`, `"knots(3)"`, `"knots(0.25:0.5:0.75)"`, `"categorical(5,2)"`, `"ordinal(4)"`.
`kernel`	covariance kernel: "gauss", "matern3_2", "matern5_2", "exp"
`regmodel`	trend: "constant", "linear", "quadratic"
`normalize`	logical; normalise continuous inputs?
`optim`	optimiser (currently only one bi-level strategy). Use `"none"` to skip optimisation and keep the values passed in `parameters` (e.g. to rebuild a model with frozen hyper-parameters).
`objective`	"LL" (log-likelihood)
`parameters`	optional named list of initial hyper-parameter values and/or optimiser knobs. Recognised entries: • `theta`: numeric vector of GP range parameters (length `feature_dim`), used as the L-BFGS start point (or kept as-is when `optim = "none"`).

- warp_params: numeric vector of packed warping parameters (see warp_params()), same convention as theta.
- noise: numeric vector of per-observation noise variances (length n); equivalent to passing noise=.
- adam_lr, max_iter_adam, max_iter_bfgs: optimiser knobs, numeric or string.

noise — numeric vector of per-observation noise variances (length n), or NULL (default) for noise-free interpolation. When set, the GP uses the NoiseKriging likelihood $diag(C) = \sigma^2 + noise_i$. (Homogeneous-nugget *estimation* is not available for WarpKriging.)

Value

An S3 object of class "WarpKriging".

Examples

```
# Continuous with Kumaraswamy warping
X <- as.matrix(c(0.0, 0.25, 0.5, 0.75, 1.0))
f <- function(x) 1 - 1/2 * (sin(12*x)/(1+x) + 2*cos(7*x)*x^5 + 0.7)
y <- f(X)
k <- WarpKriging(y, X, warping = "kumaraswamy", kernel = "gauss")
print(k)

# Mixed: 1 continuous + 1 categorical (3 levels)
n <- 15
X_mix <- cbind(runif(n), rep(0:2, length.out = n))
y_mix <- sin(2 * pi * X_mix[, 1]) * c(1, 2, 0.5)[X_mix[, 2] + 1]
k2 <- WarpKriging(y_mix, X_mix,
         warping = c("mlp(16:8,2,selu)", "categorical(3,2)"),
         kernel = "matern5_2")
```

---

warp_affine — *Affine warping: w(x) = a*x + b*

Description

Affine warping: w(x) = a*x + b

Usage

```
warp_affine()
```

Value

string "affine"

warp_boxcox *Box-Cox warping*

Description

Box-Cox warping

Usage

```
warp_boxcox()
```

Value

string "boxcox"

warp_categorical *Categorical embedding*

Description

Categorical embedding

Usage

```
warp_categorical(n_levels, embed_dim = 2)
```

Arguments

n_levels	number of levels (integer-coded 0..n_levels-1)
embed_dim	embedding dimensionality (default 2)

Value

string e.g. "categorical(5,2)"

`warp_knots` *Piecewise-linear monotone warping with knots (Xiong et al. 2007)*

Description

Implements the non-stationary input warping of Xiong, Chen, Apley & Ding (2007, *Int. J. Numer. Meth. Engng*). The domain $[0, 1]$ is split into $K + 1$ intervals by K interior knots, each carrying a learnable positive slope $s_k = \exp(r_k)$. The warp is:

$$w(x) = \sum_{j<k} s_j (t_{j+1} - t_j) + s_k (x - t_k)$$

for $x \in [t_k, t_{k+1})$, giving a continuous, monotone piecewise-linear function with $K + 1$ free parameters.

This is the same construction as the `knots` argument in **DiceKriging**.

Usage

```
warp_knots(n_knots = 3, knot_positions = NULL)
```

Arguments

`n_knots`	number of interior knots $K \geq 1$ (default 3)
`knot_positions`	optional numeric vector of K knot positions strictly inside $(0, 1)$, in increasing order. When `NULL` (default), knots are placed uniformly at $1/(K+1), 2/(K+1), \ldots, K/(K+1)$.

Value

warp specification string, e.g. `"knots(3)"` or `"knots(0.25:0.5:0.75)"`

References

Xiong, Y., Chen, W., Apley, D. & Ding, X. (2007). A non-stationary covariance-based Kriging method for metamodelling in engineering design. *International Journal for Numerical Methods in Engineering*, 71(6), 733–756.

See Also

`WarpKriging`

warp_kumaraswamy *Kumaraswamy CDF warping on [0,1]*

Description

Kumaraswamy CDF warping on [0,1]

Usage

```
warp_kumaraswamy()
```

Value

string "kumaraswamy"

warp_mlp *Per-variable MLP warping (unconstrained, multi-dim output)*

Description

Per-variable MLP warping (unconstrained, multi-dim output)

Usage

```
warp_mlp(hidden_dims, d_out = 2, activation = "selu")
```

Arguments

hidden_dims	integer vector of hidden layer sizes
d_out	output dimensionality (default 2)
activation	activation: "relu","selu","tanh","sigmoid","elu"

Value

string e.g. "mlp(16:8,3,selu)"

warp_neural_mono *Monotone neural network warping*

Description

Monotone neural network warping

Usage

```
warp_neural_mono(n_hidden = 8)
```

Arguments

n_hidden	number of hidden units (default 8)

Value

string e.g. "neural_mono(16)"

warp_none *No warping (identity)*

Description

No warping (identity)

Usage

```
warp_none()
```

Value

string "none"

warp_ordinal *Ordinal warping (learned ordered positions)*

Description

Ordinal warping (learned ordered positions)

Usage

```
warp_ordinal(n_levels)
```

Arguments

n_levels	number of ordered levels (0..n_levels-1)

Value

string e.g. "ordinal(4)"

warp_params *Get the packed warping parameters*

Description

Get the packed warping parameters

Usage

```
warp_params(object, ...)
```

Arguments

object	A WarpKriging model object.
...	Unused.

Value

numeric vector of packed per-dimension warping parameters, in the optimiser layout (concatenation of each warp's own parameters). Can be passed back through `parameters = list(warp_params = ...)`.

warp_params.WarpKriging *Get the packed warping parameters for a WarpKriging model*

Description

Get the packed warping parameters for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
warp_params(object, ...)
```

Arguments

object	A WarpKriging model object.
...	Unused.

X *Get training input matrix*

Description

Get training input matrix

Usage

```
X(object, ...)
```

Arguments

object	A fitted model object
...	ignored

Value

matrix of training inputs

X.MLPKriging *Get training input matrix*

Description

Get training input matrix

Usage

```
## S3 method for class 'MLPKriging'
X(object, ...)
```

Arguments

object	MLPKriging object
...	ignored

Value

matrix of training inputs

y *Get training output vector*

Description

Get training output vector

Usage

```
y(object, ...)
```

Arguments

object	A fitted model object
...	ignored

Value

vector of training outputs

y.MLPKriging *Get training output vector*

Description

Get training output vector

Usage

```
## S3 method for class 'MLPKriging'
y(object, ...)
```

Arguments

object	MLPKriging object
...	ignored

Value

vector of training outputs

z *Get whitened residuals z*

Description

Get whitened residuals z

Usage

```
z(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

z.MLPKriging *Get whitened residuals z for an MLPKriging model*

Description

Get whitened residuals z for an MLPKriging model

Usage

```
## S3 method for class 'MLPKriging'
z(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

z.WarpKriging *Get whitened residuals z for a WarpKriging model*

Description

Get whitened residuals z for a WarpKriging model

Usage

```
## S3 method for class 'WarpKriging'
z(object, ...)
```

Arguments

object	A Kriging/MLPKriging/WarpKriging model object.
...	Unused.

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