

Package ‘GauPro’

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Type Package

Title Gaussian Process Fitting

Version 0.2.17

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Description Fits a Gaussian process model to data. Gaussian processes are commonly used in computer experiments to fit an interpolating model. The model is stored as an 'R6' object and can be easily updated with new data. There are options to run in parallel, and 'Rcpp' has been used to speed up calculations. For more info about Gaussian process software, see Erickson et al. (2018) <[doi:10.1016/j.ejor.2017.10.002](https://doi.org/10.1016/j.ejor.2017.10.002)>.

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LinkingTo Rcpp, RcppArmadillo

Imports ggplot2, Rcpp, R6, lbfgs

RoxygenNote 7.3.2

Depends mixopt (> 0.1.0), numDeriv, rmarkdown, tidy

Suggests ContourFunctions, dplyr, ggrepel, gridExtra, knitr, lhs, MASS, microbenchmark, rlang, splitfng, testthat, testthatmulti

VignetteBuilder knitr

URL <https://github.com/CollinErickson/GauPro>

BugReports <https://github.com/CollinErickson/GauPro/issues>

Encoding UTF-8

NeedsCompilation yes

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*.GauPro_kernel	<i>Kernel product</i>
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Description

Kernel product

Usage

```
## S3 method for class 'GauPro_kernel'
k1 * k2
```

Arguments

k1	First kernel
k2	Second kernel

Value

Kernel which is product of two kernels

Examples

```
k1 <- Exponential$new(beta=1)
k2 <- Matern32$new(beta=0)
k <- k1 * k2
k$k(matrix(c(2,1), ncol=1))
```

<code>+.GauPro_kernel</code>	<i>Kernel sum</i>
------------------------------	-------------------

Description

Kernel sum

Usage

```
## S3 method for class 'GauPro_kernel'
k1 + k2
```

Arguments

<code>k1</code>	First kernel
<code>k2</code>	Second kernel

Value

Kernel which is sum of two kernels

Examples

```
k1 <- Exponential$new(beta=1)
k2 <- Matern32$new(beta=0)
k <- k1 + k2
k$k(matrix(c(2,1), ncol=1))
```

<code>arma_mult_cube_vec</code>	<i>Cube multiply over first dimension</i>
---------------------------------	---

Description

The result is transposed since that is what apply will give you

Usage

```
arma_mult_cube_vec(cub, v)
```

Arguments

<code>cub</code>	A cube (3D array)
<code>v</code>	A vector

Value

Transpose of multiplication over first dimension of cub time v

Examples

```
d1 <- 10
d2 <- 1e2
d3 <- 2e2
aa <- array(data = rnorm(d1*d2*d3), dim = c(d1, d2, d3))
bb <- rnorm(d3)
t1 <- apply(aa, 1, function(U) {U*%bb})
t2 <- arma_mult_cube_vec(aa, bb)
dd <- t1 - t2

summary(dd)
image(dd)
table(dd)
# microbenchmark::microbenchmark(apply(aa, 1, function(U) {U*%bb}),
#                                arma_mult_cube_vec(aa, bb))
```

corr_cubic_matrix_symC

Correlation Cubic matrix in C (symmetric)

Description

Correlation Cubic matrix in C (symmetric)

Usage

```
corr_cubic_matrix_symC(x, theta)
```

Arguments

x	Matrix x
theta	Theta vector

Value

Correlation matrix

Examples

```
corr_cubic_matrix_symC(matrix(c(1,0,0,1),2,2),c(1,1))
```

corr_exponential_matrix_symC

Correlation Gaussian matrix in C (symmetric)

Description

Correlation Gaussian matrix in C (symmetric)

Usage

corr_exponential_matrix_symC(x, theta)

Arguments

x	Matrix x
theta	Theta vector

Value

Correlation matrix

Examples

```
corr_gauss_matrix_symC(matrix(c(1,0,0,1),2,2),c(1,1))
```

corr_gauss_dCdX

Correlation Gaussian matrix gradient in C using Armadillo

Description

Correlation Gaussian matrix gradient in C using Armadillo

Usage

corr_gauss_dCdX(XX, X, theta, s2)

Arguments

XX	Matrix XX to get gradient for
X	Matrix X GP was fit to
theta	Theta vector
s2	Variance parameter

Value

3-dim array of correlation derivative

Examples

```
# corr_gauss_dCdX(matrix(c(1,0,0,1),2,2),c(1,1))
```

corr_gauss_matrix	<i>Gaussian correlation</i>
-------------------	-----------------------------

Description

Gaussian correlation

Usage

```
corr_gauss_matrix(x, x2 = NULL, theta)
```

Arguments

x	First data matrix
x2	Second data matrix
theta	Correlation parameter

Value

Correlation matrix

Examples

```
corr_gauss_matrix(matrix(1:10,ncol=1), matrix(6:15,ncol=1), 1e-2)
```

corr_gauss_matrixC	<i>Correlation Gaussian matrix in C using Rcpp</i>
--------------------	--

Description

Correlation Gaussian matrix in C using Rcpp

Usage

```
corr_gauss_matrixC(x, y, theta)
```

Arguments

x	Matrix x
y	Matrix y, must have same number of columns as x
theta	Theta vector

corr_gauss_matrix_symC

Correlation Gaussian matrix in C (symmetric)

Description

Correlation Gaussian matrix in C (symmetric)

Usage

corr_gauss_matrix_symC(x, theta)

Arguments

x	Matrix x
theta	Theta vector

Value

Correlation matrix

Examples

corr_gauss_matrix_symC(matrix(c(1,0,0,1),2,2),c(1,1))

corr_gauss_matrix_sym_armaC

Correlation Gaussian matrix in C using Armadillo (symmetric)

Description

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Usage

corr_gauss_matrix_sym_armaC(x, theta)

Arguments

x	Matrix x
theta	Theta vector

Value

Correlation matrix

Examples

```
corr_gauss_matrix_sym_armaC(matrix(c(1,0,0,1),2,2),c(1,1))

x3 <- matrix(runif(1e3*6), ncol=6)
th <- runif(6)
t3 <- corr_gauss_matrix_symC(x3, th)
t4 <- corr_gauss_matrix_sym_armaC(x3, th)
identical(t3, t4)
# microbenchmark::microbenchmark(corr_gauss_matrix_symC(x3, th),
#                                corr_gauss_matrix_sym_armaC(x3, th), times=50)
```

```
corr_latentfactor_matrixmatrixC
```

Correlation Latent factor matrix in C (symmetric)

Description

Correlation Latent factor matrix in C (symmetric)

Usage

```
corr_latentfactor_matrixmatrixC(x, y, theta, xindex, latentdim, offdiagequal)
```

Arguments

x	Matrix x
y	Matrix y
theta	Theta vector
xindex	Index to use
latentdim	Number of latent dimensions
offdiagequal	What to set off-diagonal values with matching values to.

Value

Correlation matrix

Examples

```
corr_latentfactor_matrixmatrixC(matrix(c(1,.5, 2,1.6, 1,0),ncol=2,byrow=TRUE),
                                matrix(c(2,1.6, 1,0),ncol=2,byrow=TRUE),
                                c(1.5,1.8), 1, 1, 1-1e-6)
corr_latentfactor_matrixmatrixC(matrix(c(0,0,0,1,0,0,0,2,0,0,0,3,0,0,0,4),
                                ncol=4, byrow=TRUE),
                                matrix(c(0,0,0,2,0,0,0,4,0,0,0,1),
                                ncol=4, byrow=TRUE),
                                c(0.101, -0.714, 0.114, -0.755, 0.117, -0.76, 0.116, -0.752),
                                4, 2, 1-1e-6) * 6.85
```

corr_latentfactor_matrix_symC
Correlation Latent factor matrix in C (symmetric)

Description

Correlation Latent factor matrix in C (symmetric)

Usage

```
corr_latentfactor_matrix_symC(x, theta, xindex, latentdim, offdiagequal)
```

Arguments

x	Matrix x
theta	Theta vector
xindex	Index to use
latentdim	Number of latent dimensions
offdiagequal	What to set off-diagonal values with matching values to.

Value

Correlation matrix

Examples

```
corr_latentfactor_matrix_symC(matrix(c(1, .5, 2, 1.6, 1, 0), ncol=2, byrow=TRUE),
                                c(1.5, 1.8), 1, 1, 1-1e-6)
corr_latentfactor_matrix_symC(matrix(c(0, 0, 0, 1, 0, 0, 0, 2, 0, 0, 0, 3, 0, 0, 0, 4),
                                ncol=4, byrow=TRUE),
                                c(0.101, -0.714, 0.114, -0.755, 0.117, -0.76, 0.116, -0.752),
                                4, 2, 1-1e-6) * 6.85
```

corr_matern32_matrix_symC
Correlation Matern 3/2 matrix in C (symmetric)

Description

Correlation Matern 3/2 matrix in C (symmetric)

Usage

```
corr_matern32_matrix_symC(x, theta)
```

Arguments

x	Matrix x
theta	Theta vector

Value

Correlation matrix

Examples

```
corr_gauss_matrix_symC(matrix(c(1,0,0,1),2,2),c(1,1))
```

```
corr_matern52_matrix_symC
```

Correlation Gaussian matrix in C (symmetric)

Description

Correlation Gaussian matrix in C (symmetric)

Usage

```
corr_matern52_matrix_symC(x, theta)
```

Arguments

x	Matrix x
theta	Theta vector

Value

Correlation matrix

Examples

```
corr_matern52_matrix_symC(matrix(c(1,0,0,1),2,2),c(1,1))
```

 corr_orderedfactor_matrixmatrixC

Correlation ordered factor matrix in C (symmetric)

Description

Correlation ordered factor matrix in C (symmetric)

Usage

```
corr_orderedfactor_matrixmatrixC(x, y, theta, xindex, offdiagequal)
```

Arguments

x	Matrix x
y	Matrix y
theta	Theta vector
xindex	Index to use
offdiagequal	What to set off-diagonal values with matching values to.

Value

Correlation matrix

Examples

```
corr_orderedfactor_matrixmatrixC(matrix(c(1,.5, 2,1.6, 1,0),ncol=2,byrow=TRUE),
  matrix(c(2,1.6, 1,0),ncol=2,byrow=TRUE),
  c(1.5,1.8), 1, 1-1e-6)
corr_orderedfactor_matrixmatrixC(matrix(c(0,0,0,1,0,0,0,2,0,0,0,3,0,0,0,4),
  ncol=4, byrow=TRUE),
  matrix(c(0,0,0,2,0,0,0,4,0,0,0,1),
  ncol=4, byrow=TRUE),
  c(0.101, -0.714, 0.114, -0.755, 0.117, -0.76, 0.116, -0.752),
  4, 1-1e-6) * 6.85
```

 corr_orderedfactor_matrix_symC

Correlation ordered factor matrix in C (symmetric)

Description

Correlation ordered factor matrix in C (symmetric)

Usage

```
corr_orderedfactor_matrix_symC(x, theta, xindex, offdiagequal)
```

Arguments

x	Matrix x
theta	Theta vector
xindex	Index to use
offdiagequal	What to set off-diagonal values with matching values to.

Value

Correlation matrix

Examples

```
corr_orderedfactor_matrix_symC(matrix(c(1,.5, 2,1.6, 1,0),ncol=2,byrow=TRUE),
                                c(1.5,1.8), 1, 1-1e-6)
corr_orderedfactor_matrix_symC(matrix(c(0,0,0,1,0,0,0,2,0,0,0,3,0,0,0,4),
                                ncol=4, byrow=TRUE),
                                c(0.101, -0.714, 0.114, -0.755, 0.117, -0.76, 0.116, -0.752),
                                4, 1-1e-6) * 6.85
```

Cubic

Cubic Kernel R6 class

Description

Cubic Kernel R6 class

Cubic Kernel R6 class

Usage

```
k_Cubic(
  beta,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
  beta_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  isotropic = FALSE
)
```

Arguments

beta	Initial beta value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster.
isotropic	If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/beta is used for each dimension.

Format

`R6Class` object.

Value

Object of `R6Class` with methods for fitting GP model.

Super classes

`GauPro::GauPro_kernel` -> `GauPro::GauPro_kernel_beta` -> `GauPro_kernel_Cubic`

Methods**Public methods:**

- `Cubic$k()`
- `Cubic$kone()`
- `Cubic$dC_dparams()`
- `Cubic$dC_dx()`
- `Cubic$print()`
- `Cubic$clone()`

Method `k()`: Calculate covariance between two points

Usage:

`Cubic$k(x, y = NULL, beta = self$beta, s2 = self$s2, params = NULL)`

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

beta Correlation parameters.

s2 Variance parameter.
 params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

`Cubic$kone(x, y, beta, theta, s2)`

Arguments:

x vector

y vector

beta correlation parameters on log scale

theta correlation parameters on regular scale

s2 Variance parameter

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

`Cubic$dC_dparams(params = NULL, X, C_nonug, C, nug)`

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method `dC_dx()`: Derivative of covariance with respect to X

Usage:

`Cubic$dC_dx(XX, X, theta, beta = self$beta, s2 = self$s2)`

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

theta Correlation parameters

beta log of theta

s2 Variance parameter

Method `print()`: Print this object

Usage:

`Cubic$print()`

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

`Cubic$clone(deep = FALSE)`

Arguments:

deep Whether to make a deep clone.

Examples

```

k1 <- Cubic$new(beta=runif(6)-.5)
plot(k1)

n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel=Cubic$new(1),
                             parallel=FALSE, restarts=0)

gp$predict(.454)

```

Exponential

Exponential Kernel R6 class

Description

Exponential Kernel R6 class

Exponential Kernel R6 class

Usage

```

k_Exponential(
  beta,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
  beta_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  isotropic = FALSE
)

```

Arguments

beta	Initial beta value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2

s2_est	Should s2 be estimated?
useC	Should C code used? Much faster.
isotropic	If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/beta is used for each dimension.

Format

R6Class object.

Value

Object of R6Class with methods for fitting GP model.

Super classes

GauPro : GauPro_kernel -> GauPro : GauPro_kernel_beta -> GauPro_kernel_Exponential

Methods**Public methods:**

- Exponential\$k()
- Exponential\$kone()
- Exponential\$dC_dparams()
- Exponential\$dC_dx()
- Exponential\$print()
- Exponential\$clone()

Method k(): Calculate covariance between two points

Usage:

Exponential\$k(x, y = NULL, beta = self\$beta, s2 = self\$s2, params = NULL)

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

beta Correlation parameters.

s2 Variance parameter.

params parameters to use instead of beta and s2.

Method kone(): Find covariance of two points

Usage:

Exponential\$kone(x, y, beta, theta, s2)

Arguments:

x vector

y vector

beta correlation parameters on log scale

theta correlation parameters on regular scale

s2 Variance parameter

Method dC_dparams(): Derivative of covariance with respect to parameters

Usage:

```
Exponential$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
Exponential$dC_dx(XX, X, theta, beta = self$beta, s2 = self$s2)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

theta Correlation parameters

beta log of theta

s2 Variance parameter

Method print(): Print this object

Usage:

```
Exponential$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
Exponential$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- Exponential$new(beta=0)
```

FactorKernel

*Factor Kernel R6 class***Description**

Initialize kernel object

Usage

```

k_FactorKernel(
  s2 = 1,
  D,
  nlevels,
  xindex,
  p_lower = 0,
  p_upper = 0.9,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  p,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)

```

Arguments

s2	Initial variance
D	Number of input dimensions of data
nlevels	Number of levels for the factor
xindex	Index of the factor (which column of X)
p_lower	Lower bound for p
p_upper	Upper bound for p
p_est	Should p be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
p	Vector of correlations
useC	Should C code used? Not implemented for FactorKernel yet.
offdiagequal	What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Format

R6Class object.

Details

For a factor that has been converted to its indices. Each factor will need a separate kernel.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro::GauPro_kernel](#) -> [GauPro_kernel_FactorKernel](#)

Public fields

`p` Parameter for correlation

`p_est` Should `p` be estimated?

`p_lower` Lower bound of `p`

`p_upper` Upper bound of `p`

`p_length` length of `p`

`s2` variance

`s2_est` Is `s2` estimated?

`logs2` Log of `s2`

`logs2_lower` Lower bound of `logs2`

`logs2_upper` Upper bound of `logs2`

`xindex` Index of the factor (which column of `X`)

`nlevels` Number of levels for the factor

`offdiagequal` What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Methods**Public methods:**

- [FactorKernel\\$new\(\)](#)
- [FactorKernel\\$k\(\)](#)
- [FactorKernel\\$kone\(\)](#)
- [FactorKernel\\$dC_dparams\(\)](#)
- [FactorKernel\\$C_dC_dparams\(\)](#)
- [FactorKernel\\$dC_dx\(\)](#)
- [FactorKernel\\$param_optim_start\(\)](#)
- [FactorKernel\\$param_optim_start0\(\)](#)
- [FactorKernel\\$param_optim_lower\(\)](#)
- [FactorKernel\\$param_optim_upper\(\)](#)
- [FactorKernel\\$set_params_from_optim\(\)](#)
- [FactorKernel\\$s2_from_params\(\)](#)

- `FactorKernel$print()`
- `FactorKernel$clone()`

Method `new()`: Initialize kernel object

Usage:

```
FactorKernel$new(
  s2 = 1,
  D,
  nlevels,
  xindex,
  p_lower = 0,
  p_upper = 0.9,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  p,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)
```

Arguments:

`s2` Initial variance

`D` Number of input dimensions of data

`nlevels` Number of levels for the factor

`xindex` Index of the factor (which column of X)

`p_lower` Lower bound for p

`p_upper` Upper bound for p

`p_est` Should p be estimated?

`s2_lower` Lower bound for s2

`s2_upper` Upper bound for s2

`s2_est` Should s2 be estimated?

`p` Vector of correlations

`useC` Should C code used? Not implemented for FactorKernel yet.

`offdiagequal` What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Method `k()`: Calculate covariance between two points

Usage:

```
FactorKernel$k(x, y = NULL, p = self$p, s2 = self$s2, params = NULL)
```

Arguments:

`x` vector.

`y` vector, optional. If excluded, find correlation of x with itself.

`p` Correlation parameters.

`s2` Variance parameter.

params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

```
FactorKernel$kone(x, y, p, s2, isdiag = TRUE, offdiagequal = self$offdiagequal)
```

Arguments:

x vector

y vector

p correlation parameters on regular scale

s2 Variance parameter

isdiag Is this on the diagonal of the covariance?

offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

```
FactorKernel$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method `C_dC_dparams()`: Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
FactorKernel$C_dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters

X matrix of points in rows

nug Value of nugget

Method `dC_dx()`: Derivative of covariance with respect to X

Usage:

```
FactorKernel$dC_dx(XX, X, ...)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

... Additional args, not used

Method `param_optim_start()`: Starting point for parameters for optimization

Usage:

```
FactorKernel$param_optim_start(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?

y Output

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

```
FactorKernel$param_optim_start0(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?

y Output

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

```
FactorKernel$param_optim_lower(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```
FactorKernel$param_optim_upper(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:


```
FactorKernel$set_params_from_optim(
  optim_out,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

optim_out Output from optimization
 p_est Is p being estimated?
 s2_est Is s2 being estimated?

Method s2_from_params(): Get s2 from params vector

Usage:

```
FactorKernel$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

params parameter vector
 s2_est Is s2 being estimated?

Method print(): Print this object

Usage:

```
FactorKernel$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
FactorKernel$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
kk <- FactorKernel$new(D=1, nlevels=5, xindex=1)
kk$p <- (1:10)/100
kmat <- outer(1:5, 1:5, Vectorize(kk$k))
kmat
kk$plot()

# 2D, Gaussian on 1D, index on 2nd dim
if (requireNamespace("dplyr", quietly=TRUE)) {
  library(dplyr)
  n <- 20
  X <- cbind(matrix(runif(n,2,6), ncol=1),
             matrix(sample(1:2, size=n, replace=TRUE), ncol=1))
  X <- rbind(X, c(3.3,3))
  n <- nrow(X)
  Z <- X[,1] - (X[,2]-1.8)^2 + rnorm(n,0,.1)
  tibble(X=X, Z) %>% arrange(X,Z)
  k2a <- IgnoreIndsKernel$new(k=Gaussian$new(D=1), ignoreinds = 2)
```

```

k2b <- FactorKernel$new(D=2, nlevels=3, xind=2)
k2 <- k2a * k2b
k2b$p_upper <- .65*k2b$p_upper
gp <- GauPro_kernel_model$new(X=X, Z=Z, kernel = k2, verbose = 5,
                              nug.min=1e-2, restarts=0)

gp$kernel$k1$kernel$beta
gp$kernel$k2$p
gp$kernel$k(x = gp$X)
tibble(X=X, Z=Z, pred=gp$predict(X)) %>% arrange(X, Z)
tibble(X=X[,2], Z) %>% group_by(X) %>% summarize(n=n(), mean(Z))
curve(gp$pred(cbind(matrix(x,ncol=1),1)),2,6, ylim=c(min(Z), max(Z)))
points(X[X[,2]==1,1], Z[X[,2]==1])
curve(gp$pred(cbind(matrix(x,ncol=1),2)), add=TRUE, col=2)
points(X[X[,2]==2,1], Z[X[,2]==2], col=2)
curve(gp$pred(cbind(matrix(x,ncol=1),3)), add=TRUE, col=3)
points(X[X[,2]==3,1], Z[X[,2]==3], col=3)
legend(legend=1:3, fill=1:3, x="topleft")
# See which points affect (5.5, 3) the most
data.frame(X, cov=gp$kernel$k(X, c(5.5,3))) %>% arrange(-cov)
plot(k2b)
}

```

GauPro

GauPro_selector

Description

GauPro_selector

Usage

```
GauPro(..., type = "Gauss")
```

Arguments

...	Pass on
type	Type of Gaussian process, or the kind of correlation function.

Value

A GauPro object

Examples

```

n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
#y <- sin(2*pi*x) + rnorm(n,0,1e-1)
y <- (2*x) %1
gp <- GauPro(X=x, Z=y, parallel=FALSE)

```

GauPro_base

*Class providing object with methods for fitting a GP model***Description**

Class providing object with methods for fitting a GP model

Class providing object with methods for fitting a GP model

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Methods

`new(X, Z, corr="Gauss", verbose=0, separable=T, useC=F, useGrad=T, parallel=T, nug.est=T, ...)`

This method is used to create object of this class with X and Z as the data.

`update(Xnew=NULL, Znew=NULL, Xall=NULL, Zall=NULL, restarts = 5, param_update = T, nug.update = self$nug.`

This method updates the model, adding new data if given, then running optimization again.

Public fields

X Design matrix

Z Responses

N Number of data points

D Dimension of data

nug.min Minimum value of nugget

nug Value of the nugget, is estimated unless told otherwise

verbose 0 means nothing printed, 1 prints some, 2 prints most.

useGrad Should grad be used?

useC Should C code be used?

parallel Should the code be run in parallel?

parallel_cores How many cores are there? It will self detect, do not set yourself.

nug.est Should the nugget be estimated?

param.est Should the parameters be estimated?

mu_hat Mean estimate

s2_hat Variance estimate

K Covariance matrix

Kchol Cholesky factorization of K

Kinv Inverse of K

Methods

Public methods:

- `GauPro_base$corr_func()`
- `GauPro_base$new()`
- `GauPro_base$initialize_GauPr()`
- `GauPro_base$fit()`
- `GauPro_base$update_K_and_estimates()`
- `GauPro_base$predict()`
- `GauPro_base$pred()`
- `GauPro_base$pred_one_matrix()`
- `GauPro_base$pred_mean()`
- `GauPro_base$pred_meanC()`
- `GauPro_base$pred_var()`
- `GauPro_base$pred_L00()`
- `GauPro_base$plot()`
- `GauPro_base$cool1Dplot()`
- `GauPro_base$plot1D()`
- `GauPro_base$plot2D()`
- `GauPro_base$loglikelihood()`
- `GauPro_base$optim()`
- `GauPro_base$optimRestart()`
- `GauPro_base$update()`
- `GauPro_base$update_data()`
- `GauPro_base$update_corrparams()`
- `GauPro_base$update_nugget()`
- `GauPro_base$deviance_searchnug()`
- `GauPro_base$nugget_update()`
- `GauPro_base$grad_norm()`
- `GauPro_base$sample()`
- `GauPro_base$print()`
- `GauPro_base$clone()`

Method `corr_func()`: Correlation function

Usage:

```
GauPro_base$corr_func(...)
```

Arguments:

... Does nothing

Method `new()`: Create GauPro object

Usage:

```
GauPro_base$new(
  X,
  Z,
  verbose = 0,
  useC = F,
  useGrad = T,
  parallel = FALSE,
  nug = 1e-06,
  nug.min = 1e-08,
  nug.est = T,
  param.est = TRUE,
  ...
)
```

Arguments:

X Matrix whose rows are the input points

Z Output points corresponding to X

verbose Amount of stuff to print. 0 is little, 2 is a lot.

useC Should C code be used when possible? Should be faster.

useGrad Should the gradient be used?

parallel Should code be run in parallel? Make optimization faster but uses more computer resources.

nug Value for the nugget. The starting value if estimating it.

nug.min Minimum allowable value for the nugget.

nug.est Should the nugget be estimated?

param.est Should the kernel parameters be estimated?

... Not used

Method initialize_GauPr(): Not used

Usage:

```
GauPro_base$initialize_GauPr()
```

Method fit(): Fit the model, never use this function

Usage:

```
GauPro_base$fit(X, Z)
```

Arguments:

X Not used

Z Not used

Method update_K_and_estimates(): Update Covariance matrix and estimated parameters

Usage:

```
GauPro_base$update_K_and_estimates()
```

Method predict(): Predict mean and se for given matrix

Usage:

```
GauPro_base$predict(XX, se.fit = F, covmat = F, split_speed = T)
```

Arguments:

XX Points to predict at

se.fit Should the se be returned?

covmat Should the covariance matrix be returned?

split_speed Should the predictions be split up for speed

Method `pred()`: Predict mean and se for given matrix

Usage:

```
GauPro_base$pred(XX, se.fit = F, covmat = F, split_speed = T)
```

Arguments:

XX Points to predict at

se.fit Should the se be returned?

covmat Should the covariance matrix be returned?

split_speed Should the predictions be split up for speed

Method `pred_one_matrix()`: Predict mean and se for given matrix

Usage:

```
GauPro_base$pred_one_matrix(XX, se.fit = F, covmat = F)
```

Arguments:

XX Points to predict at

se.fit Should the se be returned?

covmat Should the covariance matrix be returned?

Method `pred_mean()`: Predict mean

Usage:

```
GauPro_base$pred_mean(XX, kx.xx)
```

Arguments:

XX Points to predict at

kx.xx Covariance matrix between X and XX

Method `pred_meanC()`: Predict mean using C code

Usage:

```
GauPro_base$pred_meanC(XX, kx.xx)
```

Arguments:

XX Points to predict at

kx.xx Covariance matrix between X and XX

Method `pred_var()`: Predict variance

Usage:

```
GauPro_base$pred_var(XX, kxx, kx.xx, covmat = F)
```

Arguments:

XX Points to predict at

kxx Covariance matrix of XX with itself
 kx.xx Covariance matrix between X and XX
 covmat Not used

Method `pred_L00()`: Predict at X using leave-one-out. Can use for diagnostics.

Usage:

```
GauPro_base$pred_L00(se.fit = FALSE)
```

Arguments:

`se.fit` Should the standard error and t values be returned?

Method `plot()`: Plot the object

Usage:

```
GauPro_base$plot(...)
```

Arguments:

... Parameters passed to `cool1Dplot()`, `plot2D()`, or `plotmarginal()`

Method `cool1Dplot()`: Make cool 1D plot

Usage:

```
GauPro_base$cool1Dplot(
  n2 = 20,
  nn = 201,
  col2 = "gray",
  xlab = "x",
  ylab = "y",
  xmin = NULL,
  xmax = NULL,
  ymin = NULL,
  ymax = NULL
)
```

Arguments:

`n2` Number of things to plot

`nn` Number of things to plot

`col2` color

`xlab` x label

`ylab` y label

`xmin` xmin

`xmax` xmax

`ymin` ymin

`ymax` ymax

Method `plot1D()`: Make 1D plot

Usage:

```
GauPro_base$plot1D(
  n2 = 20,
  nn = 201,
  col2 = 2,
  xlab = "x",
  ylab = "y",
  xmin = NULL,
  xmax = NULL,
  ymin = NULL,
  ymax = NULL
)
```

Arguments:

n2 Number of things to plot
 nn Number of things to plot
 col2 Color of the prediction interval
 xlab x label
 ylab y label
 xmin xmin
 xmax xmax
 ymin ymin
 ymax ymax

Method plot2D(): Make 2D plot

Usage:

```
GauPro_base$plot2D()
```

Method loglikelihood(): Calculate the log likelihood, don't use this

Usage:

```
GauPro_base$loglikelihood(mu = self$mu_hat, s2 = self$s2_hat)
```

Arguments:

mu Mean vector
 s2 s2 param

Method optim(): Optimize parameters

Usage:

```
GauPro_base$optim(
  restarts = 5,
  param_update = T,
  nug.update = self$nug.est,
  parallel = self$parallel,
  parallel_cores = self$parallel_cores
)
```

Arguments:

restarts Number of restarts to do

param_update Should parameters be updated?
 nug.update Should nugget be updated?
 parallel Should restarts be done in parallel?
 parallel_cores If running parallel, how many cores should be used?

Method optimRestart(): Run a single optimization restart.

Usage:

```
GauPro_base$optimRestart(
  start.par,
  start.par0,
  param_update,
  nug.update,
  optim.func,
  optim.grad,
  optim.fngr,
  lower,
  upper,
  jit = T
)
```

Arguments:

start.par Starting parameters
 start.par0 Starting parameters
 param_update Should parameters be updated?
 nug.update Should nugget be updated?
 optim.func Function to optimize.
 optim.grad Gradient of function to optimize.
 optim.fngr Function that returns the function value and its gradient.
 lower Lower bounds for optimization
 upper Upper bounds for optimization
 jit Is jitter being used?

Method update(): Update the model, can be data and parameters

Usage:

```
GauPro_base$update(
  Xnew = NULL,
  Znew = NULL,
  Xall = NULL,
  Zall = NULL,
  restarts = 5,
  param_update = self$param.est,
  nug.update = self$nug.est,
  no_update = FALSE
)
```

Arguments:

Xnew New X matrix

Znew New Z values
Xall Matrix with all X values
Zall All Z values
restarts Number of optimization restarts
param_update Should the parameters be updated?
nug.update Should the nugget be updated?
no_update Should none of the parameters/nugget be updated?

Method update_data(): Update the data

Usage:

```
GauPro_base$update_data(Xnew = NULL, Znew = NULL, Xall = NULL, Zall = NULL)
```

Arguments:

Xnew New X matrix
Znew New Z values
Xall Matrix with all X values
Zall All Z values

Method update_corrparams(): Update the correlation parameters

Usage:

```
GauPro_base$update_corrparams(...)
```

Arguments:

... Args passed to update

Method update_nugget(): Update the nugget

Usage:

```
GauPro_base$update_nugget(...)
```

Arguments:

... Args passed to update

Method deviance_searchnug(): Optimize deviance for nugget

Usage:

```
GauPro_base$deviance_searchnug()
```

Method nugget_update(): Update the nugget

Usage:

```
GauPro_base$nugget_update()
```

Method grad_norm(): Calculate the norm of the gradient at XX

Usage:

```
GauPro_base$grad_norm(XX)
```

Arguments:

XX Points to calculate at

Method `sample()`: Sample at XX

Usage:

```
GauPro_base$sample(XX, n = 1)
```

Arguments:

XX Input points to sample at

n Number of samples

Method `print()`: Print object

Usage:

```
GauPro_base$print()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
GauPro_base$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
#n <- 12
#x <- matrix(seq(0,1,length.out = n), ncol=1)
#y <- sin(2*pi*x) + rnorm(n,0,1e-1)
#gp <- GauPro(X=x, Z=y, parallel=FALSE)
```

GauPro_Gauss

Corr Gauss GP using inherited optim

Description

Corr Gauss GP using inherited optim

Corr Gauss GP using inherited optim

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro::GauPro_base](#) -> GauPro_Gauss

Public fields

corr Name of correlation
 theta Correlation parameters
 theta_length Length of theta
 theta_map Map for theta
 theta_short Short vector for theta
 separable Are the dimensions separable?

Methods**Public methods:**

- `GauPro_Gauss$new()`
- `GauPro_Gauss$corr_func()`
- `GauPro_Gauss$deviance_theta()`
- `GauPro_Gauss$deviance_theta_log()`
- `GauPro_Gauss$deviance()`
- `GauPro_Gauss$deviance_grad()`
- `GauPro_Gauss$deviance_fngr()`
- `GauPro_Gauss$deviance_log()`
- `GauPro_Gauss$deviance_log2()`
- `GauPro_Gauss$deviance_log_grad()`
- `GauPro_Gauss$deviance_log2_grad()`
- `GauPro_Gauss$deviance_log2_fngr()`
- `GauPro_Gauss$get_optim_functions()`
- `GauPro_Gauss$param_optim_lower()`
- `GauPro_Gauss$param_optim_upper()`
- `GauPro_Gauss$param_optim_start()`
- `GauPro_Gauss$param_optim_start0()`
- `GauPro_Gauss$param_optim_jitter()`
- `GauPro_Gauss$update_params()`
- `GauPro_Gauss$grad()`
- `GauPro_Gauss$grad_dist()`
- `GauPro_Gauss$hessian()`
- `GauPro_Gauss$print()`
- `GauPro_Gauss$clone()`

Method `new()`: Create GauPro object

Usage:

```
GauPro_Gauss$new(
  X,
  Z,
  verbose = 0,
```

```

    separable = T,
    useC = F,
    useGrad = T,
    parallel = FALSE,
    nug = 1e-06,
    nug.min = 1e-08,
    nug.est = T,
    param.est = T,
    theta = NULL,
    theta_short = NULL,
    theta_map = NULL,
    ...
)

```

Arguments:

X Matrix whose rows are the input points

Z Output points corresponding to *X*

verbose Amount of stuff to print. 0 is little, 2 is a lot.

separable Are dimensions separable?

useC Should C code be used when possible? Should be faster.

useGrad Should the gradient be used?

parallel Should code be run in parallel? Make optimization faster but uses more computer resources.

nug Value for the nugget. The starting value if estimating it.

nug.min Minimum allowable value for the nugget.

nug.est Should the nugget be estimated?

param.est Should the kernel parameters be estimated?

theta Correlation parameters

theta_short Correlation parameters, not recommended

theta_map Correlation parameters, not recommended

... Not used

Method `corr_func()`: Correlation function*Usage:*

```
GauPro_Gauss$corr_func(x, x2 = NULL, theta = self$theta)
```

Arguments:

x First point

x2 Second point

theta Correlation parameter

Method `deviance_theta()`: Calculate deviance*Usage:*

```
GauPro_Gauss$deviance_theta(theta)
```

Arguments:

theta Correlation parameter

Method `deviance_theta_log()`: Calculate deviance

Usage:

```
GauPro_Gauss$deviance_theta_log(beta)
```

Arguments:

beta Correlation parameter on log scale

Method `deviance()`: Calculate deviance

Usage:

```
GauPro_Gauss$deviance(theta = self$theta, nug = self$nug)
```

Arguments:

theta Correlation parameter

nug Nugget

Method `deviance_grad()`: Calculate deviance gradient

Usage:

```
GauPro_Gauss$deviance_grad(
  theta = NULL,
  nug = self$nug,
  joint = NULL,
  overwhat = if (self$nug.est) "joint" else "theta"
)
```

Arguments:

theta Correlation parameter

nug Nugget

joint Calculate over theta and nug at same time?

overwhat Calculate over theta and nug at same time?

Method `deviance_fngr()`: Calculate deviance and gradient at same time

Usage:

```
GauPro_Gauss$deviance_fngr(
  theta = NULL,
  nug = NULL,
  overwhat = if (self$nug.est) "joint" else "theta"
)
```

Arguments:

theta Correlation parameter

nug Nugget

overwhat Calculate over theta and nug at same time?

joint Calculate over theta and nug at same time?

Method `deviance_log()`: Calculate deviance gradient

Usage:

```
GauPro_Gauss$deviance_log(beta = NULL, nug = self$nug, joint = NULL)
```

Arguments:

beta Correlation parameter on log scale
 nug Nugget
 joint Calculate over theta and nug at same time?

Method deviance_log2(): Calculate deviance on log scale

Usage:

```
GauPro_Gauss$deviance_log2(beta = NULL, lognug = NULL, joint = NULL)
```

Arguments:

beta Correlation parameter on log scale
 lognug Log of nugget
 joint Calculate over theta and nug at same time?

Method deviance_log_grad(): Calculate deviance gradient on log scale

Usage:

```
GauPro_Gauss$deviance_log_grad(
  beta = NULL,
  nug = self$nug,
  joint = NULL,
  overwhat = if (self$nug.est) "joint" else "theta"
)
```

Arguments:

beta Correlation parameter
 nug Nugget
 joint Calculate over theta and nug at same time?
 overwhat Calculate over theta and nug at same time?

Method deviance_log2_grad(): Calculate deviance gradient on log scale

Usage:

```
GauPro_Gauss$deviance_log2_grad(
  beta = NULL,
  lognug = NULL,
  joint = NULL,
  overwhat = if (self$nug.est) "joint" else "theta"
)
```

Arguments:

beta Correlation parameter
 lognug Log of nugget
 joint Calculate over theta and nug at same time?
 overwhat Calculate over theta and nug at same time?

Method deviance_log2_fngr(): Calculate deviance and gradient on log scale

Usage:

```
GauPro_Gauss$deviance_log2_fngr(
  beta = NULL,
  lognug = NULL,
  joint = NULL,
  overwhat = if (self$nug.est) "joint" else "theta"
)
```

Arguments:

beta Correlation parameter
 lognug Log of nugget
 joint Calculate over theta and nug at same time?
 overwhat Calculate over theta and nug at same time?

Method get_optim_functions(): Get optimization functions

Usage:

```
GauPro_Gauss$get_optim_functions(param_update, nug.update)
```

Arguments:

param_update Should the parameters be updated?
 nug.update Should the nugget be updated?

Method param_optim_lower(): Lower bound of params

Usage:

```
GauPro_Gauss$param_optim_lower()
```

Method param_optim_upper(): Upper bound of params

Usage:

```
GauPro_Gauss$param_optim_upper()
```

Method param_optim_start(): Start value of params for optim

Usage:

```
GauPro_Gauss$param_optim_start()
```

Method param_optim_start0(): Start value of params for optim

Usage:

```
GauPro_Gauss$param_optim_start0()
```

Method param_optim_jitter(): Jitter value of params for optim

Usage:

```
GauPro_Gauss$param_optim_jitter(param_value)
```

Arguments:

param_value param value to add jitter to

Method update_params(): Update value of params after optim

Usage:

```
GauPro_Gauss$update_params(restarts, param_update, nug.update)
```


Arguments:

restarts Number of restarts
param_update Are the params being updated?
nug.update Is the nugget being updated?

Method grad(): Calculate the gradient

Usage:

```
GauPro_Gauss$grad(XX)
```

Arguments:

XX Points to calculate grad at

Method grad_dist(): Calculate the gradient distribution

Usage:

```
GauPro_Gauss$grad_dist(XX)
```

Arguments:

XX Points to calculate grad at

Method hessian(): Calculate the hessian

Usage:

```
GauPro_Gauss$hessian(XX, useC = self$useC)
```

Arguments:

XX Points to calculate grad at
useC Should C code be used to speed up?

Method print(): Print this object

Usage:

```
GauPro_Gauss$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
GauPro_Gauss$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
n <- 12  
x <- matrix(seq(0,1,length.out = n), ncol=1)  
y <- sin(2*pi*x) + rnorm(n,0,1e-1)  
gp <- GauPro_Gauss$new(X=x, Z=y, parallel=FALSE)
```

GauPro_Gauss_LOO

Corr Gauss GP using inherited optim

Description

Corr Gauss GP using inherited optim

Corr Gauss GP using inherited optim

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super classes

[GauPro::GauPro_base](#) -> [GauPro::GauPro_Gauss](#) -> GauPro_Gauss_LOO

Public fields

use_LOO Should the leave-one-out correction be used?

tmod Second GP model fit to the t-values of leave-one-out predictions

Methods**Public methods:**

- [GauPro_Gauss_LOO\\$update\(\)](#)
- [GauPro_Gauss_LOO\\$pred_one_matrix\(\)](#)
- [GauPro_Gauss_LOO\\$print\(\)](#)
- [GauPro_Gauss_LOO\\$clone\(\)](#)

Method `update()`: Update the model, can be data and parameters

Usage:

```
GauPro_Gauss_LOO$update(
  Xnew = NULL,
  Znew = NULL,
  Xall = NULL,
  Zall = NULL,
  restarts = 5,
  param_update = self$param.est,
  nug.update = self$nug.est,
  no_update = FALSE
)
```

Arguments:

Xnew New X matrix
 Znew New Z values
 Xall Matrix with all X values
 Zall All Z values
 restarts Number of optimization restarts
 param_update Should the parameters be updated?
 nug.update Should the nugget be updated?
 no_update Should none of the parameters/nugget be updated?

Method `pred_one_matrix()`: Predict mean and se for given matrix

Usage:

```
GauPro_Gauss_L00$pred_one_matrix(XX, se.fit = F, covmat = F)
```

Arguments:

XX Points to predict at
 se.fit Should the se be returned?
 covmat Should the covariance matrix be returned?

Method `print()`: Print this object

Usage:

```
GauPro_Gauss_L00$print()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
GauPro_Gauss_L00$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_Gauss_L00$new(X=x, Z=y, parallel=FALSE)
```

GauPro_kernel

Kernel R6 class

Description

Kernel R6 class

Kernel R6 class

Format

R6Class object.

Value

Object of R6Class with methods for fitting GP model.

Public fields

D Number of input dimensions of data

useC Should C code be used when possible? Can be much faster.

Methods**Public methods:**

- `GauPro_kernel$plot()`
- `GauPro_kernel$print()`
- `GauPro_kernel$clone()`

Method `plot()`: Plot kernel decay.

Usage:

```
GauPro_kernel$plot(X = NULL)
```

Arguments:

X Matrix of points the kernel is used with. Some will be used to demonstrate how the covariance changes.

Method `print()`: Print this object

Usage:

```
GauPro_kernel$print()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
GauPro_kernel$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
#k <- GauPro_kernel$new()
```

GauPro_kernel_beta	<i>Beta Kernel R6 class</i>
--------------------	-----------------------------

Description

Beta Kernel R6 class

Beta Kernel R6 class

Format

[R6Class](#) object.

Details

This is the base structure for a kernel that uses $\beta = \log_{10}(\theta)$ for the lengthscale parameter. It standardizes the params because they all use the same underlying structure. Kernels that inherit this only need to implement `kone` and `dC_dparams`.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro:::GauPro_kernel](#) -> `GauPro_kernel_beta`

Public fields

`beta` Parameter for correlation. Log of theta.

`beta_est` Should beta be estimated?

`beta_lower` Lower bound of beta

`beta_upper` Upper bound of beta

`beta_length` length of beta

`s2` variance

`logs2` Log of s2

`logs2_lower` Lower bound of logs2

`logs2_upper` Upper bound of logs2

`s2_est` Should s2 be estimated?

`useC` Should C code used? Much faster.

`isotropic` If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/beta is used for each dimension.

Methods

Public methods:

- `GauPro_kernel_beta$new()`
- `GauPro_kernel_beta$k()`
- `GauPro_kernel_beta$kone()`
- `GauPro_kernel_beta$param_optim_start()`
- `GauPro_kernel_beta$param_optim_start0()`
- `GauPro_kernel_beta$param_optim_lower()`
- `GauPro_kernel_beta$param_optim_upper()`
- `GauPro_kernel_beta$set_params_from_optim()`
- `GauPro_kernel_beta$C_dC_dparams()`
- `GauPro_kernel_beta$s2_from_params()`
- `GauPro_kernel_beta$clone()`

Method `new()`: Initialize kernel object

Usage:

```
GauPro_kernel_beta$new(
  beta,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
  beta_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  isotropic = FALSE
)
```

Arguments:

`beta` Initial beta value

`s2` Initial variance

`D` Number of input dimensions of data

`beta_lower` Lower bound for beta

`beta_upper` Upper bound for beta

`beta_est` Should beta be estimated?

`s2_lower` Lower bound for s2

`s2_upper` Upper bound for s2

`s2_est` Should s2 be estimated?

`useC` Should C code used? Much faster.

`isotropic` If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/beta is used for each dimension.

Method `k()`: Calculate covariance between two points

Usage:

```
GauPro_kernel_beta$k(
  x,
  y = NULL,
  beta = self$beta,
  s2 = self$s2,
  params = NULL
)
```

Arguments:

x vector.
y vector, optional. If excluded, find correlation of x with itself.
beta Correlation parameters. Log of theta.
s2 Variance parameter.
params parameters to use instead of beta and s2.

Method `kone()`: Calculate covariance between two points

Usage:

```
GauPro_kernel_beta$kone(x, y, beta, theta, s2)
```

Arguments:

x vector.
y vector.
beta Correlation parameters. Log of theta.
theta Correlation parameters.
s2 Variance parameter.

Method `param_optim_start()`: Starting point for parameters for optimization

Usage:

```
GauPro_kernel_beta$param_optim_start(
  jitter = F,
  y,
  beta_est = self$beta_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
y Output
beta_est Is beta being estimated?
s2_est Is s2 being estimated?

Method `param_optim_start0()`: Starting point for parameters for optimization

Usage:

```
GauPro_kernel_beta$param_optim_start0(
  jitter = F,
  y,
```

```

    beta_est = self$beta_est,
    s2_est = self$s2_est
  )

```

Arguments:

jitter Should there be a jitter?
 y Output
 beta_est Is beta being estimated?
 s2_est Is s2 being estimated?

Method param_optim_lower(): Upper bounds of parameters for optimization

Usage:

```

GauPro_kernel_beta$param_optim_lower(
  beta_est = self$beta_est,
  s2_est = self$s2_est
)

```

Arguments:

beta_est Is beta being estimated?
 s2_est Is s2 being estimated?
 p_est Is p being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```

GauPro_kernel_beta$param_optim_upper(
  beta_est = self$beta_est,
  s2_est = self$s2_est
)

```

Arguments:

beta_est Is beta being estimated?
 s2_est Is s2 being estimated?
 p_est Is p being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```

GauPro_kernel_beta$set_params_from_optim(
  optim_out,
  beta_est = self$beta_est,
  s2_est = self$s2_est
)

```

Arguments:

optim_out Output from optimization
 beta_est Is beta being estimated?
 s2_est Is s2 being estimated?

Method C_dC_dparams(): Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
GauPro_kernel_beta$dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 nug Value of nugget

Method `s2_from_params()`: Get s2 from params vector

Usage:

```
GauPro_kernel_beta$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

params parameter vector
 s2_est Is s2 being estimated?

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
GauPro_kernel_beta$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
#k1 <- Matern52$new(beta=0)
```

GauPro_kernel_model *Gaussian process model with kernel*

Description

Class providing object with methods for fitting a GP model. Allows for different kernel and trend functions to be used. The object is an R6 object with many methods that can be called.

‘gpkm()’ is equivalent to ‘GauPro_kernel_model\$new()’, but is easier to type and gives parameter autocomplete suggestions.

Format

R6Class object.

Value

Object of R6Class with methods for fitting GP model.

Methods

`new(X, Z, corr="Gauss", verbose=0, separable=T, useC=F, useGrad=T, parallel=T, nug.est=T, ...)`

This method is used to create object of this class with X and Z as the data.

`update(Xnew=NULL, Znew=NULL, Xall=NULL, Zall=NULL, restarts = 0, param_update = T, nug.update = self$nug.)`

This method updates the model, adding new data if given, then running optimization again.

Public fields

X Design matrix

Z Responses

N Number of data points

D Dimension of data

nug.min Minimum value of nugget

nug.max Maximum value of the nugget.

nug.est Should the nugget be estimated?

nug Value of the nugget, is estimated unless told otherwise

param.est Should the kernel parameters be estimated?

verbose 0 means nothing printed, 1 prints some, 2 prints most.

useGrad Should grad be used?

useC Should C code be used?

parallel Should the code be run in parallel?

parallel_cores How many cores are there? By default it detects.

kernel The kernel to determine the correlations.

trend The trend.

mu_hatX Predicted trend value for each point in X.

s2_hat Variance parameter estimate

K Covariance matrix

Kchol Cholesky factorization of K

Kinv Inverse of K

Kinv_Z_minus_mu_hatX K inverse times Z minus the predicted trend at X.

restarts Number of optimization restarts to do when updating.

normalize Should the inputs be normalized?

normalize_mean If using normalize, the mean of each column.

normalize_sd If using normalize, the standard deviation of each column.

optimizer What algorithm should be used to optimize the parameters.

track_optim Should it track the parameters evaluated while optimizing?

track_optim_inputs If track_optim is TRUE, this will keep a list of parameters evaluated. View them with `plot_track_optim`.

track_optim_dev If track_optim is TRUE, this will keep a vector of the deviance values calculated while optimizing parameters. View them with `plot_track_optim`.

formula Formula

convert_formula_data List for storing data to convert data using the formula

Methods**Public methods:**

- `GauPro_kernel_model$new()`
- `GauPro_kernel_model$fit()`
- `GauPro_kernel_model$update_K_and_estimates()`
- `GauPro_kernel_model$predict()`
- `GauPro_kernel_model$pred()`
- `GauPro_kernel_model$pred_one_matrix()`
- `GauPro_kernel_model$pred_mean()`
- `GauPro_kernel_model$pred_meanC()`
- `GauPro_kernel_model$pred_var()`
- `GauPro_kernel_model$pred_LOO()`
- `GauPro_kernel_model$pred_var_after_adding_points()`
- `GauPro_kernel_model$pred_var_after_adding_points_sep()`
- `GauPro_kernel_model$pred_var_reduction()`
- `GauPro_kernel_model$pred_var_reductions()`
- `GauPro_kernel_model$plot()`
- `GauPro_kernel_model$cool1Dplot()`
- `GauPro_kernel_model$plot1D()`
- `GauPro_kernel_model$plot2D()`
- `GauPro_kernel_model$plotmarginal()`
- `GauPro_kernel_model$plotmarginalrandom()`
- `GauPro_kernel_model$plotkernel()`
- `GauPro_kernel_model$plotLOO()`
- `GauPro_kernel_model$plot_track_optim()`
- `GauPro_kernel_model$loglikelihood()`
- `GauPro_kernel_model$AIC()`
- `GauPro_kernel_model$get_optim_functions()`
- `GauPro_kernel_model$param_optim_lower()`
- `GauPro_kernel_model$param_optim_upper()`
- `GauPro_kernel_model$param_optim_start()`
- `GauPro_kernel_model$param_optim_start0()`
- `GauPro_kernel_model$param_optim_start_mat()`
- `GauPro_kernel_model$optim()`
- `GauPro_kernel_model$optimRestart()`
- `GauPro_kernel_model$update()`
- `GauPro_kernel_model$update_fast()`
- `GauPro_kernel_model$update_params()`
- `GauPro_kernel_model$update_data()`
- `GauPro_kernel_model$update_corrparams()`
- `GauPro_kernel_model$update_nugget()`
- `GauPro_kernel_model$deviance()`

- `GauPro_kernel_model$deviance_grad()`
- `GauPro_kernel_model$deviance_fngr()`
- `GauPro_kernel_model$grad()`
- `GauPro_kernel_model$grad_norm()`
- `GauPro_kernel_model$grad_dist()`
- `GauPro_kernel_model$grad_sample()`
- `GauPro_kernel_model$grad_norm2_mean()`
- `GauPro_kernel_model$grad_norm2_dist()`
- `GauPro_kernel_model$grad_norm2_sample()`
- `GauPro_kernel_model$hessian()`
- `GauPro_kernel_model$gradpredvar()`
- `GauPro_kernel_model$sample()`
- `GauPro_kernel_model$optimize_fn()`
- `GauPro_kernel_model$EI()`
- `GauPro_kernel_model$maxEI()`
- `GauPro_kernel_model$maxqEI()`
- `GauPro_kernel_model$KG()`
- `GauPro_kernel_model$AugmentedEI()`
- `GauPro_kernel_model$CorrectedEI()`
- `GauPro_kernel_model$importance()`
- `GauPro_kernel_model$print()`
- `GauPro_kernel_model$summary()`
- `GauPro_kernel_model$clone()`

Method `new()`: Create `kernel_model` object

Usage:

```
GauPro_kernel_model$new(
  X,
  Z,
  kernel,
  trend,
  verbose = 0,
  useC = TRUE,
  useGrad = TRUE,
  parallel = FALSE,
  parallel_cores = "detect",
  nug = 1e-06,
  nug.min = 1e-08,
  nug.max = 100,
  nug.est = TRUE,
  param.est = TRUE,
  restarts = 0,
  normalize = FALSE,
  optimizer = "L-BFGS-B",
  track_optim = FALSE,
```

```

    formula,
    data,
    ...
)

```

Arguments:

X Matrix whose rows are the input points

Z Output points corresponding to *X*

kernel The kernel to use. E.g., `Gaussian$new()`.

trend Trend to use. E.g., `trend_constant$new()`.

verbose Amount of stuff to print. 0 is little, 2 is a lot.

useC Should C code be used when possible? Should be faster.

useGrad Should the gradient be used?

parallel Should code be run in parallel? Make optimization faster but uses more computer resources.

parallel_cores When using parallel, how many cores should be used?

nug Value for the nugget. The starting value if estimating it.

nug.min Minimum allowable value for the nugget.

nug.max Maximum allowable value for the nugget.

nug.est Should the nugget be estimated?

param.est Should the kernel parameters be estimated?

restarts How many optimization restarts should be used when estimating parameters?

normalize Should the data be normalized?

optimizer What algorithm should be used to optimize the parameters.

track_optim Should it track the parameters evaluated while optimizing?

formula Formula for the data if giving in a data frame.

data Data frame of data. Use in conjunction with *formula*.

... Not used

Method `fit()`: Fit model*Usage:*

```
GauPro_kernel_model$fit(X, Z)
```

Arguments:

X Inputs

Z Outputs

Method `update_K_and_estimates()`: Update covariance matrix and estimates*Usage:*

```
GauPro_kernel_model$update_K_and_estimates()
```

Method `predict()`: Predict for a matrix of points*Usage:*

```
GauPro_kernel_model$predict(
  XX,
  se.fit = F,
  covmat = F,
  split_speed = F,
  mean_dist = FALSE,
  return_df = TRUE
)
```

Arguments:

XX points to predict at

se.fit Should standard error be returned?

covmat Should covariance matrix be returned?

split_speed Should the matrix be split for faster predictions?

mean_dist Should the error be for the distribution of the mean?

return_df When returning se.fit, should it be returned in a data frame? Otherwise it will be a list, which is faster.

Method `pred()`: Predict for a matrix of points

Usage:

```
GauPro_kernel_model$pred(
  XX,
  se.fit = F,
  covmat = F,
  split_speed = F,
  mean_dist = FALSE,
  return_df = TRUE
)
```

Arguments:

XX points to predict at

se.fit Should standard error be returned?

covmat Should covariance matrix be returned?

split_speed Should the matrix be split for faster predictions?

mean_dist Should the error be for the distribution of the mean?

return_df When returning se.fit, should it be returned in a data frame? Otherwise it will be a list, which is faster.

Method `pred_one_matrix()`: Predict for a matrix of points

Usage:

```
GauPro_kernel_model$pred_one_matrix(
  XX,
  se.fit = F,
  covmat = F,
  return_df = FALSE,
  mean_dist = FALSE
)
```

Arguments:

XX points to predict at
se.fit Should standard error be returned?
covmat Should covariance matrix be returned?
return_df When returning se.fit, should it be returned in a data frame? Otherwise it will be a list, which is faster.
mean_dist Should the error be for the distribution of the mean?

Method pred_mean(): Predict mean*Usage:*

```
GauPro_kernel_model$pred_mean(XX, kx.xx)
```

Arguments:

XX points to predict at
kx.xx Covariance of X with XX

Method pred_meanC(): Predict mean using C*Usage:*

```
GauPro_kernel_model$pred_meanC(XX, kx.xx)
```

Arguments:

XX points to predict at
kx.xx Covariance of X with XX

Method pred_var(): Predict variance*Usage:*

```
GauPro_kernel_model$pred_var(XX, kxx, kx.xx, covmat = F)
```

Arguments:

XX points to predict at
kxx Covariance of XX with itself
kx.xx Covariance of X with XX
covmat Should the covariance matrix be returned?

Method pred_LOO(): leave one out predictions*Usage:*

```
GauPro_kernel_model$pred_LOO(se.fit = FALSE)
```

Arguments:

se.fit Should standard errors be included?

Method pred_var_after_adding_points(): Predict variance after adding points*Usage:*

```
GauPro_kernel_model$pred_var_after_adding_points(add_points, pred_points)
```

Arguments:

add_points Points to add

pred_points Points to predict at

Method pred_var_after_adding_points_sep(): Predict variance reductions after adding each point separately

Usage:

```
GauPro_kernel_model$pred_var_after_adding_points_sep(add_points, pred_points)
```

Arguments:

add_points Points to add

pred_points Points to predict at

Method pred_var_reduction(): Predict variance reduction for a single point

Usage:

```
GauPro_kernel_model$pred_var_reduction(add_point, pred_points)
```

Arguments:

add_point Point to add

pred_points Points to predict at

Method pred_var_reductions(): Predict variance reductions

Usage:

```
GauPro_kernel_model$pred_var_reductions(add_points, pred_points)
```

Arguments:

add_points Points to add

pred_points Points to predict at

Method plot(): Plot the object

Usage:

```
GauPro_kernel_model$plot(...)
```

Arguments:

... Parameters passed to cool1Dplot(), plot2D(), or plotmarginal()

Method cool1Dplot(): Make cool 1D plot

Usage:

```
GauPro_kernel_model$cool1Dplot(
  n2 = 20,
  nn = 201,
  col2 = "green",
  xlab = "x",
  ylab = "y",
  xmin = NULL,
  xmax = NULL,
  ymin = NULL,
  ymax = NULL,
  gg = TRUE
)
```


Arguments:

n2 Number of things to plot
 nn Number of things to plot
 col2 color
 xlab x label
 ylab y label
 xmin xmin
 xmax xmax
 ymin ymin
 ymax ymax
 gg Should ggplot2 be used to make plot?

Method plot1D(): Make 1D plot*Usage:*

```
GauPro_kernel_model$plot1D(
  n2 = 20,
  nn = 201,
  col2 = 2,
  col3 = 3,
  xlab = "x",
  ylab = "y",
  xmin = NULL,
  xmax = NULL,
  ymin = NULL,
  ymax = NULL,
  gg = TRUE
)
```

Arguments:

n2 Number of things to plot
 nn Number of things to plot
 col2 Color of the prediction interval
 col3 Color of the interval for the mean
 xlab x label
 ylab y label
 xmin xmin
 xmax xmax
 ymin ymin
 ymax ymax
 gg Should ggplot2 be used to make plot?

Method plot2D(): Make 2D plot*Usage:*

```
GauPro_kernel_model$plot2D(se = FALSE, mean = TRUE, horizontal = TRUE, n = 50)
```

Arguments:

se Should the standard error of prediction be plotted?
 mean Should the mean be plotted?
 horizontal If plotting mean and se, should they be next to each other?
 n Number of points along each dimension

Method `plotmarginal()`: Plot marginal. For each input, hold all others at a constant value and adjust it along it's range to see how the prediction changes.

Usage:

```
GauPro_kernel_model$plotmarginal(npt = 5, ncol = NULL)
```

Arguments:

npt Number of lines to make. Each line represents changing a single variable while holding the others at the same values.
 ncol Number of columns for the plot

Method `plotmarginalrandom()`: Plot marginal prediction for random sample of inputs

Usage:

```
GauPro_kernel_model$plotmarginalrandom(npt = 100, ncol = NULL)
```

Arguments:

npt Number of random points to evaluate
 ncol Number of columns in the plot

Method `plotkernel()`: Plot the kernel

Usage:

```
GauPro_kernel_model$plotkernel(X = self$X)
```

Arguments:

X X matrix for kernel plot

Method `plotL00()`: Plot leave one out predictions for design points

Usage:

```
GauPro_kernel_model$plotL00()
```

Method `plot_track_optim()`: If track_optim, this will plot the parameters in the order they were evaluated.

Usage:

```
GauPro_kernel_model$plot_track_optim(minindex = NULL)
```

Arguments:

minindex Minimum index to plot.

Method `loglikelihood()`: Calculate loglikelihood of parameters

Usage:

```
GauPro_kernel_model$loglikelihood(mu = self$mu_hatX, s2 = self$s2_hat)
```

Arguments:

mu Mean parameters

s2 Variance parameter

Method AIC(): AIC (Akaike information criterion)

Usage:

GauPro_kernel_model\$AIC()

Method get_optim_functions(): Get optimization functions

Usage:

GauPro_kernel_model\$get_optim_functions(param.update, nug.update)

Arguments:

param.update Should parameters be updated?

nug.update Should nugget be updated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

GauPro_kernel_model\$param_optim_lower(nug.update)

Arguments:

nug.update Is the nugget being updated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

GauPro_kernel_model\$param_optim_upper(nug.update)

Arguments:

nug.update Is the nugget being updated?

Method param_optim_start(): Starting point for parameters for optimization

Usage:

GauPro_kernel_model\$param_optim_start(nug.update, jitter)

Arguments:

nug.update Is nugget being updated?

jitter Should there be a jitter?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

GauPro_kernel_model\$param_optim_start0(nug.update, jitter)

Arguments:

nug.update Is nugget being updated?

jitter Should there be a jitter?

Method param_optim_start_mat(): Get matrix for starting points of optimization

Usage:

GauPro_kernel_model\$param_optim_start_mat(restarts, nug.update, l)

Arguments:

restarts Number of restarts to use
 nug.update Is nugget being updated?
 1 Not used

Method `optim()`: Optimize parameters

Usage:

```
GauPro_kernel_model$optim(
  restarts = self$restarts,
  n0 = 5 * self$D,
  param_update = T,
  nug.update = self$nug.est,
  parallel = self$parallel,
  parallel_cores = self$parallel_cores
)
```

Arguments:

restarts Number of restarts to do
 n0 This many starting parameters are chosen and evaluated. The best ones are used as the starting points for optimization.
 param_update Should parameters be updated?
 nug.update Should nugget be updated?
 parallel Should restarts be done in parallel?
 parallel_cores If running parallel, how many cores should be used?

Method `optimRestart()`: Run a single optimization restart.

Usage:

```
GauPro_kernel_model$optimRestart(
  start.par,
  start.par0,
  param_update,
  nug.update,
  optim.func,
  optim.grad,
  optim.fngr,
  lower,
  upper,
  jit = T,
  start.par.i
)
```

Arguments:

start.par Starting parameters
 start.par0 Starting parameters
 param_update Should parameters be updated?
 nug.update Should nugget be updated?
 optim.func Function to optimize.
 optim.grad Gradient of function to optimize.

optim.fngr Function that returns the function value and its gradient.
 lower Lower bounds for optimization
 upper Upper bounds for optimization
 jit Is jitter being used?
 start.par.i Starting parameters for this restart

Method update(): Update the model. Should only give in (Xnew and Znew) or (Xall and Zall).

Usage:

```
GauPro_kernel_model$update(
  Xnew = NULL,
  Znew = NULL,
  Xall = NULL,
  Zall = NULL,
  restarts = self$restarts,
  param_update = self$param.est,
  nug.update = self$nug.est,
  no_update = FALSE
)
```

Arguments:

Xnew New X values to add.
 Znew New Z values to add.
 Xall All X values to be used. Will replace existing X.
 Zall All Z values to be used. Will replace existing Z.
 restarts Number of optimization restarts.
 param_update Are the parameters being updated?
 nug.update Is the nugget being updated?
 no_update Are no parameters being updated?

Method update_fast(): Fast update when adding new data.

Usage:

```
GauPro_kernel_model$update_fast(Xnew = NULL, Znew = NULL)
```

Arguments:

Xnew New X values to add.
 Znew New Z values to add.

Method update_params(): Update the parameters.

Usage:

```
GauPro_kernel_model$update_params(..., nug.update)
```

Arguments:

... Passed to optim.
 nug.update Is the nugget being updated?

Method update_data(): Update the data. Should only give in (Xnew and Znew) or (Xall and Zall).

Usage:

```
GauPro_kernel_model$update_data(
  Xnew = NULL,
  Znew = NULL,
  Xall = NULL,
  Zall = NULL
)
```

Arguments:

Xnew New X values to add.
 Znew New Z values to add.
 Xall All X values to be used. Will replace existing X.
 Zall All Z values to be used. Will replace existing Z.

Method update_corrparams(): Update correlation parameters. Not the nugget.

Usage:

```
GauPro_kernel_model$update_corrparams(...)
```

Arguments:

... Passed to self\$update()

Method update_nugget(): Update nugget Not the correlation parameters.

Usage:

```
GauPro_kernel_model$update_nugget(...)
```

Arguments:

... Passed to self\$update()

Method deviance(): Calculate the deviance.

Usage:

```
GauPro_kernel_model$deviance(
  params = NULL,
  nug = self$nug,
  nuglog,
  trend_params = NULL
)
```

Arguments:

params Kernel parameters
 nug Nugget
 nuglog Log of nugget. Only give in nug or nuglog.
 trend_params Parameters for the trend.

Method deviance_grad(): Calculate the gradient of the deviance.

Usage:

```
GauPro_kernel_model$deviance_grad(
  params = NULL,
  kernel_update = TRUE,
  X = self$X,
  nug = self$nug,
  nug.update,
  nuglog,
  trend_params = NULL,
  trend_update = TRUE
)
```

Arguments:

params Kernel parameters

kernel_update Is the kernel being updated? If yes, it's part of the gradient.

X Input matrix

nug Nugget

nug.update Is the nugget being updated? If yes, it's part of the gradient.

nuglog Log of the nugget.

trend_params Trend parameters

trend_update Is the trend being updated? If yes, it's part of the gradient.

Method deviance_fngr(): Calculate the deviance along with its gradient.

Usage:

```
GauPro_kernel_model$deviance_fngr(
  params = NULL,
  kernel_update = TRUE,
  X = self$X,
  nug = self$nug,
  nug.update,
  nuglog,
  trend_params = NULL,
  trend_update = TRUE
)
```

Arguments:

params Kernel parameters

kernel_update Is the kernel being updated? If yes, it's part of the gradient.

X Input matrix

nug Nugget

nug.update Is the nugget being updated? If yes, it's part of the gradient.

nuglog Log of the nugget.

trend_params Trend parameters

trend_update Is the trend being updated? If yes, it's part of the gradient.

Method grad(): Calculate gradient

Usage:

```
GauPro_kernel_model$grad(XX, X = self$X, Z = self$Z)
```

Arguments:

XX points to calculate at

X X points

Z output points

Method grad_norm(): Calculate norm of gradient

Usage:

GauPro_kernel_model\$grad_norm(XX)

Arguments:

XX points to calculate at

Method grad_dist(): Calculate distribution of gradient

Usage:

GauPro_kernel_model\$grad_dist(XX)

Arguments:

XX points to calculate at

Method grad_sample(): Sample gradient at points

Usage:

GauPro_kernel_model\$grad_sample(XX, n)

Arguments:

XX points to calculate at

n Number of samples

Method grad_norm2_mean(): Calculate mean of gradient norm squared

Usage:

GauPro_kernel_model\$grad_norm2_mean(XX)

Arguments:

XX points to calculate at

Method grad_norm2_dist(): Calculate distribution of gradient norm squared

Usage:

GauPro_kernel_model\$grad_norm2_dist(XX)

Arguments:

XX points to calculate at

Method grad_norm2_sample(): Get samples of squared norm of gradient

Usage:

GauPro_kernel_model\$grad_norm2_sample(XX, n)

Arguments:

XX points to sample at

n Number of samples

Method `hessian()`: Calculate Hessian

Usage:

```
GauPro_kernel_model$hessian(XX, as_array = FALSE)
```

Arguments:

XX Points to calculate Hessian at

as_array Should result be an array?

Method `gradpredvar()`: Calculate gradient of the predictive variance

Usage:

```
GauPro_kernel_model$gradpredvar(XX)
```

Arguments:

XX points to calculate at

Method `sample()`: Sample at rows of XX

Usage:

```
GauPro_kernel_model$sample(XX, n = 1)
```

Arguments:

XX Input matrix

n Number of samples

Method `optimize_fn()`: Optimize any function of the GP prediction over the valid input space. If there are inputs that should only be optimized over a discrete set of values, specify 'mopar' for all parameters. Factor inputs will be handled automatically.

Usage:

```
GauPro_kernel_model$optimize_fn(
  fn = NULL,
  lower = apply(self$X, 2, min),
  upper = apply(self$X, 2, max),
  n0 = 100,
  minimize = FALSE,
  fn_args = NULL,
  gr = NULL,
  fngr = NULL,
  mopar = NULL,
  groupeval = FALSE
)
```

Arguments:

fn Function to optimize

lower Lower bounds to search within

upper Upper bounds to search within

n0 Number of points to evaluate in initial stage

minimize Are you trying to minimize the output?

fn_args Arguments to pass to the function fn.

gr Gradient of function to optimize.

`fngr` Function that returns list with names elements "fn" for the function value and "gr" for the gradient. Useful when it is slow to evaluate and fn/gr would duplicate calculations if done separately.

`mopar` List of parameters using mixopt

`groupeval` Can a matrix of points be evaluated? Otherwise just a single point at a time.

Method `EI()`: Calculate expected improvement

Usage:

```
GauPro_kernel_model$EI(x, minimize = FALSE, eps = 0, return_grad = FALSE, ...)
```

Arguments:

`x` Vector to calculate EI of, or matrix for whose rows it should be calculated

`minimize` Are you trying to minimize the output?

`eps` Exploration parameter

`return_grad` Should the gradient be returned?

... Additional args

Method `maxEI()`: Find the point that maximizes the expected improvement. If there are inputs that should only be optimized over a discrete set of values, specify 'mopar' for all parameters.

Usage:

```
GauPro_kernel_model$maxEI(
  lower = apply(self$X, 2, min),
  upper = apply(self$X, 2, max),
  n0 = 100,
  minimize = FALSE,
  eps = 0,
  dontconvertback = FALSE,
  EItype = "corrected",
  mopar = NULL,
  usegrad = FALSE
)
```

Arguments:

`lower` Lower bounds to search within

`upper` Upper bounds to search within

`n0` Number of points to evaluate in initial stage

`minimize` Are you trying to minimize the output?

`eps` Exploration parameter

`dontconvertback` If data was given in with a formula, should it converted back to the original scale?

`EItype` Type of EI to calculate. One of "EI", "Augmented", or "Corrected"

`mopar` List of parameters using mixopt

`usegrad` Should the gradient be used when optimizing? Can make it faster.

Method `maxqEI()`: Find the multiple points that maximize the expected improvement. Currently only implements the constant liar method.

Usage:

```
GauPro_kernel_model$maxqEI(
  npoints,
  method = "pred",
  lower = apply(self$X, 2, min),
  upper = apply(self$X, 2, max),
  n0 = 100,
  minimize = FALSE,
  eps = 0,
  EItype = "corrected",
  dontconvertback = FALSE,
  mopar = NULL
)
```

Arguments:

npoints Number of points to add

method Method to use for setting the output value for the points chosen as a placeholder. Can be one of: "CL" for constant liar, which uses the best value seen yet; or "pred", which uses the predicted value, also called the Believer method in literature.

lower Lower bounds to search within

upper Upper bounds to search within

n0 Number of points to evaluate in initial stage

minimize Are you trying to minimize the output?

eps Exploration parameter

EItype Type of EI to calculate. One of "EI", "Augmented", or "Corrected"

dontconvertback If data was given in with a formula, should it converted back to the original scale?

mopar List of parameters using mixopt

Method KG(): Calculate Knowledge Gradient*Usage:*

```
GauPro_kernel_model$KG(x, minimize = FALSE, eps = 0, current_extreme = NULL)
```

Arguments:

x Point to calculate at

minimize Is the objective to minimize?

eps Exploration parameter

current_extreme Used for recursive solving

Method AugmentedEI(): Calculated Augmented EI*Usage:*

```
GauPro_kernel_model$AugmentedEI(
  x,
  minimize = FALSE,
  eps = 0,
  return_grad = F,
  ...
)
```

Arguments:

x Vector to calculate EI of, or matrix for whose rows it should be calculated
 minimize Are you trying to minimize the output?
 eps Exploration parameter
 return_grad Should the gradient be returned?
 ... Additional args
 f The reference max, user shouldn't change this.

Method CorrectedEI(): Calculated Augmented EI*Usage:*

```
GauPro_kernel_model$CorrectedEI(
  x,
  minimize = FALSE,
  eps = 0,
  return_grad = F,
  ...
)
```

Arguments:

x Vector to calculate EI of, or matrix for whose rows it should be calculated
 minimize Are you trying to minimize the output?
 eps Exploration parameter
 return_grad Should the gradient be returned?
 ... Additional args

Method importance(): Feature importance*Usage:*

```
GauPro_kernel_model$importance(plot = TRUE, printBars = TRUE)
```

Arguments:

plot Should the plot be made?
 printBars Should the importances be printed as bars?

Method print(): Print this object*Usage:*

```
GauPro_kernel_model$print()
```

Method summary(): Summary*Usage:*

```
GauPro_kernel_model$summary(...)
```

Arguments:

... Additional arguments

Method clone(): The objects of this class are cloneable with this method.*Usage:*

```
GauPro_kernel_model$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

References

https://scikit-learn.org/stable/modules/permutation_importance.html#id2

Examples

```
n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel="gauss")
gp$predict(.454)
gp$plot1D()
gp$cool1Dplot()

n <- 200
d <- 7
x <- matrix(runif(n*d), ncol=d)
f <- function(x) {x[1]*x[2] + cos(x[3]) + x[4]^2}
y <- apply(x, 1, f)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel=Gaussian)
```

GauPro_kernel_model_LOO

Corr Gauss GP using inherited optim

Description

Corr Gauss GP using inherited optim

Corr Gauss GP using inherited optim

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro::GauPro](#) -> GauPro_kernel_model_LOO

Public fields

tmod A second GP model for the t-values of leave-one-out predictions

use_LOO Should the leave-one-out error corrections be used?

Methods

Public methods:

- `GauPro_kernel_model_LOO$new()`
- `GauPro_kernel_model_LOO$update()`
- `GauPro_kernel_model_LOO$pred_one_matrix()`
- `GauPro_kernel_model_LOO$clone()`

Method `new()`: Create a kernel model that uses a leave-one-out GP model to fix the standard error predictions.

Usage:

```
GauPro_kernel_model_LOO$new(..., L00_kernel, L00_options = list())
```

Arguments:

... Passed to `super$initialize`.

`L00_kernel` The kernel that should be used for the leave-one-out model. Shouldn't be too smooth.

`L00_options` Options passed to the leave-one-out model.

Method `update()`: Update the model. Should only give in (`Xnew` and `Znew`) or (`Xall` and `Zall`).

Usage:

```
GauPro_kernel_model_LOO$update(
  Xnew = NULL,
  Znew = NULL,
  Xall = NULL,
  Zall = NULL,
  restarts = 5,
  param_update = self$param.est,
  nug.update = self$nug.est,
  no_update = FALSE
)
```

Arguments:

`Xnew` New X values to add.

`Znew` New Z values to add.

`Xall` All X values to be used. Will replace existing X.

`Zall` All Z values to be used. Will replace existing Z.

`restarts` Number of optimization restarts.

`param_update` Are the parameters being updated?

`nug.update` Is the nugget being updated?

`no_update` Are no parameters being updated?

Method `pred_one_matrix()`: Predict for a matrix of points

Usage:

```
GauPro_kernel_model_L00$pred_one_matrix(
  XX,
  se.fit = F,
  covmat = F,
  return_df = FALSE,
  mean_dist = FALSE
)
```

Arguments:

XX points to predict at

se.fit Should standard error be returned?

covmat Should covariance matrix be returned?

return_df When returning *se.fit*, should it be returned in a data frame?

mean_dist Should mean distribution be returned?

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
GauPro_kernel_model_L00$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model_L00$new(X=x, Z=y, kernel=Gaussian)
y <- x^2 * sin(2*pi*x) + rnorm(n,0,1e-3)
gp <- GauPro_kernel_model_L00$new(X=x, Z=y, kernel=Matern52)
y <- exp(-1.4*x)*cos(7*pi*x/2)
gp <- GauPro_kernel_model_L00$new(X=x, Z=y, kernel=Matern52)
```

GauPro_trend

Trend R6 class

Description

Trend R6 class

Trend R6 class

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Public fields

D Number of input dimensions of data

Methods**Public methods:**

- [GauPro_trend\\$clone\(\)](#)

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
GauPro_trend$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
#k <- GauPro_trend$new()
```

Gaussian

Gaussian Kernel R6 class

Description

Gaussian Kernel R6 class

Gaussian Kernel R6 class

Usage

```
k_Gaussian(  
  beta,  
  s2 = 1,  
  D,  
  beta_lower = -8,  
  beta_upper = 6,  
  beta_est = TRUE,  
  s2_lower = 1e-08,  
  s2_upper = 1e+08,  
  s2_est = TRUE,  
  useC = TRUE,  
  isotropic = FALSE  
)
```


Arguments

beta	Initial beta value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster.
isotropic	If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/beta is used for each dimension.

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super classes

[GauPro::GauPro_kernel](#) -> [GauPro::GauPro_kernel_beta](#) -> [GauPro_kernel_Gaussian](#)

Methods**Public methods:**

- [Gaussian\\$k\(\)](#)
- [Gaussian\\$kone\(\)](#)
- [Gaussian\\$dC_dparams\(\)](#)
- [Gaussian\\$C_dC_dparams\(\)](#)
- [Gaussian\\$dC_dx\(\)](#)
- [Gaussian\\$d2C_dx2\(\)](#)
- [Gaussian\\$d2C_dudv\(\)](#)
- [Gaussian\\$d2C_dudv_ueqvrows\(\)](#)
- [Gaussian\\$print\(\)](#)
- [Gaussian\\$clone\(\)](#)

Method k(): Calculate covariance between two points

Usage:

`Gaussian$k(x, y = NULL, beta = self$beta, s2 = self$s2, params = NULL)`

Arguments:

x vector.
y vector, optional. If excluded, find correlation of x with itself.
beta Correlation parameters.
s2 Variance parameter.
params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

`Gaussian$kone(x, y, beta, theta, s2)`

Arguments:

x vector
y vector
beta correlation parameters on log scale
theta correlation parameters on regular scale
s2 Variance parameter

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

`Gaussian$dC_dparams(params = NULL, X, C_nonug, C, nug)`

Arguments:

params Kernel parameters
X matrix of points in rows
C_nonug Covariance without nugget added to diagonal
C Covariance with nugget
nug Value of nugget

Method `C_dC_dparams()`: Calculate covariance matrix and its derivative with respect to parameters

Usage:

`Gaussian$C_dC_dparams(params = NULL, X, nug)`

Arguments:

params Kernel parameters
X matrix of points in rows
nug Value of nugget

Method `dC_dx()`: Derivative of covariance with respect to X

Usage:

`Gaussian$dC_dx(XX, X, theta, beta = self$beta, s2 = self$s2)`

Arguments:

XX matrix of points
X matrix of points to take derivative with respect to

theta Correlation parameters
beta log of theta
s2 Variance parameter

Method `d2C_dx2()`: Second derivative of covariance with respect to X

Usage:

`Gaussian$d2C_dx2(XX, X, theta, beta = self$beta, s2 = self$s2)`

Arguments:

XX matrix of points
X matrix of points to take derivative with respect to
theta Correlation parameters
beta log of theta
s2 Variance parameter

Method `d2C_dudv()`: Second derivative of covariance with respect to X and XX each once.

Usage:

`Gaussian$d2C_dudv(XX, X, theta, beta = self$beta, s2 = self$s2)`

Arguments:

XX matrix of points
X matrix of points to take derivative with respect to
theta Correlation parameters
beta log of theta
s2 Variance parameter

Method `d2C_dudv_ueqvrows()`: Second derivative of covariance with respect to X and XX when they equal the same value

Usage:

`Gaussian$d2C_dudv_ueqvrows(XX, theta, beta = self$beta, s2 = self$s2)`

Arguments:

XX matrix of points
theta Correlation parameters
beta log of theta
s2 Variance parameter

Method `print()`: Print this object

Usage:

`Gaussian$print()`

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

`Gaussian$clone(deep = FALSE)`

Arguments:

deep Whether to make a deep clone.

Examples

```

k1 <- Gaussian$new(beta=0)
plot(k1)
k1 <- Gaussian$new(beta=c(0,-1, 1))
plot(k1)

n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel=Gaussian$new(1),
                             parallel=FALSE)

gp$predict(.454)
gp$plot1D()
gp$cool1Dplot()

```

Gaussian_devianceC *Calculate the Gaussian deviance in C*

Description

Calculate the Gaussian deviance in C

Usage

```
Gaussian_devianceC(theta, nug, X, Z)
```

Arguments

theta	Theta vector
nug	Nugget
X	Matrix X
Z	Matrix Z

Value

Correlation matrix

Examples

```
Gaussian_devianceC(c(1,1), 1e-8, matrix(c(1,0,0,1),2,2), matrix(c(1,0),2,1))
```

Gaussian_hessianC *Calculate Hessian for a GP with Gaussian correlation*

Description

Calculate Hessian for a GP with Gaussian correlation

Usage

```
Gaussian_hessianC(XX, X, Z, Kinv, mu_hat, theta)
```

Arguments

XX	The vector at which to calculate the Hessian
X	The input points
Z	The output values
Kinv	The inverse of the correlation matrix
mu_hat	Estimate of mu
theta	Theta parameters for the correlation

Value

Matrix, the Hessian at XX

Examples

```
set.seed(0)
n <- 40
x <- matrix(runif(n*2), ncol=2)
f1 <- function(a) {sin(2*pi*a[1]) + sin(6*pi*a[2])}
y <- apply(x,1,f1) + rnorm(n,0,.01)
gp <- GauPro(x,y, verbose=2, parallel=FALSE);gp$theta
gp$hessian(c(.2,.75), useC=TRUE) # Should be -38.3, -5.96, -5.96, -389.4 as 2x2 matrix
```

Gaussian_hessianCC *Gaussian hessian in C*

Description

Gaussian hessian in C

Usage

```
Gaussian_hessianCC(XX, X, Z, Kinv, mu_hat, theta)
```

Arguments

XX	point to find Hessian at
X	matrix of data points
Z	matrix of output
Kinv	inverse of correlation matrix
mu_hat	mean estimate
theta	correlation parameters

Value

Hessian matrix

Gaussian_hessianR *Calculate Hessian for a GP with Gaussian correlation*

Description

Calculate Hessian for a GP with Gaussian correlation

Usage

```
Gaussian_hessianR(XX, X, Z, Kinv, mu_hat, theta)
```

Arguments

XX	The vector at which to calculate the Hessian
X	The input points
Z	The output values
Kinv	The inverse of the correlation matrix
mu_hat	Estimate of mu
theta	Theta parameters for the correlation

Value

Matrix, the Hessian at XX

Examples

```
set.seed(0)
n <- 40
x <- matrix(runif(n*2), ncol=2)
f1 <- function(a) {sin(2*pi*a[1]) + sin(6*pi*a[2])}
y <- apply(x,1,f1) + rnorm(n,0,.01)
gp <- GauPro(x,y, verbose=2, parallel=FALSE);gp$theta
gp$hessian(c(.2,.75), useC=FALSE) # Should be -38.3, -5.96, -5.96, -389.4 as 2x2 matrix
```

GowerFactorKernel *Gower factor Kernel R6 class*

Description

Gower factor Kernel R6 class

Gower factor Kernel R6 class

Usage

```
k_GowerFactorKernel(
  s2 = 1,
  D,
  nlevels,
  xindex,
  p_lower = 0,
  p_upper = 0.9,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  p,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)
```

Arguments

s2	Initial variance
D	Number of input dimensions of data
nlevels	Number of levels for the factor
xindex	Index of the factor (which column of X)
p_lower	Lower bound for p
p_upper	Upper bound for p
p_est	Should p be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
p	Vector of correlations
useC	Should C code used? Not implemented for FactorKernel yet.
offdiagequal	What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Format

R6Class object.

Details

For a factor that has been converted to its indices. Each factor will need a separate kernel.

Value

Object of R6Class with methods for fitting GP model.

Super class

GauPro::GauPro_kernel -> GauPro_kernel_GowerFactorKernel

Public fields

p Parameter for correlation
 p_est Should p be estimated?
 p_lower Lower bound of p
 p_upper Upper bound of p
 s2 variance
 s2_est Is s2 estimated?
 logs2 Log of s2
 logs2_lower Lower bound of logs2
 logs2_upper Upper bound of logs2
 xindex Index of the factor (which column of X)
 nlevels Number of levels for the factor
 offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Methods**Public methods:**

- GowerFactorKernel\$new()
- GowerFactorKernel\$k()
- GowerFactorKernel\$kone()
- GowerFactorKernel\$dC_dparams()
- GowerFactorKernel\$C_dC_dparams()
- GowerFactorKernel\$dC_dx()
- GowerFactorKernel\$param_optim_start()
- GowerFactorKernel\$param_optim_start0()
- GowerFactorKernel\$param_optim_lower()
- GowerFactorKernel\$param_optim_upper()

- `GowerFactorKernel$set_params_from_optim()`
- `GowerFactorKernel$s2_from_params()`
- `GowerFactorKernel$print()`
- `GowerFactorKernel$clone()`

Method `new()`: Initialize kernel object

Usage:

```
GowerFactorKernel$new(
  s2 = 1,
  D,
  nlevels,
  xindex,
  p_lower = 0,
  p_upper = 0.9,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  p,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)
```

Arguments:

`s2` Initial variance

`D` Number of input dimensions of data

`nlevels` Number of levels for the factor

`xindex` Index of the factor (which column of X)

`p_lower` Lower bound for p

`p_upper` Upper bound for p

`p_est` Should p be estimated?

`s2_lower` Lower bound for s2

`s2_upper` Upper bound for s2

`s2_est` Should s2 be estimated?

`p` Vector of correlations

`useC` Should C code used? Not implemented for FactorKernel yet.

`offdiagequal` What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Method `k()`: Calculate covariance between two points

Usage:

```
GowerFactorKernel$k(x, y = NULL, p = self$p, s2 = self$s2, params = NULL)
```

Arguments:

`x` vector.

`y` vector, optional. If excluded, find correlation of x with itself.

p Correlation parameters.
 s2 Variance parameter.
 params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

```
GowerFactorKernel$kone(
  x,
  y,
  p,
  s2,
  isdiag = TRUE,
  offdiagequal = self$offdiagequal
)
```

Arguments:

x vector
 y vector
 p correlation parameters on regular scale
 s2 Variance parameter
 isdiag Is this on the diagonal of the covariance?
 offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

```
GowerFactorKernel$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 C_nonug Covariance without nugget added to diagonal
 C Covariance with nugget
 nug Value of nugget

Method `C_dC_dparams()`: Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
GowerFactorKernel$C_dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 nug Value of nugget

Method `dC_dx()`: Derivative of covariance with respect to X

Usage:

```
GowerFactorKernel$dC_dx(XX, X, ...)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

... Additional args, not used

Method param_optim_start(): Starting point for parameters for optimization

Usage:

```
GowerFactorKernel$param_optim_start(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?

y Output

p_est Is p being estimated?

s2_est Is s2 being estimated?

alpha_est Is alpha being estimated?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

```
GowerFactorKernel$param_optim_start0(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?

y Output

p_est Is p being estimated?

s2_est Is s2 being estimated?

alpha_est Is alpha being estimated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

```
GowerFactorKernel$param_optim_lower(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?

s2_est Is s2 being estimated?

alpha_est Is alpha being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```
GowerFactorKernel$param_optim_upper(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?

s2_est Is s2 being estimated?

alpha_est Is alpha being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```
GowerFactorKernel$set_params_from_optim(  
  optim_out,  
  p_est = self$p_est,  
  s2_est = self$s2_est  
)
```

Arguments:

optim_out Output from optimization

p_est Is p being estimated?

s2_est Is s2 being estimated?

alpha_est Is alpha being estimated?

Method s2_from_params(): Get s2 from params vector

Usage:

```
GowerFactorKernel$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

params parameter vector

s2_est Is s2 being estimated?

Method print(): Print this object

Usage:

```
GowerFactorKernel$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
GowerFactorKernel$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```

kk <- GowerFactorKernel$new(D=1, nlevels=5, xindex=1, p=.2)
kmat <- outer(1:5, 1:5, Vectorize(kk$k))
kmat
kk$plot()

# 2D, Gaussian on 1D, index on 2nd dim
if (requireNamespace("dplyr", quietly=TRUE)) {
  library(dplyr)
  n <- 20
  X <- cbind(matrix(runif(n,2,6), ncol=1),
             matrix(sample(1:2, size=n, replace=TRUE), ncol=1))
  X <- rbind(X, c(3.3,3))
  n <- nrow(X)
  Z <- X[,1] - (X[,2]-1.8)^2 + rnorm(n,0,.1)
  tibble(X=X, Z) %>% arrange(X,Z)
  k2a <- IgnoreIndsKernel$new(k=Gaussian$new(D=1), ignoreinds = 2)
  k2b <- GowerFactorKernel$new(D=2, nlevels=3, xind=2)
  k2 <- k2a * k2b
  k2b$p_upper <- .65*k2b$p_upper
  gp <- GauPro_kernel_model$new(X=X, Z=Z, kernel = k2, verbose = 5,
                               nug.min=1e-2, restarts=0)

  gp$kernel$k1$kernel$beta
  gp$kernel$k2$p
  gp$kernel$k(x = gp$X)
  tibble(X=X, Z=Z, pred=gp$predict(X)) %>% arrange(X, Z)
  tibble(X=X[,2], Z) %>% group_by(X) %>% summarize(n=n(), mean(Z))
  curve(gp$pred(cbind(matrix(x,ncol=1),1)),2,6, ylim=c(min(Z), max(Z)))
  points(X[X[,2]==1,1], Z[X[,2]==1])
  curve(gp$pred(cbind(matrix(x,ncol=1),2)), add=TRUE, col=2)
  points(X[X[,2]==2,1], Z[X[,2]==2], col=2)
  curve(gp$pred(cbind(matrix(x,ncol=1),3)), add=TRUE, col=3)
  points(X[X[,2]==3,1], Z[X[,2]==3], col=3)
  legend(legend=1:3, fill=1:3, x="topleft")
  # See which points affect (5.5, 3) the most
  data.frame(X, cov=gp$kernel$k(X, c(5.5,3))) %>% arrange(-cov)
  plot(k2b)
}

```

Description

Fits a Gaussian process regression model to data.

An R6 object is returned with many methods.

'gpkm()' is an alias for 'GauPro_kernel_model\$new()'. For full documentation, see documentation for 'GauPro_kernel_model'.

Standard methods that work include 'plot()', 'summary()', and 'predict()'.

Usage

```
gpkm(
  X,
  Z,
  kernel,
  trend,
  verbose = 0,
  useC = TRUE,
  useGrad = TRUE,
  parallel = FALSE,
  parallel_cores = "detect",
  nug = 1e-06,
  nug.min = 1e-08,
  nug.max = 100,
  nug.est = TRUE,
  param.est = TRUE,
  restarts = 0,
  normalize = FALSE,
  optimizer = "L-BFGS-B",
  track_optim = FALSE,
  formula,
  data,
  ...
)
```

Arguments

X	Matrix whose rows are the input points
Z	Output points corresponding to X
kernel	The kernel to use. E.g., Gaussian\$new().
trend	Trend to use. E.g., trend_constant\$new().
verbose	Amount of stuff to print. 0 is little, 2 is a lot.
useC	Should C code be used when possible? Should be faster.
useGrad	Should the gradient be used?
parallel	Should code be run in parallel? Make optimization faster but uses more computer resources.
parallel_cores	When using parallel, how many cores should be used?
nug	Value for the nugget. The starting value if estimating it.
nug.min	Minimum allowable value for the nugget.
nug.max	Maximum allowable value for the nugget.

nug.est	Should the nugget be estimated?
param.est	Should the kernel parameters be estimated?
restarts	How many optimization restarts should be used when estimating parameters?
normalize	Should the data be normalized?
optimizer	What algorithm should be used to optimize the parameters.
track_optim	Should it track the parameters evaluated while optimizing?
formula	Formula for the data if giving in a data frame.
data	Data frame of data. Use in conjunction with formula.
...	Not used

Details

The default kernel is a Matern 5/2 kernel, but factor/character inputs will be given factor kernels.

gradfuncarray	<i>Calculate gradfunc in optimization to speed up. NEEDS TO APERM dC_dparams Doesn't need to be exported, should only be useful in functions.</i>
---------------	---

Description

Calculate gradfunc in optimization to speed up. NEEDS TO APERM dC_dparams Doesn't need to be exported, should only be useful in functions.

Usage

```
gradfuncarray(dC_dparams, Cinv, Cinv_yminusmu)
```

Arguments

dC_dparams	Derivative matrix for covariance function wrt kernel parameters
Cinv	Inverse of covariance matrix
Cinv_yminusmu	Vector that is the inverse of C times y minus the mean.

Value

Vector, one value for each parameter

Examples

```
gradfuncarray(array(dim=c(2,4,4), data=rnorm(32)), matrix(rnorm(16),4,4), rnorm(4))
```

gradfuncarrayR	<i>Calculate gradfunc in optimization to speed up. NEEDS TO APERM dC_dparams Doesn't need to be exported, should only be useful in functions.</i>
----------------	---

Description

Calculate gradfunc in optimization to speed up. NEEDS TO APERM dC_dparams Doesn't need to be exported, should only be useful in functions.

Usage

```
gradfuncarrayR(dC_dparams, Cinv, Cinv_yminusmu)
```

Arguments

dC_dparams	Derivative matrix for covariance function wrt kernel parameters
Cinv	Inverse of covariance matrix
Cinv_yminusmu	Vector that is the inverse of C times y minus the mean.

Value

Vector, one value for each parameter

Examples

```
a1 <- array(dim=c(2,4,4), data=rnorm(32))
a2 <- matrix(rnorm(16),4,4)
a3 <- rnorm(4)
#gradfuncarray(a1, a2, a3)
#gradfuncarrayR(a1, a2, a3)
```

IgnoreIndsKernel	<i>Kernel R6 class</i>
------------------	------------------------

Description

Kernel R6 class

Kernel R6 class

Usage

```
k_IgnoreIndsKernel(k, ignoreinds, useC = TRUE)
```


Arguments

k	Kernel to use on the non-ignored indices
ignoreinds	Indices of columns of X to ignore.
useC	Should C code used? Not implemented for IgnoreInds.

Format

R6Class object.

Value

Object of R6Class with methods for fitting GP model.

Super class

GauPro::GauPro_kernel -> GauPro_kernel_IgnoreInds

Public fields

D Number of input dimensions of data
kernel Kernel to use on indices that aren't ignored
ignoreinds Indices to ignore. For a matrix X, these are the columns to ignore. For example, when those dimensions will be given a different kernel, such as for factors.

Active bindings

s2_est Is s2 being estimated?
s2 Value of s2 (variance)

Methods**Public methods:**

- IgnoreIndsKernel\$new()
- IgnoreIndsKernel\$k()
- IgnoreIndsKernel\$kone()
- IgnoreIndsKernel\$dC_dparams()
- IgnoreIndsKernel\$C_dC_dparams()
- IgnoreIndsKernel\$dC_dx()
- IgnoreIndsKernel\$param_optim_start()
- IgnoreIndsKernel\$param_optim_start0()
- IgnoreIndsKernel\$param_optim_lower()
- IgnoreIndsKernel\$param_optim_upper()
- IgnoreIndsKernel\$set_params_from_optim()
- IgnoreIndsKernel\$s2_from_params()
- IgnoreIndsKernel\$print()

- [IgnoreIndsKernel\\$clone\(\)](#)

Method new(): Initialize kernel object

Usage:

```
IgnoreIndsKernel$new(k, ignoreinds, useC = TRUE)
```

Arguments:

k Kernel to use on the non-ignored indices
 ignoreinds Indices of columns of X to ignore.
 useC Should C code used? Not implemented for IgnoreInds.

Method k(): Calculate covariance between two points

Usage:

```
IgnoreIndsKernel$k(x, y = NULL, ...)
```

Arguments:

x vector.
 y vector, optional. If excluded, find correlation of x with itself.
 ... Passed to kernel

Method kone(): Find covariance of two points

Usage:

```
IgnoreIndsKernel$kone(x, y, ...)
```

Arguments:

x vector
 y vector
 ... Passed to kernel

Method dC_dparams(): Derivative of covariance with respect to parameters

Usage:

```
IgnoreIndsKernel$dC_dparams(params = NULL, X, ...)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 ... Passed to kernel

Method C_dC_dparams(): Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
IgnoreIndsKernel$C_dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 nug Value of nugget

Method `dC_dx()`: Derivative of covariance with respect to X

Usage:

`IgnoreIndsKernel$dC_dx(XX, X, ...)`

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

... Additional arguments passed on to the kernel

Method `param_optim_start()`: Starting point for parameters for optimization

Usage:

`IgnoreIndsKernel$param_optim_start(...)`

Arguments:

... Passed to kernel

Method `param_optim_start0()`: Starting point for parameters for optimization

Usage:

`IgnoreIndsKernel$param_optim_start0(...)`

Arguments:

... Passed to kernel

Method `param_optim_lower()`: Lower bounds of parameters for optimization

Usage:

`IgnoreIndsKernel$param_optim_lower(...)`

Arguments:

... Passed to kernel

Method `param_optim_upper()`: Upper bounds of parameters for optimization

Usage:

`IgnoreIndsKernel$param_optim_upper(...)`

Arguments:

... Passed to kernel

Method `set_params_from_optim()`: Set parameters from optimization output

Usage:

`IgnoreIndsKernel$set_params_from_optim(...)`

Arguments:

... Passed to kernel

Method `s2_from_params()`: Get s2 from params vector

Usage:

`IgnoreIndsKernel$s2_from_params(...)`

Arguments:

... Passed to kernel

Method print(): Print this object

Usage:

IgnoreIndsKernel\$print()

Method clone(): The objects of this class are cloneable with this method.

Usage:

IgnoreIndsKernel\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Examples

```
kg <- Gaussian$new(D=3)
kig <- GauPro::IgnoreIndsKernel$new(k = Gaussian$new(D=3), ignoreinds = 2)
Xtmp <- as.matrix(expand.grid(1:2, 1:2, 1:2))
cbind(Xtmp, kig$k(Xtmp))
cbind(Xtmp, kg$k(Xtmp))
```

kernel_cubic_dC

Derivative of cubic kernel covariance matrix in C

Description

Derivative of cubic kernel covariance matrix in C

Usage

```
kernel_cubic_dC(x, theta, C_nonug, s2_est, beta_est, lenparams_D, s2_nug, s2)
```

Arguments

x	Matrix x
theta	Theta vector
C_nonug	cov mat without nugget
s2_est	whether s2 is being estimated
beta_est	Whether theta/beta is being estimated
lenparams_D	Number of parameters the derivative is being calculated for
s2_nug	s2 times the nug
s2	s2

Value

Correlation matrix

kernel_exponential_dC *Derivative of Matern 5/2 kernel covariance matrix in C*

Description

Derivative of Matern 5/2 kernel covariance matrix in C

Usage

```
kernel_exponential_dC(
  x,
  theta,
  C_nonug,
  s2_est,
  beta_est,
  lenparams_D,
  s2_nug,
  s2
)
```

Arguments

x	Matrix x
theta	Theta vector
C_nonug	cov mat without nugget
s2_est	whether s2 is being estimated
beta_est	Whether theta/beta is being estimated
lenparams_D	Number of parameters the derivative is being calculated for
s2_nug	s2 times the nug
s2	s2 parameter

Value

Correlation matrix

kernel_gauss_dC *Derivative of Gaussian kernel covariance matrix in C*

Description

Derivative of Gaussian kernel covariance matrix in C

Usage

```
kernel_gauss_dC(x, theta, C_nonug, s2_est, beta_est, lenparams_D, s2_nug)
```

Arguments

x	Matrix x
theta	Theta vector
C_nonug	cov mat without nugget
s2_est	whether s2 is being estimated
beta_est	Whether theta/beta is being estimated
lenparams_D	Number of parameters the derivative is being calculated for
s2_nug	s2 times the nug

Value

Correlation matrix

kernel_latentFactor_dC
Derivative of covariance matrix of X with respect to kernel parameters for the Latent Factor Kernel

Description

Derivative of covariance matrix of X with respect to kernel parameters for the Latent Factor Kernel

Usage

```
kernel_latentFactor_dC(
  x,
  pf,
  C_nonug,
  s2_est,
  p_est,
  lenparams_D,
  s2_nug,
```

```

    latentdim,
    xindex,
    nlevels,
    s2
)

```

Arguments

x	Matrix x
pf	pf vector
C_nonug	cov mat without nugget
s2_est	whether s2 is being estimated
p_est	Whether theta/beta is being estimated
lenparams_D	Number of parameters the derivative is being calculated for
s2_nug	s2 times the nug
latentdim	Number of latent dimensions
xindex	Which column of x is the indexing variable
nlevels	Number of levels
s2	Value of s2

Value

Correlation matrix

kernel_matern32_dC	<i>Derivative of Matern 5/2 kernel covariance matrix in C</i>
--------------------	---

Description

Derivative of Matern 5/2 kernel covariance matrix in C

Usage

```
kernel_matern32_dC(x, theta, C_nonug, s2_est, beta_est, lenparams_D, s2_nug)
```

Arguments

x	Matrix x
theta	Theta vector
C_nonug	cov mat without nugget
s2_est	whether s2 is being estimated
beta_est	Whether theta/beta is being estimated
lenparams_D	Number of parameters the derivative is being calculated for
s2_nug	s2 times the nug

Value

Correlation matrix

kernel_matern52_dC *Derivative of Matern 5/2 kernel covariance matrix in C*

Description

Derivative of Matern 5/2 kernel covariance matrix in C

Usage

```
kernel_matern52_dC(x, theta, C_nonug, s2_est, beta_est, lenparams_D, s2_nug)
```

Arguments

x	Matrix x
theta	Theta vector
C_nonug	cov mat without nugget
s2_est	whether s2 is being estimated
beta_est	Whether theta/beta is being estimated
lenparams_D	Number of parameters the derivative is being calculated for
s2_nug	s2 times the nug

Value

Correlation matrix

kernel_orderedFactor_dC
*Derivative of covariance matrix of X with respect to kernel parameters
for the Ordered Factor Kernel*

Description

Derivative of covariance matrix of X with respect to kernel parameters for the Ordered Factor Kernel

Usage

```
kernel_orderedFactor_dC(
  x,
  pf,
  C_nonug,
  s2_est,
  p_est,
  lenparams_D,
  s2_nug,
  xindex,
  nlevels,
  s2
)
```

Arguments

x	Matrix x
pf	pf vector
C_nonug	cov mat without nugget
s2_est	whether s2 is being estimated
p_est	Whether theta/beta is being estimated
lenparams_D	Number of parameters the derivative is being calculated for
s2_nug	s2 times the nug
xindex	Which column of x is the indexing variable
nlevels	Number of levels
s2	Value of s2

Value

Correlation matrix

kernel_product	<i>Gaussian Kernel R6 class</i>
----------------	---------------------------------

Description

Gaussian Kernel R6 class
 Gaussian Kernel R6 class

Format

[R6Class](#) object.

Value

Object of `R6Class` with methods for fitting GP model.

Super class

`GauPro`: `GauPro_kernel` -> `GauPro_kernel_product`

Public fields

k1 kernel 1
k2 kernel 2
s2 Variance

Active bindings

k1p1 param length of kernel 1
k2p1 param length of kernel 2
s2_est Is s2 being estimated?

Methods**Public methods:**

- `kernel_product$new()`
- `kernel_product$k()`
- `kernel_product$param_optim_start()`
- `kernel_product$param_optim_start0()`
- `kernel_product$param_optim_lower()`
- `kernel_product$param_optim_upper()`
- `kernel_product$set_params_from_optim()`
- `kernel_product$dC_dparams()`
- `kernel_product$C_dC_dparams()`
- `kernel_product$dC_dx()`
- `kernel_product$s2_from_params()`
- `kernel_product$print()`
- `kernel_product$clone()`

Method `new()`: Is s2 being estimated?

Length of the parameters of k1

Length of the parameters of k2

Initialize kernel

Usage:

`kernel_product$new(k1, k2, useC = TRUE)`

Arguments:

k1 Kernel 1

k2 Kernel 2

useC Should C code used? Not applicable for kernel product.

Method k(): Calculate covariance between two points

Usage:

kernel_product\$k(x, y = NULL, params, ...)

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

params parameters to use instead of beta and s2.

... Not used

Method param_optim_start(): Starting point for parameters for optimization

Usage:

kernel_product\$param_optim_start(jitter = F, y)

Arguments:

jitter Should there be a jitter?

y Output

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

kernel_product\$param_optim_start0(jitter = F, y)

Arguments:

jitter Should there be a jitter?

y Output

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

kernel_product\$param_optim_lower()

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

kernel_product\$param_optim_upper()

Method set_params_from_optim(): Set parameters from optimization output

Usage:

kernel_product\$set_params_from_optim(optim_out)

Arguments:

optim_out Output from optimization

Method dC_dparams(): Derivative of covariance with respect to parameters

Usage:

kernel_product\$dC_dparams(params = NULL, C, X, C_nonug, nug)

Arguments:

params Kernel parameters
 C Covariance with nugget
 X matrix of points in rows
 C_nonug Covariance without nugget added to diagonal
 nug Value of nugget

Method C_dc_dparams(): Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
kernel_product$C_dc_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
kernel_product$dC_dx(XX, X)
```

Arguments:

XX matrix of points
 X matrix of points to take derivative with respect to

Method s2_from_params(): Get s2 from params vector

Usage:

```
kernel_product$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

params parameter vector
 s2_est Is s2 being estimated?

Method print(): Print this object

Usage:

```
kernel_product$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
kernel_product$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- Exponential$new(beta=1)
k2 <- Matern32$new(beta=2)
k <- k1 * k2
k$k(matrix(c(2,1), ncol=1))
```

kernel_sum	<i>Gaussian Kernel R6 class</i>
------------	---------------------------------

Description

Gaussian Kernel R6 class

Gaussian Kernel R6 class

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro](#): :[GauPro_kernel](#) -> [GauPro_kernel_sum](#)

Public fields

k1 kernel 1

k2 kernel 2

k1_param_length param length of kernel 1

k2_param_length param length of kernel 2

k1p1 param length of kernel 1

k2p1 param length of kernel 2

s2 variance

s2_est Is s2 being estimated?

Methods**Public methods:**

- [kernel_sum\\$new\(\)](#)
- [kernel_sum\\$k\(\)](#)
- [kernel_sum\\$param_optim_start\(\)](#)
- [kernel_sum\\$param_optim_start0\(\)](#)
- [kernel_sum\\$param_optim_lower\(\)](#)
- [kernel_sum\\$param_optim_upper\(\)](#)
- [kernel_sum\\$set_params_from_optim\(\)](#)
- [kernel_sum\\$dC_dparams\(\)](#)
- [kernel_sum\\$C_dC_dparams\(\)](#)

- `kernel_sum$dC_dx()`
- `kernel_sum$s2_from_params()`
- `kernel_sum$print()`
- `kernel_sum$clone()`

Method `new()`: Initialize kernel

Usage:

```
kernel_sum$new(k1, k2, useC = TRUE)
```

Arguments:

k1 Kernel 1

k2 Kernel 2

useC Should C code used? Not applicable for kernel sum.

Method `k()`: Calculate covariance between two points

Usage:

```
kernel_sum$k(x, y = NULL, params, ...)
```

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

params parameters to use instead of beta and s2.

... Not used

Method `param_optim_start()`: Starting point for parameters for optimization

Usage:

```
kernel_sum$param_optim_start(jitter = F, y)
```

Arguments:

jitter Should there be a jitter?

y Output

Method `param_optim_start0()`: Starting point for parameters for optimization

Usage:

```
kernel_sum$param_optim_start0(jitter = F, y)
```

Arguments:

jitter Should there be a jitter?

y Output

Method `param_optim_lower()`: Lower bounds of parameters for optimization

Usage:

```
kernel_sum$param_optim_lower()
```

Method `param_optim_upper()`: Upper bounds of parameters for optimization

Usage:

```
kernel_sum$param_optim_upper()
```

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```
kernel_sum$set_params_from_optim(optim_out)
```

Arguments:

optim_out Output from optimization

Method dC_dparams(): Derivative of covariance with respect to parameters

Usage:

```
kernel_sum$dC_dparams(params = NULL, C, X, C_nonug, nug)
```

Arguments:

params Kernel parameters

C Covariance with nugget

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

nug Value of nugget

Method C_dC_dparams(): Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
kernel_sum$C_dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters

X matrix of points in rows

nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
kernel_sum$dC_dx(XX, X)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

Method s2_from_params(): Get s2 from params vector

Usage:

```
kernel_sum$s2_from_params(params)
```

Arguments:

params parameter vector

s2_est Is s2 being estimated?

Method print(): Print this object

Usage:

```
kernel_sum$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
kernel_sum$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- Exponential$new(beta=1)
k2 <- Matern32$new(beta=2)
k <- k1 + k2
k$k(matrix(c(2,1), ncol=1))
```

LatentFactorKernel *Latent Factor Kernel R6 class*

Description

Latent Factor Kernel R6 class

Latent Factor Kernel R6 class

Usage

```
k_LatentFactorKernel(
  s2 = 1,
  D,
  nlevels,
  xindex,
  latentdim,
  p_lower = 0,
  p_upper = 1,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)
```

Arguments

s2	Initial variance
D	Number of input dimensions of data
nlevels	Number of levels for the factor
xindex	Index of X to use the kernel on

latentdim	Dimension of embedding space
p_lower	Lower bound for p
p_upper	Upper bound for p
p_est	Should p be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster.
offdiagequal	What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Format

[R6Class](#) object.

Details

Used for factor variables, a single dimension. Each level of the factor gets mapped into a latent space, then the distances in that space determine their correlations.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro](#): [GauPro_kernel](#) -> [GauPro_kernel_LatentFactorKernel](#)

Public fields

p Parameter for correlation
 p_est Should p be estimated?
 p_lower Lower bound of p
 p_upper Upper bound of p
 p_length length of p
 s2 variance
 s2_est Is s2 estimated?
 logs2 Log of s2
 logs2_lower Lower bound of logs2
 logs2_upper Upper bound of logs2
 xindex Index of the factor (which column of X)
 nlevels Number of levels for the factor
 latentdim Dimension of embedding space

`pf_to_p_log` Logical vector used to convert pf to p
`p_to_pf_inds` Vector of indexes used to convert p to pf
`offdiagequal` What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Methods

Public methods:

- `LatentFactorKernel$new()`
- `LatentFactorKernel$k()`
- `LatentFactorKernel$kone()`
- `LatentFactorKernel$dC_dparams()`
- `LatentFactorKernel$C_dC_dparams()`
- `LatentFactorKernel$dC_dx()`
- `LatentFactorKernel$param_optim_start()`
- `LatentFactorKernel$param_optim_start0()`
- `LatentFactorKernel$param_optim_lower()`
- `LatentFactorKernel$param_optim_upper()`
- `LatentFactorKernel$set_params_from_optim()`
- `LatentFactorKernel$p_to_pf()`
- `LatentFactorKernel$s2_from_params()`
- `LatentFactorKernel$plotLatent()`
- `LatentFactorKernel$print()`
- `LatentFactorKernel$clone()`

Method `new()`: Initialize kernel object

Usage:

```

LatentFactorKernel$new(
  s2 = 1,
  D,
  nlevels,
  xindex,
  latentdim,
  p_lower = 0,
  p_upper = 1,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)
  
```

Arguments:

`s2` Initial variance
`D` Number of input dimensions of data

nlevels Number of levels for the factor
xindex Index of X to use the kernel on
latentdim Dimension of embedding space
p_lower Lower bound for p
p_upper Upper bound for p
p_est Should p be estimated?
s2_lower Lower bound for s2
s2_upper Upper bound for s2
s2_est Should s2 be estimated?
useC Should C code used? Much faster.
offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Method `k()`: Calculate covariance between two points

Usage:

```
LatentFactorKernel$k(x, y = NULL, p = self$p, s2 = self$s2, params = NULL)
```

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

p Correlation parameters.

s2 Variance parameter.

params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

```
LatentFactorKernel$kone(
  x,
  y,
  pf,
  s2,
  isdiag = TRUE,
  offdiagequal = self$offdiagequal
)
```

Arguments:

x vector

y vector

pf correlation parameters on regular scale, includes zeroes for first level.

s2 Variance parameter

isdiag Is this on the diagonal of the covariance?

offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

```
LatentFactorKernel$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 C_nonug Covariance without nugget added to diagonal
 C Covariance with nugget
 nug Value of nugget

Method C_dC_dparams(): Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
LatentFactorKernel$C_dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
LatentFactorKernel$dC_dx(XX, X, ...)
```

Arguments:

XX matrix of points
 X matrix of points to take derivative with respect to
 ... Additional args, not used

Method param_optim_start(): Starting point for parameters for optimization

Usage:

```
LatentFactorKernel$param_optim_start(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
 y Output
 p_est Is p being estimated?
 s2_est Is s2 being estimated?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

```
LatentFactorKernel$param_optim_start0(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?

y Output

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

```
LatentFactorKernel$param_optim_lower(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```
LatentFactorKernel$param_optim_upper(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```
LatentFactorKernel$set_params_from_optim(
  optim_out,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

optim_out Output from optimization

p_est Is p being estimated?

s2_est Is s2 being estimated?

Method p_to_pf(): Convert p (short parameter vector) to pf (long parameter vector with zeros).

Usage:

```
LatentFactorKernel$p_to_pf(p)
```

Arguments:

p Parameter vector

Method `s2_from_params()`: Get `s2` from `params` vector

Usage:

```
LatentFactorKernel$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

`params` parameter vector
`s2_est` Is `s2` being estimated?

Method `plotLatent()`: Plot the points in the latent space

Usage:

```
LatentFactorKernel$plotLatent()
```

Method `print()`: Print this object

Usage:

```
LatentFactorKernel$print()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
LatentFactorKernel$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

References

<https://stackoverflow.com/questions/27086195/linear-index-upper-triangular-matrix>

Examples

```
# Create a new kernel for a single factor with 5 levels,
# mapped into two latent dimensions.
kk <- LatentFactorKernel$new(D=1, nlevels=5, xindex=1, latentdim=2)
# Random initial parameter values
kk$p
# Plots to understand
kk$plotLatent()
kk$plot()

# 5 levels, 1/4 are similar and 2/3/5 are similar
n <- 30
x <- matrix(sample(1:5, n, TRUE))
y <- c(ifelse(x == 1 | x == 4, 4, -3) + rnorm(n,0,.1))
plot(c(x), y)
m5 <- GauPro_kernel_model$new(
  X=x, Z=y,
  kernel=LatentFactorKernel$new(D=1, nlevels = 5, xindex = 1, latentdim = 2))
m5$kernel$p
# We should see 1/4 and 2/3/4 in separate clusters
m5$kernel$plotLatent()
```

```

if (requireNamespace("dplyr", quietly=TRUE)) {
  library(dplyr)
  n <- 20
  X <- cbind(matrix(runif(n,2,6), ncol=1),
             matrix(sample(1:2, size=n, replace=TRUE), ncol=1))
  X <- rbind(X, c(3.3,3), c(3.7,3))
  n <- nrow(X)
  Z <- X[,1] - (4-X[,2])^2 + rnorm(n,0,.1)
  plot(X[,1], Z, col=X[,2])
  tibble(X=X, Z) %>% arrange(X,Z)
  k2a <- IgnoreIndsKernel$new(k=Gaussian$new(D=1), ignoreinds = 2)
  k2b <- LatentFactorKernel$new(D=2, nlevels=3, xind=2, latentdim=2)
  k2 <- k2a * k2b
  k2b$p_upper <- .65*k2b$p_upper
  gp <- GauPro_kernel_model$new(X=X, Z=Z, kernel = k2, verbose = 5,
                                nug.min=1e-2, restarts=1)
  gp$kernel$k1$kernel$beta
  gp$kernel$k2$p
  gp$kernel$k(x = gp$X)
  tibble(X=X, Z=Z, pred=gp$predict(X)) %>% arrange(X, Z)
  tibble(X=X[,2], Z) %>% group_by(X) %>% summarize(n=n(), mean(Z))
  curve(gp$pred(cbind(matrix(x,ncol=1),1)),2,6, ylim=c(min(Z), max(Z)))
  points(X[X[,2]==1,1], Z[X[,2]==1])
  curve(gp$pred(cbind(matrix(x,ncol=1),2)), add=TRUE, col=2)
  points(X[X[,2]==2,1], Z[X[,2]==2], col=2)
  curve(gp$pred(cbind(matrix(x,ncol=1),3)), add=TRUE, col=3)
  points(X[X[,2]==3,1], Z[X[,2]==3], col=3)
  legend(legend=1:3, fill=1:3, x="topleft")
  # See which points affect (5.5, 3) the most
  data.frame(X, cov=gp$kernel$k(X, c(5.5,3))) %>% arrange(-cov)
  plot(k2b)
}

```

Matern32

Matern 3/2 Kernel R6 class

Description

Matern 3/2 Kernel R6 class

Matern 3/2 Kernel R6 class

Usage

```

k_Matern32(
  beta,
  s2 = 1,
  D,
  beta_lower = -8,

```

```

beta_upper = 6,
beta_est = TRUE,
s2_lower = 1e-08,
s2_upper = 1e+08,
s2_est = TRUE,
useC = TRUE,
isotropic = FALSE
)

```

Arguments

beta	Initial beta value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster.
isotropic	If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/beta is used for each dimension.

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super classes

[GauPro::GauPro_kernel](#) -> [GauPro::GauPro_kernel_beta](#) -> [GauPro_kernel_Matern32](#)

Public fields

sqrt3 Saved value of square root of 3

Methods

Public methods:

- [Matern32\\$k\(\)](#)
- [Matern32\\$kone\(\)](#)
- [Matern32\\$dC_dparams\(\)](#)

- [Matern32\\$dC_dx\(\)](#)
- [Matern32\\$print\(\)](#)
- [Matern32\\$clone\(\)](#)

Method `k()`: Calculate covariance between two points

Usage:

```
Matern32$k(x, y = NULL, beta = self$beta, s2 = self$s2, params = NULL)
```

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

beta Correlation parameters.

s2 Variance parameter.

params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

```
Matern32$kone(x, y, beta, theta, s2)
```

Arguments:

x vector

y vector

beta correlation parameters on log scale

theta correlation parameters on regular scale

s2 Variance parameter

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

```
Matern32$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method `dC_dx()`: Derivative of covariance with respect to X

Usage:

```
Matern32$dC_dx(XX, X, theta, beta = self$beta, s2 = self$s2)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

theta Correlation parameters

beta log of theta

s2 Variance parameter

Method print(): Print this object

Usage:

```
Matern32$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
Matern32$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- Matern32$new(beta=0)
plot(k1)

n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel=Matern32$new(1),
                             parallel=FALSE)

gp$predict(.454)
gp$plot1D()
gp$cool1Dplot()
```

Matern52

Matern 5/2 Kernel R6 class

Description

Matern 5/2 Kernel R6 class

Matern 5/2 Kernel R6 class

Usage

```
k_Matern52(
  beta,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
  beta_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  isotropic = FALSE
)
```

Arguments

beta	Initial beta value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster.
isotropic	If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/theta is used for each dimension.

Format

[R6Class](#) object.

Details

$k(x, y) = s2 * (1 + t1 + t1^2/3) * exp(-t1)$ where $t1 = sqrt(5) * sqrt(sum(theta * (x - y)^2))$

Value

Object of [R6Class](#) with methods for fitting GP model.

Super classes

[GauPro::GauPro_kernel](#) -> [GauPro::GauPro_kernel_beta](#) -> [GauPro_kernel_Matern52](#)

Public fields

sqrt5 Saved value of square root of 5

Methods**Public methods:**

- [Matern52\\$k\(\)](#)
- [Matern52\\$kone\(\)](#)
- [Matern52\\$dC_dparams\(\)](#)
- [Matern52\\$dC_dx\(\)](#)
- [Matern52\\$print\(\)](#)
- [Matern52\\$clone\(\)](#)

Method k(): Calculate covariance between two points

Usage:

Matern52\$k(x, y = NULL, beta = self\$beta, s2 = self\$s2, params = NULL)

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

beta Correlation parameters.

s2 Variance parameter.

params parameters to use instead of beta and s2.

Method kone(): Find covariance of two points*Usage:*

Matern52\$kone(x, y, beta, theta, s2)

Arguments:

x vector

y vector

beta correlation parameters on log scale

theta correlation parameters on regular scale

s2 Variance parameter

Method dC_dparams(): Derivative of covariance with respect to parameters*Usage:*

Matern52\$dC_dparams(params = NULL, X, C_nonug, C, nug)

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X*Usage:*

Matern52\$dC_dx(XX, X, theta, beta = self\$beta, s2 = self\$s2)

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

theta Correlation parameters

beta log of theta

s2 Variance parameter

Method print(): Print this object*Usage:*

Matern52\$print()

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
Matern52$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- Matern52$new(beta=0)
plot(k1)

n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel=Matern52$new(1),
                             parallel=FALSE)

gp$predict(.454)
gp$plot1D()
gp$cool1Dplot()
```

OrderedFactorKernel *Ordered Factor Kernel R6 class*

Description

Ordered Factor Kernel R6 class

Ordered Factor Kernel R6 class

Usage

```
k_OrderedFactorKernel(
  s2 = 1,
  D,
  nlevels,
  xindex,
  p_lower = 1e-08,
  p_upper = 5,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)
```

Arguments

s2	Initial variance
D	Number of input dimensions of data
nlevels	Number of levels for the factor
xindex	Index of the factor (which column of X)
p_lower	Lower bound for p
p_upper	Upper bound for p
p_est	Should p be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Not implemented for FactorKernel yet.
offdiagequal	What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Format

[R6Class](#) object.

Details

Use for factor inputs that are considered to have an ordering

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro::GauPro_kernel](#) -> GauPro_kernel_OrderedFactorKernel

Public fields

p Parameter for correlation
 p_est Should p be estimated?
 p_lower Lower bound of p
 p_upper Upper bound of p
 p_length length of p
 s2 variance
 s2_est Is s2 estimated?
 logs2 Log of s2
 logs2_lower Lower bound of logs2
 logs2_upper Upper bound of logs2

xindex Index of the factor (which column of X)
 nlevels Number of levels for the factor
 offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Methods

Public methods:

- `OrderedFactorKernel$new()`
- `OrderedFactorKernel$k()`
- `OrderedFactorKernel$kone()`
- `OrderedFactorKernel$dC_dparams()`
- `OrderedFactorKernel$C_dC_dparams()`
- `OrderedFactorKernel$dC_dx()`
- `OrderedFactorKernel$param_optim_start()`
- `OrderedFactorKernel$param_optim_start0()`
- `OrderedFactorKernel$param_optim_lower()`
- `OrderedFactorKernel$param_optim_upper()`
- `OrderedFactorKernel$set_params_from_optim()`
- `OrderedFactorKernel$s2_from_params()`
- `OrderedFactorKernel$plotLatent()`
- `OrderedFactorKernel$print()`
- `OrderedFactorKernel$clone()`

Method `new()`: Initialize kernel object

Usage:

```
OrderedFactorKernel$new(
  s2 = 1,
  D = NULL,
  nlevels,
  xindex,
  p_lower = 1e-08,
  p_upper = 5,
  p_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE,
  offdiagequal = 1 - 1e-06
)
```

Arguments:

s2 Initial variance
 D Number of input dimensions of data
 nlevels Number of levels for the factor

xindex Index of X to use the kernel on
 p_lower Lower bound for p
 p_upper Upper bound for p
 p_est Should p be estimated?
 s2_lower Lower bound for s2
 s2_upper Upper bound for s2
 s2_est Should s2 be estimated?
 useC Should C code used? Much faster.
 offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.
 p Vector of distances in latent space

Method `k()`: Calculate covariance between two points

Usage:

```
OrderedFactorKernel$k(x, y = NULL, p = self$p, s2 = self$s2, params = NULL)
```

Arguments:

x vector.
 y vector, optional. If excluded, find correlation of x with itself.
 p Correlation parameters.
 s2 Variance parameter.
 params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

```
OrderedFactorKernel$kone(
  x,
  y,
  p,
  s2,
  isdiag = TRUE,
  offdiagequal = self$offdiagequal
)
```

Arguments:

x vector
 y vector
 p correlation parameters on regular scale
 s2 Variance parameter
 isdiag Is this on the diagonal of the covariance?
 offdiagequal What should offdiagonal values be set to when the indices are the same? Use to avoid decomposition errors, similar to adding a nugget.

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

```
OrderedFactorKernel$dC_dparams(params = NULL, X, C_nonug, C, nug)
```


Arguments:

params Kernel parameters
 X matrix of points in rows
 C_nonug Covariance without nugget added to diagonal
 C Covariance with nugget
 nug Value of nugget

Method C_dC_dparams(): Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
OrderedFactorKernel$C_dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
OrderedFactorKernel$dC_dx(XX, X, ...)
```

Arguments:

XX matrix of points
 X matrix of points to take derivative with respect to
 ... Additional args, not used

Method param_optim_start(): Starting point for parameters for optimization

Usage:

```
OrderedFactorKernel$param_optim_start(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
 y Output
 p_est Is p being estimated?
 s2_est Is s2 being estimated?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

```
OrderedFactorKernel$param_optim_start0(
  jitter = F,
  y,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
 y Output
 p_est Is p being estimated?
 s2_est Is s2 being estimated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

```
OrderedFactorKernel$param_optim_lower(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?
 s2_est Is s2 being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```
OrderedFactorKernel$param_optim_upper(p_est = self$p_est, s2_est = self$s2_est)
```

Arguments:

p_est Is p being estimated?
 s2_est Is s2 being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```
OrderedFactorKernel$set_params_from_optim(
  optim_out,
  p_est = self$p_est,
  s2_est = self$s2_est
)
```

Arguments:

optim_out Output from optimization
 p_est Is p being estimated?
 s2_est Is s2 being estimated?

Method s2_from_params(): Get s2 from params vector

Usage:

```
OrderedFactorKernel$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

params parameter vector
 s2_est Is s2 being estimated?

Method plotLatent(): Plot the points in the latent space

Usage:

```
OrderedFactorKernel$plotLatent()
```

Method print(): Print this object

Usage:

```
OrderedFactorKernel$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
OrderedFactorKernel$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

References

<https://stackoverflow.com/questions/27086195/linear-index-upper-triangular-matrix>

Examples

```
kk <- OrderedFactorKernel$new(D=1, nlevels=5, xindex=1)
kk$p <- (1:10)/100
kmat <- outer(1:5, 1:5, Vectorize(kk$k))
kmat

if (requireNamespace("dplyr", quietly=TRUE)) {
  library(dplyr)
  n <- 20
  X <- cbind(matrix(runif(n,2,6), ncol=1),
             matrix(sample(1:2, size=n, replace=TRUE), ncol=1))
  X <- rbind(X, c(3.3,3), c(3.7,3))
  n <- nrow(X)
  Z <- X[,1] - (4-X[,2])^2 + rnorm(n,0,.1)
  plot(X[,1], Z, col=X[,2])
  tibble(X=X, Z) %>% arrange(X,Z)
  k2a <- IgnoreIndsKernel$new(k=Gaussian$new(D=1), ignoreinds = 2)
  k2b <- OrderedFactorKernel$new(D=2, nlevels=3, xind=2)
  k2 <- k2a * k2b
  k2b$p_upper <- .65*k2b$p_upper
  gp <- GauPro_kernel_model$new(X=X, Z=Z, kernel = k2, verbose = 5,
                                nug.min=1e-2, restarts=0)
  gp$kernel$k1$kernel$beta
  gp$kernel$k2$p
  gp$kernel$k(x = gp$X)
  tibble(X=X, Z=Z, pred=gp$predict(X)) %>% arrange(X, Z)
  tibble(X=X[,2], Z) %>% group_by(X) %>% summarize(n=n(), mean(Z))
  curve(gp$pred(cbind(matrix(x,ncol=1),1)),2,6, ylim=c(min(Z), max(Z)))
  points(X[X[,2]==1,1], Z[X[,2]==1])
  curve(gp$pred(cbind(matrix(x,ncol=1),2)), add=TRUE, col=2)
  points(X[X[,2]==2,1], Z[X[,2]==2], col=2)
  curve(gp$pred(cbind(matrix(x,ncol=1),3)), add=TRUE, col=3)
  points(X[X[,2]==3,1], Z[X[,2]==3], col=3)
  legend(legend=1:3, fill=1:3, x="topleft")
  # See which points affect (5.5, 3) the most
  data.frame(X, cov=gp$kernel$k(X, c(5.5,3))) %>% arrange(-cov)
```

```
plot(k2b)
}
```

Periodic

Periodic Kernel R6 class

Description

Periodic Kernel R6 class

Periodic Kernel R6 class

Usage

```
k_Periodic(
  p,
  alpha = 1,
  s2 = 1,
  D,
  p_lower = 0,
  p_upper = 100,
  p_est = TRUE,
  alpha_lower = 0,
  alpha_upper = 100,
  alpha_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE
)
```

Arguments

p	Periodic parameter
alpha	Periodic parameter
s2	Initial variance
D	Number of input dimensions of data
p_lower	Lower bound for p
p_upper	Upper bound for p
p_est	Should p be estimated?
alpha_lower	Lower bound for alpha
alpha_upper	Upper bound for alpha
alpha_est	Should alpha be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster if implemented.

Format

[R6Class](#) object.

Details

p is the period for each dimension, a is a single number for scaling

$$k(x, y) = s^2 * \exp(-\text{sum}(\alpha * \sin(p * (x - y))^2))$$

$$k(x, y) = \sigma^2 * \exp(-\sum(\alpha_i * \sin(p * (x_i - y_i))^2))$$

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro::GauPro_kernel](#) -> [GauPro_kernel_Periodic](#)

Public fields

p Parameter for correlation
 p_est Should p be estimated?
 $\log p$ Log of p
 $\log p_lower$ Lower bound of $\log p$
 $\log p_upper$ Upper bound of $\log p$
 p_length length of p
 α Parameter for correlation
 α_est Should α be estimated?
 $\log \alpha$ Log of α
 $\log \alpha_lower$ Lower bound of $\log \alpha$
 $\log \alpha_upper$ Upper bound of $\log \alpha$
 s^2 variance
 s^2_est Is s^2 estimated?
 $\log s^2$ Log of s^2
 $\log s^2_lower$ Lower bound of $\log s^2$
 $\log s^2_upper$ Upper bound of $\log s^2$

Methods**Public methods:**

- [Periodic\\$new\(\)](#)
- [Periodic\\$k\(\)](#)
- [Periodic\\$kone\(\)](#)
- [Periodic\\$dC_dparams\(\)](#)

- `Periodic$dC_dparams()`
- `Periodic$dC_dx()`
- `Periodic$param_optim_start()`
- `Periodic$param_optim_start0()`
- `Periodic$param_optim_lower()`
- `Periodic$param_optim_upper()`
- `Periodic$set_params_from_optim()`
- `Periodic$s2_from_params()`
- `Periodic$print()`
- `Periodic$clone()`

Method `new()`: Initialize kernel object

Usage:

```
Periodic$new(
  p,
  alpha = 1,
  s2 = 1,
  D,
  p_lower = 0,
  p_upper = 100,
  p_est = TRUE,
  alpha_lower = 0,
  alpha_upper = 100,
  alpha_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE
)
```

Arguments:

`p` Periodic parameter
`alpha` Periodic parameter
`s2` Initial variance
`D` Number of input dimensions of data
`p_lower` Lower bound for `p`
`p_upper` Upper bound for `p`
`p_est` Should `p` be estimated?
`alpha_lower` Lower bound for `alpha`
`alpha_upper` Upper bound for `alpha`
`alpha_est` Should `alpha` be estimated?
`s2_lower` Lower bound for `s2`
`s2_upper` Upper bound for `s2`
`s2_est` Should `s2` be estimated?
`useC` Should C code used? Much faster if implemented.

Method `k()`: Calculate covariance between two points

Usage:

```
Periodic$k(
  x,
  y = NULL,
  logp = self$logp,
  logalpha = self$logalpha,
  s2 = self$s2,
  params = NULL
)
```

Arguments:

`x` vector.

`y` vector, optional. If excluded, find correlation of `x` with itself.

`logp` Correlation parameters.

`logalpha` Correlation parameters.

`s2` Variance parameter.

`params` parameters to use instead of `beta` and `s2`.

Method `kone()`: Find covariance of two points

Usage:

```
Periodic$kone(x, y, logp, p, alpha, s2)
```

Arguments:

`x` vector

`y` vector

`logp` correlation parameters on log scale

`p` correlation parameters on regular scale

`alpha` correlation parameter

`s2` Variance parameter

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

```
Periodic$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

`params` Kernel parameters

`X` matrix of points in rows

`C_nonug` Covariance without nugget added to diagonal

`C` Covariance with nugget

`nug` Value of nugget

Method `C_dC_dparams()`: Calculate covariance matrix and its derivative with respect to parameters

Usage:

```
Periodic$C_dC_dparams(params = NULL, X, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
Periodic$dC_dx(XX, X, logp = self$logp, logalpha = self$logalpha, s2 = self$s2)
```

Arguments:

XX matrix of points
 X matrix of points to take derivative with respect to
 logp log of p
 logalpha log of alpha
 s2 Variance parameter

Method param_optim_start(): Starting point for parameters for optimization

Usage:

```
Periodic$param_optim_start(
  jitter = F,
  y,
  p_est = self$p_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
 y Output
 p_est Is p being estimated?
 alpha_est Is alpha being estimated?
 s2_est Is s2 being estimated?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

```
Periodic$param_optim_start0(
  jitter = F,
  y,
  p_est = self$p_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
 y Output
 p_est Is p being estimated?

alpha_est Is alpha being estimated?
s2_est Is s2 being estimated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

```
Periodic$param_optim_lower(  
  p_est = self$p_est,  
  alpha_est = self$alpha_est,  
  s2_est = self$s2_est  
)
```

Arguments:

p_est Is p being estimated?
alpha_est Is alpha being estimated?
s2_est Is s2 being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```
Periodic$param_optim_upper(  
  p_est = self$p_est,  
  alpha_est = self$alpha_est,  
  s2_est = self$s2_est  
)
```

Arguments:

p_est Is p being estimated?
alpha_est Is alpha being estimated?
s2_est Is s2 being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```
Periodic$set_params_from_optim(  
  optim_out,  
  p_est = self$p_est,  
  alpha_est = self$alpha_est,  
  s2_est = self$s2_est  
)
```

Arguments:

optim_out Output from optimization
p_est Is p being estimated?
alpha_est Is alpha being estimated?
s2_est Is s2 being estimated?

Method s2_from_params(): Get s2 from params vector

Usage:

```
Periodic$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

params parameter vector
s2_est Is s2 being estimated?

Method print(): Print this object

Usage:

Periodic\$print()

Method clone(): The objects of this class are cloneable with this method.

Usage:

Periodic\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- Periodic$new(p=1, alpha=1)
plot(k1)

n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel=Periodic$new(D=1),
                             parallel=FALSE)

gp$predict(.454)
gp$plot1D()
gp$cool1Dplot()
plot(gp$kernel)
```

PowerExp

Power Exponential Kernel R6 class

Description

Power Exponential Kernel R6 class

Power Exponential Kernel R6 class

Usage

```
k_PowerExp(
  alpha = 1.95,
  beta,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
```

```

    beta_est = TRUE,
    alpha_lower = 1e-08,
    alpha_upper = 2,
    alpha_est = TRUE,
    s2_lower = 1e-08,
    s2_upper = 1e+08,
    s2_est = TRUE,
    useC = TRUE
)

```

Arguments

alpha	Initial alpha value (the exponent). Between 0 and 2.
beta	Initial beta value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
alpha_lower	Lower bound for alpha
alpha_upper	Upper bound for alpha
alpha_est	Should alpha be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster if implemented.

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super classes

[GauPro::GauPro_kernel](#) -> [GauPro::GauPro_kernel_beta](#) -> [GauPro_kernel_PowerExp](#)

Public fields

alpha alpha value (the exponent). Between 0 and 2.
alpha_lower Lower bound for alpha
alpha_upper Upper bound for alpha
alpha_est Should alpha be estimated?

Methods**Public methods:**

- [PowerExp\\$new\(\)](#)
- [PowerExp\\$k\(\)](#)
- [PowerExp\\$kone\(\)](#)
- [PowerExp\\$dC_dparams\(\)](#)
- [PowerExp\\$dC_dx\(\)](#)
- [PowerExp\\$param_optim_start\(\)](#)
- [PowerExp\\$param_optim_start0\(\)](#)
- [PowerExp\\$param_optim_lower\(\)](#)
- [PowerExp\\$param_optim_upper\(\)](#)
- [PowerExp\\$set_params_from_optim\(\)](#)
- [PowerExp\\$print\(\)](#)
- [PowerExp\\$clone\(\)](#)

Method `new()`: Initialize kernel object

Usage:

```
PowerExp$new(
  alpha = 1.95,
  beta,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
  beta_est = TRUE,
  alpha_lower = 1e-08,
  alpha_upper = 2,
  alpha_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE
)
```

Arguments:

`alpha` Initial alpha value (the exponent). Between 0 and 2.

`beta` Initial beta value

`s2` Initial variance

`D` Number of input dimensions of data

`beta_lower` Lower bound for beta

`beta_upper` Upper bound for beta

`beta_est` Should beta be estimated?

`alpha_lower` Lower bound for alpha

`alpha_upper` Upper bound for alpha

`alpha_est` Should alpha be estimated?

s2_lower Lower bound for s2
 s2_upper Upper bound for s2
 s2_est Should s2 be estimated?
 useC Should C code used? Much faster if implemented.

Method k(): Calculate covariance between two points

Usage:

```
PowerExp$k(
  x,
  y = NULL,
  beta = self$beta,
  alpha = self$alpha,
  s2 = self$s2,
  params = NULL
)
```

Arguments:

x vector.
 y vector, optional. If excluded, find correlation of x with itself.
 beta Correlation parameters.
 alpha alpha value (the exponent). Between 0 and 2.
 s2 Variance parameter.
 params parameters to use instead of beta and s2.

Method kone(): Find covariance of two points

Usage:

```
PowerExp$kone(x, y, beta, theta, alpha, s2)
```

Arguments:

x vector
 y vector
 beta correlation parameters on log scale
 theta correlation parameters on regular scale
 alpha alpha value (the exponent). Between 0 and 2.
 s2 Variance parameter

Method dC_dparams(): Derivative of covariance with respect to parameters

Usage:

```
PowerExp$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters
 X matrix of points in rows
 C_nonug Covariance without nugget added to diagonal
 C Covariance with nugget
 nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
PowerExp$dC_dx(
  XX,
  X,
  theta,
  beta = self$beta,
  alpha = self$alpha,
  s2 = self$s2
)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

theta Correlation parameters

beta log of theta

alpha alpha value (the exponent). Between 0 and 2.

s2 Variance parameter

Method param_optim_start(): Starting point for parameters for optimization

Usage:

```
PowerExp$param_optim_start(
  jitter = F,
  y,
  beta_est = self$beta_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?

y Output

beta_est Is beta being estimated?

alpha_est Is alpha being estimated?

s2_est Is s2 being estimated?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

```
PowerExp$param_optim_start0(
  jitter = F,
  y,
  beta_est = self$beta_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
y Output
beta_est Is beta being estimated?
alpha_est Is alpha being estimated?
s2_est Is s2 being estimated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

```
PowerExp$param_optim_lower(  
  beta_est = self$beta_est,  
  alpha_est = self$alpha_est,  
  s2_est = self$s2_est  
)
```

Arguments:

beta_est Is beta being estimated?
alpha_est Is alpha being estimated?
s2_est Is s2 being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```
PowerExp$param_optim_upper(  
  beta_est = self$beta_est,  
  alpha_est = self$alpha_est,  
  s2_est = self$s2_est  
)
```

Arguments:

beta_est Is beta being estimated?
alpha_est Is alpha being estimated?
s2_est Is s2 being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```
PowerExp$set_params_from_optim(  
  optim_out,  
  beta_est = self$beta_est,  
  alpha_est = self$alpha_est,  
  s2_est = self$s2_est  
)
```

Arguments:

optim_out Output from optimization
beta_est Is beta estimate?
alpha_est Is alpha estimated?
s2_est Is s2 estimated?

Method print(): Print this object

Usage:

```
PowerExp$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
PowerExp$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- PowerExp$new(beta=0, alpha=0)
```

predict.GauPro	<i>Predict for class GauPro</i>
----------------	---------------------------------

Description

Predict for class GauPro

Usage

```
## S3 method for class 'GauPro'
predict(object, XX, se.fit = F, covmat = F, split_speed = T, ...)
```

Arguments

object	Object of class GauPro
XX	new points to predict
se.fit	Should standard error be returned (and variance)?
covmat	Should the covariance matrix be returned?
split_speed	Should the calculation be split up to speed it up?
...	Additional parameters

Value

Prediction from object at XX

Examples

```
n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro(X=x, Z=y, parallel=FALSE)
predict(gp, .448)
```

predict.GauPro_base *Predict for class GauPro_base*

Description

Predict mean and se for given matrix

Usage

```
## S3 method for class 'GauPro_base'
predict(object, XX, se.fit = F, covmat = F, split_speed = T, ...)
```

Arguments

object	Object of class GauPro_base
XX	Points to predict at
se.fit	Should the se be returned?
covmat	Should the covariance matrix be returned?
split_speed	Should the predictions be split up for speed
...	Additional parameters

Value

Prediction from object at XX

print.summary.GauPro *Print summary.GauPro*

Description

Print summary.GauPro

Usage

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

Arguments

x	summary.GauPro object
...	Additional args

Value

prints, returns invisible object

RatQuad

*Rational Quadratic Kernel R6 class***Description**

Rational Quadratic Kernel R6 class

Rational Quadratic Kernel R6 class

Usage

```

k_RatQuad(
  beta,
  alpha = 1,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
  beta_est = TRUE,
  alpha_lower = 1e-08,
  alpha_upper = 100,
  alpha_est = TRUE,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE
)

```

Arguments

beta	Initial beta value
alpha	Initial alpha value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
alpha_lower	Lower bound for alpha
alpha_upper	Upper bound for alpha
alpha_est	Should alpha be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster if implemented.

Format

R6Class object.

Value

Object of R6Class with methods for fitting GP model.

Super classes

GauPro::GauPro_kernel -> GauPro::GauPro_kernel_beta -> GauPro_kernel_RatQuad

Public fields

alpha alpha value (the exponent). Between 0 and 2.

logalpha Log of alpha

logalpha_lower Lower bound for log of alpha

logalpha_upper Upper bound for log of alpha

alpha_est Should alpha be estimated?

Methods**Public methods:**

- RatQuad\$new()
- RatQuad\$k()
- RatQuad\$kone()
- RatQuad\$dC_dparams()
- RatQuad\$dC_dx()
- RatQuad\$param_optim_start()
- RatQuad\$param_optim_start0()
- RatQuad\$param_optim_lower()
- RatQuad\$param_optim_upper()
- RatQuad\$set_params_from_optim()
- RatQuad\$print()
- RatQuad\$clone()

Method new(): Initialize kernel object

Usage:

```
RatQuad$new(
  beta,
  alpha = 1,
  s2 = 1,
  D,
  beta_lower = -8,
  beta_upper = 6,
  beta_est = TRUE,
```

```

    alpha_lower = 1e-08,
    alpha_upper = 100,
    alpha_est = TRUE,
    s2_lower = 1e-08,
    s2_upper = 1e+08,
    s2_est = TRUE,
    useC = TRUE
)

```

Arguments:

beta Initial beta value
 alpha Initial alpha value
 s2 Initial variance
 D Number of input dimensions of data
 beta_lower Lower bound for beta
 beta_upper Upper bound for beta
 beta_est Should beta be estimated?
 alpha_lower Lower bound for alpha
 alpha_upper Upper bound for alpha
 alpha_est Should alpha be estimated?
 s2_lower Lower bound for s2
 s2_upper Upper bound for s2
 s2_est Should s2 be estimated?
 useC Should C code used? Much faster if implemented.

Method `k()`: Calculate covariance between two points

Usage:

```

RatQuad$k(
  x,
  y = NULL,
  beta = self$beta,
  logalpha = self$logalpha,
  s2 = self$s2,
  params = NULL
)

```

Arguments:

x vector.
 y vector, optional. If excluded, find correlation of x with itself.
 beta Correlation parameters.
 logalpha A correlation parameter
 s2 Variance parameter.
 params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

```
RatQuad$kone(x, y, beta, theta, alpha, s2)
```

Arguments:

x vector

y vector

beta correlation parameters on log scale

theta correlation parameters on regular scale

alpha A correlation parameter

s2 Variance parameter

Method dC_dparams(): Derivative of covariance with respect to parameters

Usage:

```
RatQuad$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

```
RatQuad$dC_dx(XX, X, theta, beta = self$beta, alpha = self$alpha, s2 = self$s2)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

theta Correlation parameters

beta log of theta

alpha parameter

s2 Variance parameter

Method param_optim_start(): Starting point for parameters for optimization

Usage:

```
RatQuad$param_optim_start(
  jitter = F,
  y,
  beta_est = self$beta_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?

y Output

beta_est Is beta being estimated?

alpha_est Is alpha being estimated?
 s2_est Is s2 being estimated?

Method param_optim_start0(): Starting point for parameters for optimization

Usage:

```
RatQuad$param_optim_start0(
  jitter = F,
  y,
  beta_est = self$beta_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

jitter Should there be a jitter?
 y Output
 beta_est Is beta being estimated?
 alpha_est Is alpha being estimated?
 s2_est Is s2 being estimated?

Method param_optim_lower(): Lower bounds of parameters for optimization

Usage:

```
RatQuad$param_optim_lower(
  beta_est = self$beta_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

beta_est Is beta being estimated?
 alpha_est Is alpha being estimated?
 s2_est Is s2 being estimated?

Method param_optim_upper(): Upper bounds of parameters for optimization

Usage:

```
RatQuad$param_optim_upper(
  beta_est = self$beta_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

beta_est Is beta being estimated?
 alpha_est Is alpha being estimated?
 s2_est Is s2 being estimated?

Method set_params_from_optim(): Set parameters from optimization output

Usage:

```
RatQuad$set_params_from_optim(
  optim_out,
  beta_est = self$beta_est,
  alpha_est = self$alpha_est,
  s2_est = self$s2_est
)
```

Arguments:

optim_out Output from optimization
 beta_est Is beta being estimated?
 alpha_est Is alpha being estimated?
 s2_est Is s2 being estimated?

Method print(): Print this object

Usage:

```
RatQuad$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
RatQuad$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- RatQuad$new(beta=0, alpha=0)
```

 sqrt_matrix

Find the square root of a matrix

Description

Same thing as 'expm::sqrtm', but faster.

Usage

```
sqrt_matrix(mat, symmetric)
```

Arguments

mat Matrix to find square root matrix of
 symmetric Is it symmetric? Passed to eigen.

Value

Square root of mat

Examples

```
mat <- matrix(c(1,.1,.1,1), 2, 2)
smat <- sqrt_matrix(mat=mat, symmetric=TRUE)
smat %**% smat
```

summary.GauPro	<i>Summary for GauPro object</i>
----------------	----------------------------------

Description

Summary for GauPro object

Usage

```
## S3 method for class 'GauPro'
summary(object, ...)
```

Arguments

object	GauPro R6 object
...	Additional arguments passed to summary

Value

Summary

trend_0	<i>Trend R6 class</i>
---------	-----------------------

Description

Trend R6 class
Trend R6 class

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro::GauPro_trend](#) -> GauPro_trend_0

Public fields

m Trend parameters
 m_lower m lower bound
 m_upper m upper bound
 m_est Should m be estimated?

Methods**Public methods:**

- trend_0\$new()
- trend_0\$Z()
- trend_0\$dZ_dparams()
- trend_0\$dZ_dx()
- trend_0\$param_optim_start()
- trend_0\$param_optim_start0()
- trend_0\$param_optim_lower()
- trend_0\$param_optim_upper()
- trend_0\$set_params_from_optim()
- trend_0\$clone()

Method new(): Initialize trend object

Usage:

trend_0\$new(m = 0, m_lower = 0, m_upper = 0, m_est = FALSE, D = NA)

Arguments:

m trend initial parameters
 m_lower trend lower bounds
 m_upper trend upper bounds
 m_est Logical of whether each param should be estimated
 D Number of input dimensions of data

Method Z(): Get trend value for given matrix X

Usage:

trend_0\$Z(X, m = self\$m, params = NULL)

Arguments:

X matrix of points
 m trend parameters
 params trend parameters

Method dZ_dparams(): Derivative of trend with respect to trend parameters

Usage:

trend_0\$dZ_dparams(X, m = m\$est, params = NULL)

Arguments:

X matrix of points
m trend values
params overrides m

Method dZ_dx(): Derivative of trend with respect to X

Usage:

trend_0\$dZ_dx(X, m = self\$m, params = NULL)

Arguments:

X matrix of points
m trend values
params overrides m

Method param_optim_start(): Get parameter initial point for optimization

Usage:

trend_0\$param_optim_start(jitter, trend_est)

Arguments:

jitter Not used
trend_est If the trend should be estimate.

Method param_optim_start0(): Get parameter initial point for optimization

Usage:

trend_0\$param_optim_start0(jitter, trend_est)

Arguments:

jitter Not used
trend_est If the trend should be estimate.

Method param_optim_lower(): Get parameter lower bounds for optimization

Usage:

trend_0\$param_optim_lower(jitter, trend_est)

Arguments:

jitter Not used
trend_est If the trend should be estimate.

Method param_optim_upper(): Get parameter upper bounds for optimization

Usage:

trend_0\$param_optim_upper(jitter, trend_est)

Arguments:

jitter Not used
trend_est If the trend should be estimate.

Method set_params_from_optim(): Set parameters after optimization

Usage:

trend_0\$set_params_from_optim(optim_out)

Arguments:

optim_out Output from optim

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
trend_0$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
t1 <- trend_0$new()
```

trend_c	<i>Trend R6 class</i>
---------	-----------------------

Description

Trend R6 class

Trend R6 class

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro](#): [GauPro_trend](#) -> GauPro_trend_c

Public fields

m Trend parameters

m_lower m lower bound

m_upper m upper bound

m_est Should m be estimated?

Methods**Public methods:**

- `trend_c$new()`
- `trend_c$Z()`
- `trend_c$dZ_dparams()`
- `trend_c$dZ_dx()`
- `trend_c$param_optim_start()`
- `trend_c$param_optim_start0()`
- `trend_c$param_optim_lower()`
- `trend_c$param_optim_upper()`
- `trend_c$set_params_from_optim()`
- `trend_c$clone()`

Method `new()`: Initialize trend object

Usage:

```
trend_c$new(m = 0, m_lower = -Inf, m_upper = Inf, m_est = TRUE, D = NA)
```

Arguments:

`m` trend initial parameters

`m_lower` trend lower bounds

`m_upper` trend upper bounds

`m_est` Logical of whether each param should be estimated

`D` Number of input dimensions of data

Method `Z()`: Get trend value for given matrix `X`

Usage:

```
trend_c$Z(X, m = self$m, params = NULL)
```

Arguments:

`X` matrix of points

`m` trend parameters

`params` trend parameters

Method `dZ_dparams()`: Derivative of trend with respect to trend parameters

Usage:

```
trend_c$dZ_dparams(X, m = self$m, params = NULL)
```

Arguments:

`X` matrix of points

`m` trend values

`params` overrides `m`

Method `dZ_dx()`: Derivative of trend with respect to `X`

Usage:

```
trend_c$dZ_dx(X, m = self$m, params = NULL)
```

Arguments:

X matrix of points
m trend values
params overrides m

Method param_optim_start(): Get parameter initial point for optimization

Usage:

```
trend_c$param_optim_start(jitter = F, m_est = self$m_est)
```

Arguments:

jitter Not used
m_est If the trend should be estimate.

Method param_optim_start0(): Get parameter initial point for optimization

Usage:

```
trend_c$param_optim_start0(jitter = F, m_est = self$m_est)
```

Arguments:

jitter Not used
m_est If the trend should be estimate.

Method param_optim_lower(): Get parameter lower bounds for optimization

Usage:

```
trend_c$param_optim_lower(m_est = self$m_est)
```

Arguments:

m_est If the trend should be estimate.

Method param_optim_upper(): Get parameter upper bounds for optimization

Usage:

```
trend_c$param_optim_upper(m_est = self$m_est)
```

Arguments:

m_est If the trend should be estimate.

Method set_params_from_optim(): Set parameters after optimization

Usage:

```
trend_c$set_params_from_optim(optim_out)
```

Arguments:

optim_out Output from optim

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
trend_c$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
t1 <- trend_c$new()
```

trend_LM	<i>Trend R6 class</i>
----------	-----------------------

Description

Trend R6 class

Trend R6 class

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

[GauPro](#): :[GauPro_trend](#) -> [GauPro_trend_LM](#)

Public fields

m Trend parameters

m_lower m lower bound

m_upper m upper bound

m_est Should m be estimated?

b trend parameter

b_lower trend lower bounds

b_upper trend upper bounds

b_est Should b be estimated?

Methods**Public methods:**

- [trend_LM\\$new\(\)](#)
- [trend_LM\\$Z\(\)](#)
- [trend_LM\\$dZ_dparams\(\)](#)
- [trend_LM\\$dZ_dx\(\)](#)
- [trend_LM\\$param_optim_start\(\)](#)
- [trend_LM\\$param_optim_start0\(\)](#)
- [trend_LM\\$param_optim_lower\(\)](#)
- [trend_LM\\$param_optim_upper\(\)](#)
- [trend_LM\\$set_params_from_optim\(\)](#)

- [trend_LM\\$clone\(\)](#)

Method new(): Initialize trend object

Usage:

```
trend_LM$new(
  D,
  m = rep(0, D),
  m_lower = rep(-Inf, D),
  m_upper = rep(Inf, D),
  m_est = rep(TRUE, D),
  b = 0,
  b_lower = -Inf,
  b_upper = Inf,
  b_est = TRUE
)
```

Arguments:

D Number of input dimensions of data
 m trend initial parameters
 m_lower trend lower bounds
 m_upper trend upper bounds
 m_est Logical of whether each param should be estimated
 b trend parameter
 b_lower trend lower bounds
 b_upper trend upper bounds
 b_est Should b be estimated?

Method Z(): Get trend value for given matrix X

Usage:

```
trend_LM$Z(X, m = self$m, b = self$b, params = NULL)
```

Arguments:

X matrix of points
 m trend parameters
 b trend parameters (slopes)
 params trend parameters

Method dZ_dparams(): Derivative of trend with respect to trend parameters

Usage:

```
trend_LM$dZ_dparams(X, m = self$m_est, b = self$b_est, params = NULL)
```

Arguments:

X matrix of points
 m trend values
 b trend intercept
 params overrides m

Method dZ_dx(): Derivative of trend with respect to X

Usage:

```
trend_LM$dZ_dx(X, m = self$m, params = NULL)
```

Arguments:

X matrix of points
m trend values
params overrides m

Method param_optim_start(): Get parameter initial point for optimization

Usage:

```
trend_LM$param_optim_start(
  jitter = FALSE,
  b_est = self$b_est,
  m_est = self$m_est
)
```

Arguments:

jitter Not used
b_est If the mean should be estimated.
m_est If the linear terms should be estimated.

Method param_optim_start0(): Get parameter initial point for optimization

Usage:

```
trend_LM$param_optim_start0(
  jitter = FALSE,
  b_est = self$b_est,
  m_est = self$m_est
)
```

Arguments:

jitter Not used
b_est If the mean should be estimated.
m_est If the linear terms should be estimated.

Method param_optim_lower(): Get parameter lower bounds for optimization

Usage:

```
trend_LM$param_optim_lower(b_est = self$b_est, m_est = self$m_est)
```

Arguments:

b_est If the mean should be estimated.
m_est If the linear terms should be estimated.

Method param_optim_upper(): Get parameter upper bounds for optimization

Usage:

```
trend_LM$param_optim_upper(b_est = self$b_est, m_est = self$m_est)
```

Arguments:

b_est If the mean should be estimated.
 m_est If the linear terms should be estimated.

Method `set_params_from_optim()`: Set parameters after optimization

Usage:

```
trend_LM$set_params_from_optim(optim_out)
```

Arguments:

optim_out Output from optim

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
trend_LM$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
t1 <- trend_LM$new(D=2)
```

Triangle

Triangle Kernel R6 class

Description

Triangle Kernel R6 class

Triangle Kernel R6 class

Usage

```
k_Triangle(  
  beta,  
  s2 = 1,  
  D,  
  beta_lower = -8,  
  beta_upper = 6,  
  beta_est = TRUE,  
  s2_lower = 1e-08,  
  s2_upper = 1e+08,  
  s2_est = TRUE,  
  useC = TRUE,  
  isotropic = FALSE  
)
```

Arguments

beta	Initial beta value
s2	Initial variance
D	Number of input dimensions of data
beta_lower	Lower bound for beta
beta_upper	Upper bound for beta
beta_est	Should beta be estimated?
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Much faster.
isotropic	If isotropic then a single beta/theta is used for all dimensions. If not (anisotropic) then a separate beta/beta is used for each dimension.

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super classes

[GauPro::GauPro_kernel](#) -> [GauPro::GauPro_kernel_beta](#) -> [GauPro_kernel_Triangle](#)

Methods**Public methods:**

- [Triangle\\$k\(\)](#)
- [Triangle\\$kone\(\)](#)
- [Triangle\\$dC_dparams\(\)](#)
- [Triangle\\$dC_dx\(\)](#)
- [Triangle\\$print\(\)](#)
- [Triangle\\$clone\(\)](#)

Method `k()`: Calculate covariance between two points

Usage:

```
Triangle$k(x, y = NULL, beta = self$beta, s2 = self$s2, params = NULL)
```

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

beta Correlation parameters.

s2 Variance parameter.
params parameters to use instead of beta and s2.

Method `kone()`: Find covariance of two points

Usage:

```
Triangle$kone(x, y, beta, theta, s2)
```

Arguments:

x vector

y vector

beta correlation parameters on log scale

theta correlation parameters on regular scale

s2 Variance parameter

Method `dC_dparams()`: Derivative of covariance with respect to parameters

Usage:

```
Triangle$dC_dparams(params = NULL, X, C_nonug, C, nug)
```

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method `dC_dx()`: Derivative of covariance with respect to X

Usage:

```
Triangle$dC_dx(XX, X, theta, beta = self$beta, s2 = self$s2)
```

Arguments:

XX matrix of points

X matrix of points to take derivative with respect to

theta Correlation parameters

beta log of theta

s2 Variance parameter

Method `print()`: Print this object

Usage:

```
Triangle$print()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
Triangle$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```

k1 <- Triangle$new(beta=0)
plot(k1)

n <- 12
x <- matrix(seq(0,1,length.out = n), ncol=1)
y <- sin(2*pi*x) + rnorm(n,0,1e-1)
gp <- GauPro_kernel_model$new(X=x, Z=y, kernel=Triangle$new(1),
                             parallel=FALSE)

gp$predict(.454)
gp$plot1D()
gp$cool1Dplot()

```

White

*White noise Kernel R6 class***Description**

Initialize kernel object

Usage

```

k_White(
  s2 = 1,
  D,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE
)

```

Arguments

s2	Initial variance
D	Number of input dimensions of data
s2_lower	Lower bound for s2
s2_upper	Upper bound for s2
s2_est	Should s2 be estimated?
useC	Should C code used? Not implemented for White.

Format

[R6Class](#) object.

Value

Object of [R6Class](#) with methods for fitting GP model.

Super class

`GauPro::GauPro_kernel` -> `GauPro_kernel_White`

Public fields

`s2` variance
`logs2` Log of `s2`
`logs2_lower` Lower bound of `logs2`
`logs2_upper` Upper bound of `logs2`
`s2_est` Should `s2` be estimated?

Methods**Public methods:**

- `White$new()`
- `White$k()`
- `White$kone()`
- `White$dC_dparams()`
- `White$C_dC_dparams()`
- `White$dC_dx()`
- `White$param_optim_start()`
- `White$param_optim_start0()`
- `White$param_optim_lower()`
- `White$param_optim_upper()`
- `White$set_params_from_optim()`
- `White$s2_from_params()`
- `White$print()`
- `White$clone()`

Method `new()`: Initialize kernel object

Usage:

```
White$new(
  s2 = 1,
  D,
  s2_lower = 1e-08,
  s2_upper = 1e+08,
  s2_est = TRUE,
  useC = TRUE
)
```

Arguments:

`s2` Initial variance
`D` Number of input dimensions of data
`s2_lower` Lower bound for `s2`

s2_upper Upper bound for s2
 s2_est Should s2 be estimated?
 useC Should C code used? Not implemented for White.

Method k(): Calculate covariance between two points

Usage:

White\$k(x, y = NULL, s2 = self\$s2, params = NULL)

Arguments:

x vector.

y vector, optional. If excluded, find correlation of x with itself.

s2 Variance parameter.

params parameters to use instead of beta and s2.

Method kone(): Find covariance of two points

Usage:

White\$kone(x, y, s2)

Arguments:

x vector

y vector

s2 Variance parameter

Method dC_dparams(): Derivative of covariance with respect to parameters

Usage:

White\$dC_dparams(params = NULL, X, C_nonug, C, nug)

Arguments:

params Kernel parameters

X matrix of points in rows

C_nonug Covariance without nugget added to diagonal

C Covariance with nugget

nug Value of nugget

Method C_dC_dparams(): Calculate covariance matrix and its derivative with respect to parameters

Usage:

White\$C_dC_dparams(params = NULL, X, nug)

Arguments:

params Kernel parameters

X matrix of points in rows

nug Value of nugget

Method dC_dx(): Derivative of covariance with respect to X

Usage:

White\$dC_dx(XX, X, s2 = self\$s2)

Arguments:

XX matrix of points
X matrix of points to take derivative with respect to
s2 Variance parameter
theta Correlation parameters
beta log of theta

Method `param_optim_start()`: Starting point for parameters for optimization

Usage:

```
White$param_optim_start(jitter = F, y, s2_est = self$s2_est)
```

Arguments:

jitter Should there be a jitter?
y Output
s2_est Is s2 being estimated?

Method `param_optim_start0()`: Starting point for parameters for optimization

Usage:

```
White$param_optim_start0(jitter = F, y, s2_est = self$s2_est)
```

Arguments:

jitter Should there be a jitter?
y Output
s2_est Is s2 being estimated?

Method `param_optim_lower()`: Lower bounds of parameters for optimization

Usage:

```
White$param_optim_lower(s2_est = self$s2_est)
```

Arguments:

s2_est Is s2 being estimated?

Method `param_optim_upper()`: Upper bounds of parameters for optimization

Usage:

```
White$param_optim_upper(s2_est = self$s2_est)
```

Arguments:

s2_est Is s2 being estimated?

Method `set_params_from_optim()`: Set parameters from optimization output

Usage:

```
White$set_params_from_optim(optim_out, s2_est = self$s2_est)
```

Arguments:

optim_out Output from optimization
s2_est s2 estimate

Method `s2_from_params()`: Get s2 from params vector

Usage:

```
White$s2_from_params(params, s2_est = self$s2_est)
```

Arguments:

params parameter vector

s2_est Is s2 being estimated?

Method print(): Print this object

Usage:

```
White$print()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
White$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
k1 <- White$new(s2=1e-8)
```


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