# Package ‘GPfit’

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Gaussian Processes Modeling

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**Description**  
A computationally stable approach of fitting a Gaussian Process (GP) model to a deterministic simulator.

**Imports**  
lhs (>= 0.5), lattice (>= 0.18-8)

**Suggests**  
testthat

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**GPfit-package**

*Gaussian Process Modeling*

### Description

A computationally stable approach of fitting a Gaussian process (GP) model to simulator outputs. It is assumed that the input variables are continuous and the outputs are obtained from scalar valued deterministic computer simulator.

### Details

This package implements a slightly modified version of the regularized GP model proposed in Ranjan et al. (2011). For details see MacDonald et al. (2015). A new parameterization of the Gaussian correlation is used for the ease of optimization. This package uses a multi-start gradient based search algorithm for optimizing the deviance (negative 2*log-likelihood).

For a complete list of functions, use `library(help="GPfit")`. The main function for fitting the GP model is `GP_fit`.

### Author(s)

Blake MacDoanld, Hugh Chipman, Pritam Ranjan

Maintainer: Hugh Chipman <hugh.chipman@acadiau.ca>

### References


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**corr_matrix**

*Power Exponential or Matern Correlation Matrix*

### Description

Computes the power exponential or Matern correlation matrix for a set of $n$ design points in $d$-dimensional input region and a vector of $d$ correlation hyper-parameters (beta).
Usage

corr_matrix(X, beta, corr = list(type = "exponential", power = 1.95))

Arguments

X                    the (n x d) design matrix
beta                 a (d x 1) vector of correlation hyper-parameters in (−∞, ∞)
corr                 a list that specifies the type of correlation function along with the smooth-
ness parameter. The default corresponds to power exponential correlation with smoothness parameter "power=1.95". One can specify a different power (between 1.0 and 2.0) for the power exponential, or use the Matern correlation function, specified as corr=list(type = "matern", nu=(2*k+1)/2), where k ∈ {0, 1, 2, ...}

Details

The power exponential correlation function is given by

\[ R_{ij} = \prod_{k=1}^{d} \exp(-10^{\beta_k}|x_{ik} - x_{jk}|^{\text{power}}). \]

The Matern correlation function given by Santner, Williams, and Notz (2003) is

\[ R_{ij} = \prod_{k=1}^{d} \frac{1}{\Gamma(\nu)2^{-\nu\kappa_{\nu}}}(2\sqrt{\nu}|x_{ik} - x_{jk}|10^{\beta_k})^{\nu} \kappa_{\nu}(2\sqrt{\nu}|x_{ik} - x_{jk}|10^{\beta_k}), \]

where \( \kappa_{\nu} \) is the modified Bessel function of order \( \nu \).

Value

The (n x n) correlation matrix, R, for the design matrix (X) and the hyper-parameters (beta).

Note

Both Matern and power exponential correlation functions use the new \( \beta \) parametrization of hyper-
parameters given by \( \theta_k = 10^{\beta_k} \) for easier likelihood optimization. That is, beta is a log scale
parameter (see MacDonald et al. (2015)).

Author(s)

Blake MacDonald, Hugh Chipman, Pritam Ranjan

References

http://www.jstatsoft.org/v64/i12/


Examples

```r
## 1D Example - 1
n = 5
d = 1
set.seed(3)
library(lhs)
x = maximinLHS(n,d)
beta = rnorm(1)
corr_matrix(x,beta)

## 1D Example - 2
beta = rnorm(1)
corr_matrix(x,beta, corr = list(type = "matern"))

## 2D example - 1
n = 10
d = 2
set.seed(2)
library(lhs)
x = maximinLHS(n,d)
beta = rnorm(2)
corr_matrix(x, beta,
    corr = list(type = "exponential", power = 2))

## 2D example - 2
beta = rnorm(2)
R = corr_matrix(x,beta,corr = list(type = "matern", nu = 5/2))
print(R)
```

---

**GP_deviance**  
*Computes the Deviance of a GP model*

**Description**

Evaluates the deviance (negative $2\log$-likelihood), as defined in Ranjan et al. (2011), however the correlation is reparametrized and can be either power exponential or Matern as discussed in `corr_matrix`.

**Usage**

```r
GP_deviance(beta, X, Y, nug_thres = 20, corr = list(type = "exponential", power = 1.95))
```
**Arguments**

- **beta**
  a \((d \times 1)\) vector of correlation hyper-parameters, as described in `corr_matrix`
- **X**
  the \((n \times d)\) design matrix
- **Y**
  the \((n \times 1)\) vector of simulator outputs
- **nug_thres**
  a parameter used in computing the nugget. See `GP_fit`.
- **corr**
  a list of parameters for the specifying the correlation to be used. See `corr_matrix`.

**Value**

the deviance (negative 2 * log-likelihood)

**Author(s)**

Blake MacDonald, Hugh Chipman, Pritam Ranjan

**References**


**See Also**

- `corr_matrix` for computing the correlation matrix;
- `GP_fit` for estimating the parameters of the GP model.

**Examples**

```r
## 1D Example 1
n = 5
d = 1
computer_simulator <- function(x) {
  x = 2 * x + 0.5
  y = sin(10 * pi * x)/(2 * x) + (x - 1)^4
  return(y)
}
set.seed(3)
library(lhs)
x = maximinLHS(n,d)
y = computer_simulator(x)
beta = rnorm(1)
GP_deviance(beta,x,y)
```

```r
## 1D Example 2
n = 7
d = 1
computer_simulator <- function(x) {
  y <- log(x + 0.1) + sin(5 * pi * x)
  return(y)
}
```
set.seed(1)
library(lhs)
x = maximinLHS(n, d)
y = computer_simulator(x)
beta = rnorm(1)
GP_deviance(beta, x, y,
corr = list(type = "matern", nu = 5/2))

## 2D Example: GoldPrice Function
computer_simulator <- function(x) {
  x1 = 4 * x[, 1] - 2
  x2 = 4 * x[, 2] - 2
  t1 = 1 + (x1 + x2 + 1)^2 *
       (19 - 14 * x1 + 3 * x1^2 - 14 * x2 + 6 * x1 * x2 + 3 * x2^2)
  t2 = 30 + (2 * x1 - 3 * x2)^2 *
       (18 - 32 * x1 + 12 * x1^2 + 48 * x2 - 36 * x1 * x2 + 27 * x2^2)
  y = t1 * t2
  return(y)
}

n = 10
d = 2
set.seed(1)
library(lhs)
x = maximinLHS(n, d)
y = computer_simulator(x)
beta = rnorm(2)
GP_deviance(beta, x, y)

GP_fit

Gaussian Process Model fitting

Description

For an \((n \times d)\) design matrix, \(X\), and the corresponding \((n \times 1)\) simulator output \(Y\), this function fits the GP model and returns the parameter estimates. The optimization routine assumes that the inputs are scaled to the unit hypercube \([0, 1]^d\).

Usage

\(\text{GP\_fit}(X, Y, \text{control} = c(200 * d, 80 * d, 2 * d), \text{nug\_thres} = 20,\)
\(\quad \text{trace} = \text{FALSE}, \text{maxit} = 100, \text{corr} = \text{list(type = "exponential", power = 1.95), optim\_start = NULL})\)
Arguments

- **X**
  - the \((n \times d)\) design matrix

- **Y**
  - the \((n \times 1)\) vector of simulator outputs.

- **control**
  - a vector of parameters used in the search for optimal beta (search grid size, percent, number of clusters). See ‘Details’.

- **nug_thres**
  - a parameter used in computing the nugget. See ‘Details’.

- **trace**
  - logical, if TRUE, will provide information on the optim runs

- **maxit**
  - the maximum number of iterations within optim, defaults to 100

- **corr**
  - a list of parameters for the specifying the correlation to be used. See corr_matrix.

- **optim_start**
  - a matrix of potentially likely starting values for correlation hyperparameters for the optim runs, i.e., initial guess of the d-vector beta

Details

This function fits the following GP model, 
\[ y(x) = \mu + Z(x), \quad x \in [0, 1]^d, \]
where \( Z(x) \) is a GP with mean 0, \( \text{Var}(Z(x_i)) = \sigma^2 \), and \( \text{Cov}(Z(x_i), Z(x_j)) = \sigma^2 R_{ij} \). Entries in covariance matrix \( R \) are determined by \( \text{corr} \) and parameterized by \( \beta \), a \( d \)-vector of parameters. For computational stability \( R^{-1} \) is replaced with \( R^{-1}_{\delta lb} \), where \( R_{\delta lb} = R + \delta lb I \) and \( \delta lb \) is the nugget parameter described in Ranjan et al. (2011).

The parameter estimate \( \beta \) is obtained by minimizing the deviance using a multi-start gradient based search (L-BFGS-B) algorithm. The starting points are selected using the k-means clustering algorithm on a large maximin LHD for values of \( \beta \), after discarding \( \beta \) vectors with high deviance. The control parameter determines the quality of the starting points of the L-BFGS-B algorithm.

control is a vector of three tunable parameters used in the deviance optimization algorithm. The default values correspond to choosing \( 2^d \times d \) clusters (using k-means clustering algorithm) based on \( 80d \times d \) best points (smallest deviance, refer to gp_deviance) from a \( 200^d \times d \)-point random maximin LHD in \( \beta \). One can change these values to balance the trade-off between computational cost and robustness of likelihood optimization (or prediction accuracy). For details see MacDonald et al. (2015).

The nug_thres parameter is outlined in Ranjan et al. (2011) and is used in finding the lower bound on the nugget (\( \delta lb \)).

Value

an object of class GP containing parameter estimates beta and sig2, nugget parameter delta, the data (X and Y), and a specification of the correlation structure used.

Author(s)

Blake MacDonald, Hugh Chipman, Pritam Ranjan
References

http://www.jstatsoft.org/v64/i12/


See Also

plot for plotting in 1 and 2 dimensions;
predict for predicting the response and error surfaces;
optim for information on the L-BFGS-B procedure;
GP_deviance for computing the deviance.

Examples

```r
## 1D Example 1
n = 5
d = 1
computer_simulator <- function(x){
  x = 2 * x + 0.5
  y = sin(10 * pi * x) / (2 * x) + (x - 1)^4
  return(y)
}
set.seed(3)
library(lhs)
x = maximinlhs(n, d)
y = computer_simulator(x)
GPmodel = GP_fit(x, y)
print(GPmodel)

## 1D Example 2
n = 7
d = 1
computer_simulator <- function(x) {
  y <- log(x + 0.1) + sin(5 * pi * x)
  return(y)
}
set.seed(1)
library(lhs)
x = maximinlhs(n, d)
y = computer_simulator(x)
GPmodel = GP_fit(x, y)
print(GPmodel, digits = 4)

## 2D Example: GoldPrice Function
computer_simulator <- function(x) {
```

```
\begin{verbatim}
x1 = 4 * x[, 1] - 2
x2 = 4 * x[, 2] - 2
t1 = 1 + (x1 + x2 + 1)*2 * (19 - 14 * x1 + 3 * x1^2 - 14 * x2 + 6 * x1 * x2 + 3 * x2^2)
t2 = 30 + (2 * x1 - 3 * x2)*2 * (18 - 32 * x1 + 12 * x1^2 + 48 * x2 - 36 * x1 * x2 + 27 * x2^2)
y = t1 * t2
return(y)

n = 30
d = 2
set.seed(1)
library(lhs)
x = maximinLHS(n, d)
y = computer_simulator(x)
GPmodel = GP_fit(x, y)
print(GPmodel)
\end{verbatim}

---

**plot**  
Plotting GP model fits

**Description**

Plots the predicted response and mean squared error (MSE) surfaces for simulators with 1 and 2 dimensional inputs (i.e. \( d = 1,2 \)).

**Usage**

```r
## S3 method for class 'GP'
plot(x, M = 1, range = c(0, 1), resolution = 50,
     colors = c("black", "blue", "red"), line_type = c(1, 2), pch = 20,
     cex = 1, legends = FALSE, surf_check = FALSE, response = TRUE,
     ...)```

**Arguments**

- **x**: a class GP object estimated by GP_fit
- **M**: the number of iterations for use in prediction. See predict.GP
- **range**: the input range for plotting (default set to \([0, 1]\))
- **resolution**: the number of points along a coordinate in the specified range
- **colors**: a vector of length 3 assigning colors[1] to training design points, colors[2] to model predictions, and colors[3] to the error bounds
- **line_type**: a vector of length 2 assigning line_type[1] to model predictions, and line_type[2] to the error bounds
- **pch**: a parameter defining the plotting character for the training design points, see ‘pch’ for possible options in par
**Methods (by class)**

- **GP**: The plot method creates a **graphics** plot for 1-D fits and **lattice** plot for 2-D fits.

**Author(s)**

Blake MacDonald, Hugh Chipman, Pritam Ranjan

**References**


**See Also**

- `GP_fit` for estimating the parameters of the GP model;
- `predict.GP` for predicting the response and error surfaces;
- `par` for additional plotting characters and line types for 1 dimensional plots;
- `wireframe` and `levelplot` for additional plotting settings in 2 dimensions.

**Examples**

```r
## 1D Example 1
n <- 5
d <- 1
computer_simulator <- function(x){
  x <- 2 * x + 0.5
  y <- sin(10 * pi * x) / (2 * x) + (x - 1)^4
  return(y)
}
set.seed(3)
library(lhs)
x <- maximinLHS(n,d)
y <- computer_simulator(x)
GPmodel <- GP_fit(x,y)
plot(GPmodel)

## 1D Example 2
n <- 7
d <- 1
```
predict

\textit{Model Predictions from GPfit}

\textbf{Description}

Computes the regularized predicted response $\hat{y}_{\delta,M}(x)$ and the mean squared error $s^2_{\delta,M}(x)$ for a new set of inputs using the fitted GP model.

The value of $M$ determines the number of iterations (or terms) in approximating $R^{-1} \approx R^{-1}_{\delta,M}$. The iterative use of the nugget $\delta_0$, as outlined in Ranjan et al. (2011), is used in calculating $\hat{y}_{\delta_0,M}(x)$ and $s^2_{\delta_0,M}(x)$, where $R^{-1}_{\delta,M} = \sum_{t=1}^M \delta_0^{-t}(R + \delta I)^{-t}$. 

```r
computer_simulator <- function(x) {
  y <- log(x + 0.1) + sin(5 * pi * x)
  return(y)
}
set.seed(1)
library(lhs)
x <- maximinLHS(n, d)
y <- computer_simulator(x)
GPmodel <- GP_fit(x, y)

## Plotting with changes from the default line type and characters
plot(GPmodel, resolution = 100, line_type = c(6,2), pch = 5)

## 2D Example: GoldPrice Function
computer_simulator <- function(x) {
  x1 <- 4 * x[1] - 2
  x2 <- 4 * x[2] - 2
  t1 <- 1 + (x1 + x2 + 1)^2 * (19 - 14 * x1 + 3 * x1^2 - 14 * x2 +
    6 * x1 * x2 + 3 * x2^2)
  t2 <- 30 + (2 * x1 - 3 * x2)^2 * (18 - 32 * x1 + 12 * x1^2 + 48 * x2 -
    36 * x1 * x2 + 27 * x2^2)
  y <- t1 * t2
  return(y)
}
n <- 30
d <- 2
set.seed(1)
x <- lhs::maximinLHS(n, d)
y <- computer_simulator(x)
GPmodel <- GP_fit(x, y)

## Basic level plot
plot(GPmodel)

## Adding Contours and increasing the number of levels
plot(GPmodel, contour = TRUE, cuts = 50, pretty = TRUE)

## Plotting the Response Surface
plot(GPmodel, surf_check = TRUE)

## Plotting the Error Surface with color
plot(GPmodel, surf_check = TRUE, response = FALSE, shade = TRUE)
```
### Usage

```r
## S3 method for class 'GP'
predict(object, xnew = object$X, M = 1, ...)

## S3 method for class 'GP'
fitted(object, ...)
```

### Arguments

- **object**: a class GP object estimated by GP_fit
- **xnew**: the \((n_{new} \times d)\) design matrix of test points where model predictions and MSEs are desired
- **M**: the number of iterations. See 'Details'
- **...**: for compatibility with generic method predict

### Value

Returns a list containing the predicted values (\(\hat{y}\)), the mean squared errors of the predictions (MSE), and a matrix (complete_data) containing \(x_{new}\), \(\hat{y}\), and MSE.

### Methods (by class)

- **GP**: The predict method returns a list of elements \(\hat{y}\) (fitted values), \(y\) (dependent variable), MSE (residuals), and completed_data (the matrix of independent variables, \(\hat{y}\), and MSE).
- **GP**: The fitted method extracts the complete data.

### Author(s)

Blake MacDonald, Hugh Chipman, Pritam Ranjan

### References


### See Also

- GP_fit for estimating the parameters of the GP model;
- plot for plotting the predicted and error surfaces.

### Examples

```r
## 1D Example
n <- 5
d <- 1
computer_simulator <- function(x){
  x <- 2*x+0.5
  ...}
```
\[ \frac{\sin(10\pi x)}{(2x) + (x-1)^4} \]

```r
set.seed(3)
library(lhs)
x <- maximinLHS(n, d)
y <- computer_simulator(x)
xvec <- seq(from = 0, to = 1, length.out = 10)
GPmodel <- GP_fit(x, y)
head(fitted(GPmodel))
lapply(predict(GPmodel, xvec), head)
```

```r
## 1D Example 2
n <- 7
d <- 1
computer_simulator <- function(x) {
  log(x+0.1)+sin(5*pi*x)
}
set.seed(1)
library(lhs)
x <- maximinLHS(n, d)
y <- computer_simulator(x)
xvec <- seq(from = 0, to = 1, length.out = 10)
GPmodel <- GP_fit(x, y)
head(fitted(GPmodel))
predict(GPmodel, xvec)
```

```r
## 2D Example: GoldPrice Function
computer_simulator <- function(x) {
  x1 <- 4*x[,1] - 2
  x2 <- 4*x[,2] - 2
  t1 <- 1 + (x1 + x2 + 1)^2*(19 - 14*x1 + 3*x1^2 - 14*x2 + 6*x1*x2 + 3*x2^2)
  t2 <- 30 + (2*x1 -3*x2)^2*(18 - 32*x1 + 12*x1^2 + 48*x2 - 36*x1*x2 + 27*x2^2)
  y <- t1*t2
  return(y)
}
n <- 10
d <- 2
set.seed(1)
library(lhs)
x <- maximinLHS(n, d)
y <- computer_simulator(x)
GPmodel <- GP_fit(x, y)
# fitted values
head(fitted(GPmodel))
# new data
xvector <- seq(from = 0, to = 1, length.out = 10)
xdf <- expand.grid(x = xvector, y = xvector)
predict(GPmodel, xdf)
```
print.GP

GP model fit Summary

Description
Prints the summary of a class GP object estimated by GP_fit

Usage
## S3 method for class 'GP'
print(x, ...)

Arguments
x a class GP object estimated by GP_fit
... for compatibility with generic method print

Details
Prints the summary of the class GP object. It returns the number of observations, input dimension, parameter estimates of the GP model, lower bound on the nugget, and the nugget threshold parameter (described in GP_fit).

Author(s)
Blake MacDonald, Hugh Chipman, Pritam Ranjan

See Also
GP_fit for more information on estimating the model;
print for more description on the print function.

Examples

## 1D example
n <- 5
d <- 1
computer_simulator <- function(x){
  x <- 2 * x + 0.5
  y <- sin(10 * pi * x) / (2 * x) + (x - 1)^4
  return(y)
}
set.seed(3)
x <- lhs::maximinLHS(n, d)
y <- computer_simulator(x)
GPmodel <- GP_fit(x, y)
print(GPmodel)
### 2D Example: GoldPrice Function

```r
computer_simulator <- function(x) {
  x1 <- 4*x[,1] - 2
  x2 <- 4*x[,2] - 2
  t1 <- 1 + (x1 + x2 + 1)^2*(19 - 14*x1 + 3*x1^2 - 14*x2 + 6*x1*x2 + 3*x2^2)
  t2 <- 30 + (2*x1 - 3*x2)^2*(18 - 32*x1 + 12*x1^2 + 48*x2 - 36*x1*x2 + 27*x2^2)
  y <- t1*t2
  return(y)
}

n <- 30
d <- 2
set.seed(1)
x <- lhs::maximinLHS(n, d)
y <- computer_simulator(x)
GPmodel <- GP_fit(x, y)
print(GPmodel, digits = 3)
```

---

**scale_norm**

*Scale variable into normal range 0, 1*

**Description**

Perform calculation: \((x - \text{min}(x)) / (\text{max}(x) - \text{min}(x))\)

**Usage**

```r
scale_norm(x, range = NULL)
```

**Arguments**

- `x` numeric vector
- `range` numeric vector additional values for shrinking distribution of values within the 0-1 space, without affecting limits of `x`

**Value**

numeric vector

**Examples**

```r
scale_norm(x = c(-1, 4, 10, 182))
# lower bound extended beyond -1
# upper bound still range of data
scale_norm(x = c(-1, 4, 10, 182), range = c(-100, 100))
```
### sig_invb

**Internal tools**

**Description**

shared utilities between GP_deviance and GP_fit

**Usage**

```r
delta, L, mu_hat, Sig_invb
```

**Arguments**

- `x`: the \((n \times d)\) design matrix
- `y`: the \((n \times 1)\) vector of simulator outputs
- `beta`: a \((d \times 1)\) vector of correlation hyper-parameters, as described in `corr_matrix`
- `corr`: a list of parameters for the specifying the correlation to be used. See `corr_matrix`.
- `nug_thres`: a parameter used in computing the nugget. See `GP_fit`.

**Value**

list with elements delta, L, mu_hat, Sig_invb

**Examples**

```r
gpfit:::sig_invb(x = matrix(1:10, 10, 10),
                y = runif(11),
                beta = 1.23)
```

---

### summary.GP

**Summary of GP model fit**

**Description**

Prints the summary of a class GP object estimated by GP_fit

**Usage**

```r
## S3 method for class 'GP'
summary(object, ...)
```
summary.GP

Arguments

object a class GP object estimated by GP_fit

Details

prints the summary of the GP object (object), by calling print.GP

Author(s)

Blake MacDonald, Hugh Chipman, Pritam Ranjan

See Also

print.GP for more description of the output;
GP_fit for more information on estimating the model;
summary for more description on the summary function.

Examples

## 1D example
n <- 5
d <- 1
computer_simulator <- function(x){
x <- 2 * x + 0.5
y <- sin(10 * pi * x) / (2 * x) + (x - 1)^4
return(y)
}
set.seed(3)
x <- lhs::maximinLHS(n, d)
y <- computer_simulator(x)
gpmodel <- GP_fit(x, y)
summary(gpmodel)

## 2D Example: GoldPrice Function
computer_simulator <- function(x) {
x1 = 4*x[, 1] - 2
x2 = 4*x[, 2] - 2
t1 = 1 + (x1 + x2 + 1)^2*(19 - 14*x1 + 3*x1^2 - 14*x2 + 6*x1*x2 + 3*x2^2)
t2 = 30 + (2*x1 - 3*x2)^2*(18 - 32*x1 + 12*x1^2 + 48*x2 - 36*x1*x2 + 27*x2^2)
y = t1 * t2
return(y)
}
n <- 10
d <- 2
set.seed(1)
x <- lhs::maximinLHS(n, d)
y <- computer_simulator(x)
GPmodel <- GP_fit(x, y)
summary(GPmodel)
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