Package 'rlibkriging'

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Type Package

Title Kriging Models using the 'libKriging' Library

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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.

License Apache License (>= 2)

Encoding UTF-8

LinkingTo Rcpp, RcppArmadillo

Depends R (>= 4.2)

Imports Rcpp (>= 1.0.12), methods, DiceKriging

Suggests testthat, RobustGaSP, utils, DiceDesign, foreach

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

URL https://github.com/libKriging

RoxygenNote 7.3.1

NeedsCompilation yes

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Contents

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@irsn.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.km.NoiseKriging *Coerce a* NoiseKriging *object into the* "km" *class of the* **DiceKriging** *package.*

Description

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

Usage

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

Arguments

x	An object with S3 class "NoiseKriging".
.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 NoiseKriging slot.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X)) # add noise dep. on X
## fit and print
k <- NoiseKriging(y, noise=(X/10)^2, X, kernel = "matern3_2")
print(k)

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

---

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

Description

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

Usage

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

Arguments

x	An object with S3 class "NuggetKriging".
.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 NuggetKriging slot.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))

k <- NuggetKriging(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@irsn.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"))
```

`as.list.NoiseKriging` *Coerce a* `NoiseKriging` *Object into a List*

Description

Coerce a `NoiseKriging` Object into a List

Usage

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

Arguments

`x`	An object with class "`NoiseKriging`".
`...`	Ignored

Value

A list with its elements copying the content of the `NoiseKriging` 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@irsn.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) + X/10 * rnorm(nrow(X)) # add noise dep. on X

k <- NoiseKriging(y, noise=(X/10)^2, X, kernel = "matern3_2")

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

`as.list.NuggetKriging` *Coerce a* `NuggetKriging` *Object into a List*

Description

Coerce a `NuggetKriging` Object into a List

Usage

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

Arguments

`x`	An object with class "`NuggetKriging`".
`...`	Ignored

Value

A list with its elements copying the content of the `NuggetKriging` 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@irsn.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) + 0.1 * rnorm(nrow(X))

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

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

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

classNoiseKriging *Shortcut to provide functions to the S3 class "NoiseKriging"*

Description

Shortcut to provide functions to the S3 class "NoiseKriging"

Usage

```
classNoiseKriging(nk)
```

Arguments

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

Value

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

classNuggetKriging *Shortcut to provide functions to the S3 class "NuggetKriging"*

Description

Shortcut to provide functions to the S3 class "NuggetKriging"

Usage

```
classNuggetKriging(nk)
```

Arguments

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

Value

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

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@irsn.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.NoiseKriging *Duplicate a NoiseKriging Model*

Description

Duplicate a NoiseKriging Model

Usage

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

Arguments

object	An S3 NoiseKriging object.
...	Not used.

Value

The copy of object.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X))

k <- NoiseKriging(y, (X/10)^2, X, kernel = "matern3_2", objective="LL")
print(k)

print(copy(k))
```

---

copy.NuggetKriging *Duplicate a NuggetKriging Model*

Description

Duplicate a NuggetKriging Model

Usage

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

Arguments

object	An S3 NuggetKriging object.
...	Not used.

Value

The copy of object.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))

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

print(copy(k))
```

---

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@irsn.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.NoiseKriging` *Compute Covariance Matrix of NoiseKriging Model*

Description

Compute Covariance Matrix of NoiseKriging Model

Usage

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

Arguments

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

Value

A matrix of the covariance matrix of the NoiseKriging model.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X))

k <- NoiseKriging(y, (X/10)^2, X, "matern3_2")

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

covMat(k, x1, x2)
```

`covMat.NuggetKriging` *Compute Covariance Matrix of NuggetKriging Model*

Description

Compute Covariance Matrix of NuggetKriging Model

Usage

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

Arguments

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

Value

A matrix of the covariance matrix of the NuggetKriging model.

Author(s)

Yann Richet <yann.richet@irsn.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 <- NuggetKriging(y, X, kernel = "gauss")

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

covMat(k, x1, x2)
```

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", "none"),
  normalize = FALSE,
  optim = c("BFGS", "Newton", "none"),
  objective = c("LL", "LOO", "LMP"),
  parameters = 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", "Newton" and "none", the later simply keeping the values given in parameters. The method "BFGS" uses the gradient of the objective (note that "BGFS10" means 10 multi-start of BFGS). The method "Newton" uses both the gradient and the Hessian of the objective.
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 and "LMP" for the Log-Marginal Posterior.
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.
...	Ignored.

Value

No return value. Kriging object argument is modified.

Author(s)

Yann Richet <yann.richet@irsn.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.NoiseKriging` *Fit* `NoiseKriging` *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 'NoiseKriging'
fit(
  object,
  y,
  noise,
  X,
  regmodel = c("constant", "linear", "interactive", "none"),
  normalize = FALSE,
  optim = c("BFGS", "none"),
  objective = c("LL"),
  parameters = NULL,
  ...
)
```

Arguments

`object`	S3 NoiseKriging object.
`y`	Numeric vector of response values.
`noise`	Numeric vector of response variances.
`X`	Numeric matrix of input design.
`regmodel`	Universal NoiseKriging `"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 `"BGFS10"` means 10 multi-start of BFGS).
`objective`	Character giving the objective function to optimize. Possible values are: `"LL"` for the Log-Likelihood.
`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.
`...`	Ignored.

Value

No return value. NoiseKriging object argument is modified.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X)) # add noise dep. on X
points(X, y, col = "blue", pch = 16)

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

fit(k,y,noise=(X/10)^2,X)
print(k)
```

---

fit.NuggetKriging *Fit* NuggetKriging *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 'NuggetKriging'
fit(
  object,
  y,
  X,
  regmodel = c("constant", "linear", "interactive", "none"),
  normalize = FALSE,
  optim = c("BFGS", "none"),
  objective = c("LL", "LMP"),
  parameters = NULL,
  ...
)
```

Arguments

`object`	S3 NuggetKriging object.
`y`	Numeric vector of response values.
`X`	Numeric matrix of input design.
`regmodel`	Universal NuggetKriging `"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 `"BGFS10"` means 10 multi-start of BFGS).
`objective`	Character giving the objective function to optimize. Possible values are: `"LL"` for the Log-Likelihood and `"LMP"` for the Log-Marginal Posterior.
`parameters`	Initial values for the hyper-parameters. When provided this must be named list with some elements `"sigma2"`, `"theta"`, `"nugget"` containing the initial value(s) for the variance, range and nugget parameters. If `theta` is a matrix with more than one row, each row is used as a starting point for optimization.
`...`	Ignored.

Value

No return value. NuggetKriging object argument is modified.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))
points(X, y, col = "blue", pch = 16)

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

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

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`, `nugget.estim`, `noise.var`	Not implemented yet.
`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@irsn.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 $\hat{\beta}$ 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@irsn.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", "none"),
  normalize = FALSE,
  optim = c("BFGS", "Newton", "none"),
  objective = c("LL", "LOO", "LMP"),
  parameters = 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"`, `"Newton"` and `"none"`, the later simply keeping the values given in `parameters`. The method `"BFGS"` uses the gradient of the objective (note that `"BGFS10"` means 10 multi-start of BFGS). The method `"Newton"` uses both the gradient and the Hessian of the objective.
`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 and `"LMP"` for the Log-Marginal Posterior.
`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.

Value

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

Author(s)

Yann Richet <yann.richet@irsn.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@irsn.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@irsn.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@irsn.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@irsn.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@irsn.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))
```

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

Description

Load a NoiseKriging Model from a file storage

Usage

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

Arguments

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

Value

The loaded NoiseKriging object.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X))
points(X, y, col = "blue")

k <- NoiseKriging(y, (X/10)^2, X, "matern3_2")
print(k)

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

print(load.NoiseKriging(outfile))
```

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

Description

Load a NuggetKriging Model from a file storage

Usage

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

Arguments

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

Value

The loaded NuggetKriging object.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))
points(X, y, col = "blue")

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

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

print(load.NuggetKriging(outfile))
```

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@irsn.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.NoiseKriging

Get logLikelihood of NoiseKriging Model

Description

Get logLikelihood of NoiseKriging Model

Usage

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

Arguments

object	An S3 NoiseKriging object.
...	Not used.

Value

The logLikelihood computed for fitted $theta_sigma2$.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X))

k <- NoiseKriging(y, (X/10)^2, X, kernel = "matern3_2", objective="LL")
print(k)

logLikelihood(k)
```

`logLikelihood.NuggetKriging` *Get logLikelihood of NuggetKriging Model*

Description

Get logLikelihood of NuggetKriging Model

Usage

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

Arguments

`object`	An S3 NuggetKriging object.
`...`	Not used.

Value

The logLikelihood computed for fitted $theta_alpha$.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))

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

logLikelihood(k)
```

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@irsn.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.NoiseKriging

Compute Log-Likelihood of NoiseKriging Model

Description

Compute Log-Likelihood of NoiseKriging Model

Usage

```
## S3 method for class 'NoiseKriging'
logLikelihoodFun(object, theta_sigma2, return_grad = FALSE, bench = FALSE, ...)
```

Arguments

object	An S3 NoiseKriging object.
theta_sigma2	A numeric vector of (positive) range parameters and variance at which the log-likelihood will be evaluated.
return_grad	Logical. Should the function return the gradient?
bench	Logical. Should the function display benchmarking output
...	Not used.

Value

The log-Likelihood computed for given $theta_sigma2$.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10  *rnorm(nrow(X))

k <- NoiseKriging(y, (X/10)^2, X, kernel = "matern3_2")
print(k)

theta0 = k$theta()
ll_sigma2 <- function(sigma2) logLikelihoodFun(k, cbind(theta0,sigma2))$logLikelihood
s2 <- seq(from = 0.001, to = 1, length.out = 101)
plot(s2, Vectorize(ll_sigma2)(s2), type = 'l')
abline(v = k$sigma2(), col = "blue")

sigma20 = k$sigma2()
ll_theta <- function(theta) logLikelihoodFun(k, cbind(theta,sigma20))$logLikelihood
t <- seq(from = 0.001, to = 2, length.out = 101)
plot(t, Vectorize(ll_theta)(t), type = 'l')
abline(v = k$theta(), col = "blue")

ll <- function(theta_sigma2) logLikelihoodFun(k, theta_sigma2)$logLikelihood
s2 <- seq(from = 0.001, to = 1, length.out = 31)
t <- seq(from = 0.001, to = 2, length.out = 31)
contour(t,s2,matrix(ncol=length(s2),ll(expand.grid(t,s2))),xlab="theta",ylab="sigma2")
points(k$theta(),k$sigma2(),col='blue')
```

`logLikelihoodFun.NuggetKriging` *Compute Log-Likelihood of NuggetKriging Model*

Description

Compute Log-Likelihood of NuggetKriging Model

Usage

```
## S3 method for class 'NuggetKriging'
logLikelihoodFun(object, theta_alpha, return_grad = FALSE, bench = FALSE, ...)
```

Arguments

`object`	An S3 NuggetKriging object.
`theta_alpha`	A numeric vector of (positive) range parameters and variance over variance plus nugget at which the log-likelihood will be evaluated.
`return_grad`	Logical. Should the function return the gradient?
`bench`	Logical. Should the function display benchmarking output
`...`	Not used.

Value

The log-Likelihood computed for given $theta_alpha$.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))

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

theta0 = k$theta()
ll_alpha <- function(alpha) logLikelihoodFun(k,cbind(theta0,alpha))$logLikelihood
a <- seq(from = 0.9, to = 1.0, length.out = 101)
plot(a, Vectorize(ll_alpha)(a), type = "l",xlim=c(0.9,1))
abline(v = k$sigma2()/(k$sigma2()+k$nugget()), col = "blue")

alpha0 = k$sigma2()/(k$sigma2()+k$nugget())
ll_theta <- function(theta) logLikelihoodFun(k,cbind(theta,alpha0))$logLikelihood
```

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

ll <- function(theta_alpha) logLikelihoodFun(k,theta_alpha)$logLikelihood
a <- seq(from = 0.9, to = 1.0, length.out = 31)
t <- seq(from = 0.001, to = 2, length.out = 101)
contour(t,a,matrix(ncol=length(a),ll(expand.grid(t,a))),xlab="theta",ylab="sigma2/(sigma2+nugget)")
points(k$theta(),k$sigma2()/(k$sigma2()+k$nugget()),col='blue')
```

`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 $theta$.

Author(s)

Yann Richet <yann.richet@irsn.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)
```

---

logMargPost.NuggetKriging

Get logMargPost of NuggetKriging Model

Description

Get logMargPost of NuggetKriging Model

Usage

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

Arguments

object	An S3 NuggetKriging object.
...	Not used.

Value

The logMargPost computed for fitted $theta_alpha$.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))

k <- NuggetKriging(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@irsn.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")
```

`logMargPostFun.NuggetKriging` *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 'NuggetKriging'
logMargPostFun(object, theta_alpha, return_grad = FALSE, bench = FALSE, ...)
```

Arguments

`object`	S3 NuggetKriging object.
`theta_alpha`	Numeric vector of correlation range and variance over variance plus nugget parameters at which the function is to be evaluated.
`return_grad`	Logical. Should the function return the gradient (w.r.t theta_alpha)?
`bench`	Logical. Should the function display benchmarking output
`...`	Not used.

Value

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

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))

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

```
print(k)

theta0 = k$theta()
lmp_alpha <- function(alpha) k$logMargPostFun(cbind(theta0,alpha))$logMargPost
a <- seq(from = 0.9, to = 1.0, length.out = 101)
plot(a, Vectorize(lmp_alpha)(a), type = "l",xlim=c(0.9,1))
abline(v = k$sigma2()/(k$sigma2()+k$nugget()), col = "blue")

alpha0 = k$sigma2()/(k$sigma2()+k$nugget())
lmp_theta <- function(theta) k$logMargPostFun(cbind(theta,alpha0))$logMargPost
t <- seq(from = 0.001, to = 2, length.out = 101)
plot(t, Vectorize(lmp_theta)(t), type = 'l')
abline(v = k$theta(), col = "blue")

lmp <- function(theta_alpha) k$logMargPostFun(theta_alpha)$logMargPost
t <- seq(from = 0.4, to = 0.6, length.out = 51)
a <- seq(from = 0.9, to = 1, length.out = 51)
contour(t,a,matrix(ncol=length(t),lmp(expand.grid(t,a))),
 nlevels=50,xlab="theta",ylab="sigma2/(sigma2+nugget)")
points(k$theta(),k$sigma2()/(k$sigma2()+k$nugget()),col='blue')
```

NoiseKM *Create an* NoiseKM *Object*

Description

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

Usage

```
NoiseKM(
  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,
  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 NoiseKriging. 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, nugget.estim	Not implemented.
noise.var	Vector of output values variance.
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 "NoiseKM" extends the "km" class of the **DiceKriging** package, hence has all slots of "km". It also has an extra slot "NoiseKriging" slot which contains a copy of the original object.

Value

A NoiseKM object. See **Details**.

Author(s)

Yann Richet <yann.richet@irsn.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) + rnorm(nrow(design.fact))

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

NoiseKM-class *S4 class for NoiseKriging 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 $\hat{\beta}$ 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?

`NoiseKriging` A copy of the `NoiseKriging` object used to create the current `NoiseKM` object.

Author(s)

Yann Richet <yann.richet@irsn.fr>

See Also

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

NoiseKriging *Create an object with S3 class* "NoiseKriging" *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

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

Arguments

y	Numeric vector of response values.
noise	Numeric vector of response variances.
X	Numeric matrix of input design.
kernel	Character defining the covariance model: "exp", "gauss", "matern3_2", "matern5_2".
regmodel	Universal NoiseKriging "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 "BGFS10" means 10 multi-start of BFGS).
objective	Character giving the objective function to optimize. Possible values are: "LL" for the Log-Likelihood.

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.

Value

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

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X)) # add noise dep. on X
## fit and print
k <- NoiseKriging(y, noise=(X/10)^2, 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)
```

NuggetKM *Create an* NuggetKM *Object*

Description

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

Usage

```
NuggetKM(
  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 = TRUE,
  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 NuggetKriging. 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.estim, nugget	Should nugget be estimated? (defaults TRUE) or given values.
noise.var	Not implemented.
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 "NuggetKM" extends the "km" class of the **DiceKriging** package, hence has all slots of "km". It also has an extra slot "NuggetKriging" slot which contains a copy of the original object.

Value

A NuggetKM object. See **Details**.

Author(s)

Yann Richet <yann.richet@irsn.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) + rnorm(nrow(design.fact))

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

NuggetKM-class *S4 class for NuggetKriging 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 $\hat{\beta}$ 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?

`NuggetKriging` A copy of the `NuggetKriging` object used to create the current `NuggetKM` object.

Author(s)

Yann Richet <yann.richet@irsn.fr>

See Also

`km-class` in the **DiceKriging** package. The creator `NuggetKM`.

`NuggetKriging` *Create an object with S3 class* `"NuggetKriging"` *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

```
NuggetKriging(
  y = NULL,
  X = NULL,
  kernel = NULL,
  regmodel = c("constant", "linear", "interactive", "none"),
  normalize = FALSE,
  optim = c("BFGS", "none"),
  objective = c("LL", "LMP"),
  parameters = 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 NuggetKriging "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 "BGFS10" means 10 multi-start of BFGS).
objective	Character giving the objective function to optimize. Possible values are: "LL" for the Log-Likelihood and "LMP" for the Log-Marginal Posterior.
parameters	Initial values for the hyper-parameters. When provided this must be named list with some elements "sigma2", "theta", "nugget" containing the initial value(s) for the variance, range and nugget parameters. If theta is a matrix with more than one row, each row is used as a starting point for optimization.

Value

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

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))
## fit and print
k <- NuggetKriging(y, X, kernel = "matern3_2")
print(k)

x <- sort(c(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)
```

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@irsn.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,NoiseKM-method

Prediction Method for a NoiseKM *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 'NoiseKM'
predict(
  object,
  newdata,
  type = "UK",
  se.compute = TRUE,
  cov.compute = FALSE,
  light.return = TRUE,
  bias.correct = FALSE,
  checkNames = FALSE,
```

```
  ...
)
```

Arguments

object	NoiseKM 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 "NoiseKM", 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 NoiseKM 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@irsn.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) + rnorm(nrow(design.fact))

## library(DiceKriging)
## kriging model 1 : matern5_2 covariance structure, no trend, no nugget
## m1 <- km(design = design.fact, response = y, covtype = "gauss",
##          noise.var=rep(1,nrow(design.fact)),
##          parinit = c(.5, 1), control = list(trace = FALSE))
KM1 <- NoiseKM(design = design.fact, response = y, covtype = "gauss",
               noise=rep(1,nrow(design.fact)),
               parinit = c(.5, 1))
```

```
Pred <- predict(KM1, newdata = matrix(.5,ncol = 2), type = "UK",
                checkNames = FALSE, light.return = TRUE)
```

---

predict,NuggetKM-method

Prediction Method for a NuggetKM *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 'NuggetKM'
predict(
  object,
  newdata,
  type = "UK",
  se.compute = TRUE,
  cov.compute = FALSE,
  light.return = TRUE,
  bias.correct = FALSE,
  checkNames = FALSE,
  ...
)
```

Arguments

object	NuggetKM 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 "NuggetKM", 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 NuggetKM 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@irsn.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) + rnorm(nrow(design.fact))

## library(DiceKriging)
## kriging model 1 : matern5_2 covariance structure, no trend, no nugget
## m1 <- km(design = design.fact, response = y, covtype = "gauss",
##          nugget.estim=TRUE,
##          parinit = c(.5, 1), control = list(trace = FALSE))
KM1 <- NuggetKM(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@irsn.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.NoiseKriging *Predict from a* NoiseKriging *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 'NoiseKriging'
predict(
  object,
  x,
  return_stdev = TRUE,
  return_cov = FALSE,
  return_deriv = FALSE,
  ...
)
```

Arguments

object	S3 NoiseKriging 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@irsn.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) + X/10 * rnorm(nrow(X))
points(X, y, col = "blue", pch = 16)

k <- NoiseKriging(y, (X/10)^2, 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.NuggetKriging` *Predict from a* `NuggetKriging` *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 'NuggetKriging'
predict(
  object,
  x,
  return_stdev = TRUE,
  return_cov = FALSE,
  return_deriv = FALSE,
  ...
)
```

Arguments

`object`	S3 NuggetKriging 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@irsn.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) + 0.1 * rnorm(nrow(X))
points(X, y, col = "blue", pch = 16)

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

## include design points to see interpolation
x <- sort(c(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))
```

---

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@irsn.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.NoiseKriging *Print the content of a* NoiseKriging *object.*

Description

Print the content of a NoiseKriging object.

Usage

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

Arguments

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

Value

String of printed object.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X)) # add noise dep. on X

k <- NoiseKriging(y, noise=(X/10)^2, X, kernel = "matern3_2")

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

---

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

Description

Print the content of a NuggetKriging object.

Usage

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

Arguments

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

Value

String of printed object.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))

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

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

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@irsn.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@irsn.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)
```

---

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

Description

Save a NoiseKriging Model to a file storage

Usage

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

Arguments

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

Value

The loaded NoiseKriging object.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X))

k <- NoiseKriging(y, (X/10)^2, X, "matern3_2")
print(k)

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

---

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

Description

Save a NuggetKriging Model to a file storage

Usage

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

Arguments

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

Value

The loaded NuggetKriging object.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))
points(X, y, col = "blue")

k <- NuggetKriging(y, X, "matern3_2")
print(k)
```

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

`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@irsn.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,NoiseKM-method

Simulation from a `NoiseKM` *Object*

Description

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

Usage

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

Arguments

object	A NoiseKM 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 "NoiseKM", 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 NoiseKM 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 NoiseKM

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.01*rnorm(nrow(X))
points(X, y, col = 'blue')
k <- NoiseKM(design = X, response = y, covtype = "gauss", noise=rep(0.01^2,nrow(X)))
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,NuggetKM-method

Simulation from a NuggetKM *Object*

Description

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

Usage

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

Arguments

object	A NuggetKM 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 "NuggetKM", 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 NuggetKM 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 NuggetKM

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.01*rnorm(nrow(X))
points(X, y, col = 'blue')
k <- NuggetKM(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, 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.
will_update	Set to TRUE if wish to use 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@irsn.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.NoiseKriging *Simulation from a* NoiseKriging *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 'NoiseKriging'
simulate(
  object,
  nsim = 1,
  seed = 123,
  x,
  with_noise = NULL,
  will_update = FALSE,
  ...
)
```

Arguments

object	S3 NoiseKriging object.
nsim	Number of simulations to perform.
seed	Random seed used.
x	Points in model input space where to simulate.
with_noise	Set to array of values if wish to add the noise in the simulation.
will_update	Set to TRUE if wish to use 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@irsn.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) + X/10 * rnorm(nrow(X))
points(X, y, col = "blue")

k <- NoiseKriging(y, (X/10)^2, 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.NuggetKriging` *Simulation from a* `NuggetKriging` *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 'NuggetKriging'
simulate(
  object,
  nsim = 1,
  seed = 123,
  x,
  with_nugget = TRUE,
  will_update = FALSE,
  ...
)
```

Arguments

`object`	S3 NuggetKriging object.
`nsim`	Number of simulations to perform.
`seed`	Random seed used.
`x`	Points in model input space where to simulate.
`with_nugget`	Set to FALSE if wish to remove the nugget in the simulation.
`will_update`	Set to TRUE if wish to use 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@irsn.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) + 0.1  *rnorm(nrow(X))
points(X, y, col = "blue")

k <- NuggetKriging(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")
```

---

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@irsn.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,NoiseKM-method` *Update a* `NoiseKM` *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 'NoiseKM'
update(
  object,
  newX,
  newy,
  newnoise.var,
  newX.alreadyExist = FALSE,
  cov.reestim = TRUE,
  trend.reestim = cov.reestim,
  nugget.reestim = FALSE,
  kmcontrol = NULL,
  newF = NULL,
  ...
)
```

Arguments

`object`	A NoiseKM 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.
newnoise.var	Variance of an additional noise on the new response.
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.
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 "NoiseKM", 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 NoiseKM object to a km object with as.km before calling update.

Value

The updated NoiseKM object.

Author(s)

Yann Richet <yann.richet@irsn.fr>

See Also

as.km to coerce a NoiseKM 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) + 0.01*rnorm(nrow(X))
points(X, y, col = "blue")
KMobj <- NoiseKM(design = X, response = y, noise=rep(0.01^2,5), 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) + 0.01*rnorm(nrow(newX))
points(newX, newy, col = "red")

## replace the object by its udated version
KMobj <- update(KMobj, newX=newX, newy=newy, newnoise.var=rep(0.01^2,3))

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,NuggetKM-method`

Update a `NuggetKM` *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 'NuggetKM'
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 NuggetKM 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 "NuggetKM", 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 NuggetKM object to a km object with as.km before calling update.

Value

The updated NuggetKM object.

Author(s)

Yann Richet <yann.richet@irsn.fr>

See Also

as.km to coerce a NuggetKM 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) + 0.01*rnorm(nrow(X))
points(X, y, col = "blue")
KMobj <- NuggetKM(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) + 0.01*rnorm(nrow(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, refit = TRUE, ...)
```

Arguments

`object`	S3 Kriging object.
`y_u`	Numeric vector of new responses (output).
`X_u`	Numeric matrix of new input points.
`refit`	Logical. If `TRUE` the model is refitted (default is FALSE).
`...`	Ignored.

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 the methods `update.km` in **DiceKriging** and `update,KM-method`.

Author(s)

Yann Richet <yann.richet@irsn.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.NoiseKriging *Update a* NoiseKriging *model object with new points*

Description

Update a NoiseKriging model object with new points

Usage

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

Arguments

object	S3 NoiseKriging object.
y_u	Numeric vector of new responses (output).
noise_u	Numeric vector of new noise variances (output).
X_u	Numeric matrix of new input points.
refit	Logical. If TRUE the model is refitted (default is FALSE).
...	Ignored.

Value

No return value. NoiseKriging 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 the methods update.km in **DiceKriging** and update,KM-method.

Author(s)

Yann Richet <yann.richet@irsn.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) + X/10 * rnorm(nrow(X))
points(X, y, col = "blue")

k <- NoiseKriging(y, (X/10)^2, 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) + 0.1 * rnorm(nrow(X_u))
points(X_u, y_u, col = "red")

## change the content of the object 'k'
update(k, y_u, rep(0.1^2,3), 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.NuggetKriging` *Update a* `NuggetKriging` *model object with new points*

Description

Update a `NuggetKriging` model object with new points

Usage

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

Arguments

`object`	S3 NuggetKriging object.
`y_u`	Numeric vector of new responses (output).
`X_u`	Numeric matrix of new input points.
`refit`	Logical. If `TRUE` the model is refitted (default is FALSE).
`...`	Ignored.

Value

No return value. NuggetKriging 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 the methods `update.km` in **DiceKriging** and `update,KM-method`.

Author(s)

Yann Richet <yann.richet@irsn.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) + 0.1 * rnorm(nrow(X))
points(X, y, col = "blue")

k <- NuggetKriging(y, X, "matern3_2")
```

```
## include design points to see interpolation
x <- sort(c(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) + 0.1 * rnorm(nrow(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_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, ...)
```

Arguments

object	S3 Kriging object.
y_u	Numeric vector of new responses (output).
X_u	Numeric matrix of new input points.
...	Ignored.

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@irsn.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.NoiseKriging` *Update previous simulation of a* `NoiseKriging` *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 'NoiseKriging'
update_simulate(object, y_u, noise_u, X_u, ...)
```

Arguments

`object`	S3 NoiseKriging object.
`y_u`	Numeric vector of new responses (output).
`noise_u`	Numeric vector of new noise variances (output).
`X_u`	Numeric matrix of new input points.
`...`	Ignored.

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@irsn.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) + X/10 * rnorm(nrow(X))
points(X, y, col = "blue")

k <- NoiseKriging(y, (X/10)^2, X, "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) + 0.1 * rnorm(nrow(X_u))
points(X_u, y_u, col = "red")

su <- k$update_simulate(y_u, rep(0.1^2,3), 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.NuggetKriging

Update previous simulation of a `NuggetKriging` *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 'NuggetKriging'
update_simulate(object, y_u, X_u, ...)
```

Arguments

`object`	S3 NuggetKriging object.
`y_u`	Numeric vector of new responses (output).
`X_u`	Numeric matrix of new input points.
`...`	Ignored.

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@irsn.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) + 0.1 * rnorm(nrow(X))
points(X, y, col = "blue")

k <- NuggetKriging(y, X, "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) + 0.1 * rnorm(nrow(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)
```

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