

# Package ‘GPfit’

April 2, 2015

**Title** Gaussian Processes Modeling

**Version** 1.0-0

**Date** 2015-04-01

**Author** Blake MacDoanld, Hugh Chipman, Pritam Ranjan

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

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

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

**License** GPL-2

**NeedsCompilation** no

**Repository** CRAN

**Date/Publication** 2015-04-02 17:44:08

## R topics documented:

GPfit-package . . . . .	2
corr_matrix . . . . .	2
GP_deviance . . . . .	4
GP_fit . . . . .	6
plot.GP . . . . .	9
predict.GP . . . . .	11
print.GP . . . . .	13
summary.GP . . . . .	14
<b>Index</b>	<b>17</b>

---

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  $2 \times \log$ -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

MacDonald, K.B., Ranjan, P. and Chipman, H. (2015). GPfit: An R Package for Fitting a Gaussian Process Model to Deterministic Simulator Outputs. *Journal of Statistical Software*, 64(12), 1-23. <http://www.jstatsoft.org/v64/i12/>

Ranjan, P., Haynes, R., and Karsten, R. (2011). A Computationally Stable Approach to Gaussian Process Interpolation of Deterministic Computer Simulation Data, *Technometrics*, 53(4), 366 - 378.

Santner, T.J., Williams, B., and Notz, W. (2003), *The design and analysis of computer experiments*, Springer Verlag, New York.

---

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.

**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  $(-\infty, \infty)$

**corr** a list that specifies the type of correlation function along with the smoothness 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  $k \in \{0, 1, 2, \dots\}$

**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

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

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**

MacDonald, K.B., Ranjan, P. and Chipman, H. (2015). GPfit: An R Package for Fitting a Gaussian Process Model to Deterministic Simulator Outputs. *Journal of Statistical Software*, 64(12), 1-23. <http://www.jstatsoft.org/v64/i12/>

Ranjan, P., Haynes, R., and Karsten, R. (2011). A Computationally Stable Approach to Gaussian Process Interpolation of Deterministic Computer Simulation Data, *Technometrics*, 53(4), 366 - 378.

Santner, T.J., Williams, B., and Notz, W. (2003), The design and analysis of computer experiments, Springer Verlag, New York.

### Examples

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

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

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

```
## 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  $2 \cdot \log$ -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

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

**Arguments**

beta	a (d x 1) vector of correlation hyper-parameters, as described in <a href="#">corr_matrix</a>
X	the (n x d) design matrix
Y	the (n x 1) vector of simulator outputs
nug_thres	a parameter used in computing the nugget. See <a href="#">GP_fit</a> .
corr	a list of parameters for the specifying the correlation to be used. See <a href="#">corr_matrix</a> .

**Value**

the deviance (negative  $2 \times \log$ -likelihood)

**Author(s)**

Blake MacDonald, Hugh Chipman, Pritam Ranjan

**References**

Ranjan, P., Haynes, R., and Karsten, R. (2011). A Computationally Stable Approach to Gaussian Process Interpolation of Deterministic Computer Simulation Data, *Technometrics*, 53(4), 366 - 378.

**See Also**

[corr\\_matrix](#) for computing the correlation matrix;  
[GP\\_fit](#) for estimating the parameters of the GP model.

**Examples**

```
## 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);

## 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

```

GP_fit(X, Y, control = c(200*d, 80*d, 2*d), nug_thres = 20,
trace = FALSE,maxit = 100,corr = list(type="exponential",power=1.95),
optim_start = NULL)

```

## Arguments

<code>X</code>	the $(n \times d)$ design matrix
<code>Y</code>	the $(n \times 1)$ vector of simulator outputs.
<code>control</code>	a vector of parameters used in the search for optimal beta. See ‘Details’.
<code>nug_thres</code>	a parameter used in computing the nugget. See ‘Details’.
<code>trace</code>	logical, if TRUE, will provide information on the <code>optim</code> runs
<code>maxit</code>	the maximum number of iterations within <code>optim</code> , defaults to 100

corr	a list of parameters for the specifying the correlation to be used. See <a href="#">corr_matrix</a> .
optim_start	a matrix of potentially likely starting values for correlation hyperparameters for the <a href="#">optim</a> runs, i.e., initial guess of the d-vector beta

### Details

This function fits the following GP model,  $y(x) = \mu + Z(x)$ ,  $x \in [0, 1]^d$ , where  $Z(x)$  is a GP with mean 0,  $Var(Z(x_i)) = \sigma^2$ , and  $Cov(Z(x_i), Z(x_j)) = \sigma^2 R_{ij}$ . Entries in covariance matrix R are determined by corr and parameterized by beta, a d-vector of parameters. For computational stability  $R^{-1}$  is replaced with  $R_{\delta_{lb}}^{-1}$ , 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 clusters (using k-means clustering algorithm) based on 80\*d best points (smallest deviance, refer to [GP\\_deviance](#)) from a 200\*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

MacDonald, K.B., Ranjan, P. and Chipman, H. (2015). GPfit: An R Package for Fitting a Gaussian Process Model to Deterministic Simulator Outputs. Journal of Statistical Software, 64(12), 1-23. <http://www.jstatsoft.org/v64/i12/>

Ranjan, P., Haynes, R., and Karsten, R. (2011). A Computationally Stable Approach to Gaussian Process Interpolation of Deterministic Computer Simulation Data, Technometrics, 53(4), 366 - 378.

### See Also

[plot.GP](#) for plotting in 1 and 2 dimensions;  
[predict.GP](#) for predicting the response and error surfaces;

`optim` for information on the L-BFGS-B procedure;  
`GP_deviance` for computing the deviance.

### Examples

```
## 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) {
  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)
```



---

plot.GP	<i>Plotting GP model fits</i>
---------	-------------------------------

---

**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**

```
## 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**

<code>x</code>	a class GP object estimated by <code>GP_fit</code>
<code>M</code>	the number of iterations for use in prediction. See <a href="#">predict.GP</a>
<code>range</code>	the input range for plotting (default set to <code>[0, 1]</code> )
<code>resolution</code>	the number of points along a coordinate in the specified range

**For 1 Dimensional Plotting**

<code>colors</code>	a vector of length 3 assigning <code>colors[1]</code> to training design points, <code>colors[2]</code> to model predictions, and <code>colors[3]</code> to the error bounds
<code>line_type</code>	a vector of length 2 assigning <code>line_type[1]</code> to model predictions, and <code>line_type[2]</code> to the error bounds
<code>pch</code>	a parameter defining the plotting character for the training design points, see ‘pch’ for possible options in <a href="#">par</a>
<code>cex</code>	a parameter defining the size of the pch used for plotting the training design points, see ‘cex’ for possible options in <a href="#">par</a>
<code>legends</code>	a parameter that controls the inclusion of a <a href="#">legend</a> ; by default it is ‘FALSE’

**For 2 Dimensional Plotting**

<code>surf_check</code>	logical, switch between 3d surface and 2d level/contour plotting, the default of FALSE implies level/contour plotting
<code>response</code>	logical, switch between predicted response and error (MSE) plots, the default of TRUE displays the response surface
<code>...</code>	additional arguments from <a href="#">wireframe</a> or <a href="#">levelplot</a>

**Author(s)**

Blake MacDonald, Hugh Chipman, Pritam Ranjan

## References

Ranjan, P., Haynes, R., and Karsten, R. (2011). A Computationally Stable Approach to Gaussian Process Interpolation of Deterministic Computer Simulation Data, *Technometrics*, 53(4), 366 - 378.

## 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

```
## 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.GP(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);
## Plotting with changes from the default line type and characters
plot.GP(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);
library(lhs);
library(lattice);
x = maximinLHS(n,d);
y = computer_simulator(x);
GPmodel = GP_fit(x,y);
## Basic level plot
plot.GP(GPmodel)
## Adding Contours and increasing the number of levels
plot.GP(GPmodel, contour = TRUE, cuts = 50, pretty = TRUE)
## Plotting the Response Surface
plot.GP(GPmodel, surf_check = TRUE)
## Plotting the Error Surface with color
plot.GP(GPmodel, surf_check = TRUE, response = FALSE, shade = TRUE)

```

---

predict.GP

*Model Predictions from GPfit*


---

### Description

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

### Usage

```

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

```

### Arguments

object	a class GP object estimated by GP_fit
xnew	the (n_new x 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 <a href="#">predict</a>

### Details

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

### Value

Returns a list containing the predicted values (Y\_hat), the mean squared errors of the predictions (MSE), and a matrix (complete\_data) containing xnew, Y\_hat, and MSE

**Author(s)**

Blake MacDonald, Hugh Chipman, Pritam Ranjan

**References**

Ranjan, P., Haynes, R., and Karsten, R. (2011). A Computationally Stable Approach to Gaussian Process Interpolation of Deterministic Computer Simulation Data, *Technometrics*, 53(4), 366 - 378.

**See Also**

[GP\\_fit](#) for estimating the parameters of the GP model;  
[plot.GP](#) for plotting the predicted and error surfaces.

**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);
library(lhs);
x = maximinLHS(n,d);
y = computer_simulator(x);
xvec <- seq(from=0,to=1,length.out=10);
GPmodel = GP_fit(x,y);
GPprediction = predict.GP(GPmodel,xvec);
yhat = GPprediction$Y_hat;
mse = GPprediction$MSE;
completedata = GPprediction$complete_data;
completedata;
```

```
## 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)
xvec <- seq(from=0,to=1,length.out=10);
GPmodel = GP_fit(x,y)
GPprediction = predict.GP(GPmodel,xvec);
yhat = GPprediction$Y_hat;
mse = GPprediction$MSE;
completedata = GPprediction$complete_data;
```

```

## 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);

xvector = seq(from=0,to=1,length.out=10);
xvec = expand.grid(x = xvector, y=xvector);
xvec = as.matrix(xvec);
GPprediction = predict.GP(GPmodel,xvec);
yhat = GPprediction$Y_hat;
mse = GPprediction$MSE;
completedata = GPprediction$complete_data;

```

---

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);
library(lhs);
x = maximinLHS(n,d);
y = computer_simulator(x);
GPmodel = GP_fit(x,y);
print(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);
library(lhs);
x = maximinLHS(n,d);
y = computer_simulator(x);
GPmodel = GP_fit(x,y);
print(GPmodel,digits = 3)
```

---

summary.GP

*Summary of GP model fit*

---

**Description**

Prints the summary of a class GP object estimated by GP\_fit

**Usage**

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

**Arguments**

```
object      a class GP object estimated by GP_fit
...         for compatibility with generic method summary
```

**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);
library(lhs);
x = 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);  
library(lhs);  
x = maximinLHS(n,d);  
y = computer_simulator(x);  
GPmodel = GP_fit(x,y);  
summary(GPmodel)
```



# Index

- \*Topic **Deviance**
  - GP\_deviance, 4
- \*Topic **Gaussian Correlation**
  - corr\_matrix, 2
- \*Topic **Gaussian Process Model Prediction**
  - predict.GP, 11
- \*Topic **Gaussian Process**
  - GP\_fit, 6
- \*Topic **Matern Correlation**
  - corr\_matrix, 2
- \*Topic **Power Exponential Correlation**
  - corr\_matrix, 2

corr\_matrix, 2, 4, 5, 7

GP\_deviance, 4, 7, 8

GP\_fit, 2, 5, 6, 10, 12–15

GPfit (GPfit-package), 2

GPfit-package, 2

legend, 9

levelplot, 9, 10

optim, 6–8

par, 9, 10

plot.GP, 7, 9, 12

predict, 11

predict.GP, 7, 9, 10, 11

print, 13, 14

print.GP, 13, 15

summary, 15

summary.GP, 14

wireframe, 9, 10