mlegp: an R package for Gaussian process modeling and sensitivity analysis

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1 *mlegp*: an overview

Gaussian processes (GPs) are commonly used as surrogate statistical models for predicting output of computer experiments (Santner *et al.*, 2003). Generlly, GPs are both interpolators and smoothers of data and are effective predictors when the response surface of interest is a smooth function of the parameter space. The package *mlegp* finds *m*aximum *l*ikelihood *e*stimates of *G*aussian *p*rocesses for univariate and multi-dimensional responses, for Gaussian processes with product exponential correlation structures; constant or linear regression mean functions; no nugget term, constant nugget terms, or a nugget matrix that can be specified up to a multiplicative constant. The latter is an extension of previous Gaussian process models and provides some flexibility for using GPs to model heteroscedastic responses. Diagnostic plotting functions, and the sensitivity analysis tools of Functional Analysis of Variance (FANOVA) decomposition, and plotting of main and two-way factor interaction effects are implemented. Multi-dimensional output can be modelled by fitting independent GPs to each dimension of output, or to the most important principle component weights following singular value decomposition of the output. Plotting of main effects for functional output is also implemented. From within R, a complete list of functions and vignettes can be obtained by calling 'library(help = "mlegp")'.

2 Gaussian process modeling and diagnostics

2.1 Gaussian processes

Let $z_{\text{known}} = \left[z(\theta^{(1)}), \ldots, z(\theta^{(m)}) \right]$ be a vector of *observed* responses, where $z(\theta^{(i)})$ is the response observed at the design point $\theta^{(i)}$, the parameter vector $\theta^{(i)} = \left[\theta_1^{(i)}, \ldots, \theta_p^{(i)} \right]$, and we are interested in predicting output $z(\theta^{(\text{new})})$ at the untried parameter setting $\theta^{(\text{new})}$. The correlation between any two responses (observed or unobserved) is assumed to have the (prodcut exponential) form

$$C(\beta)_{i,j} \equiv \text{cor}\left(z(\theta^{(i)}), z(\theta^{(j)}) \right) = \exp\left\{ \sum_{k=1}^{p} \left(-\beta_k \left(\theta_k^{(i)} - \theta_k^{(j)} \right)^2 \right) \right\}. \tag{1}$$

The correlation matrix $C(\beta) = [C(\beta)]_{i,j}$, and depends on the correlation parameters $\beta = [\beta_1, \ldots, \beta_p]$

Let $\mu(\cdot)$ be the mean function for the unconditional mean of any observation, and the mean matrix of z_{known} be

$$M \equiv \left[\mu\left(\theta^{(1)} \right), \ldots, \mu\left(\theta^{(m)} \right) \right]. \tag{2}$$

The vector of observed responses, z_{known}, is distributed according to

$$z_{\text{known}} \sim MVN_m(M, \sigma_{GP}^2 C(\beta) + \sigma_e^2 I), \tag{3}$$

where I is a k x k identity matrix, σ^2_{GP} is the unconditional variance of an expected response and σ^2_e, the nugget term, is variance due to the stochasticity of the response (e.g., random noise). For convenience, denote the variance-covariance matrix of z_{known} as

$$V \equiv \sigma^2_{GP}C(\beta) + \sigma^2_e I \tag{4}$$

Also define $r_i = \text{cor}(z(\theta^{(new)}), z(\theta^{(i)}))$, following equation (1), and $r = [r_1, \ldots, r_m]'$. Under the GP assumption, the predictive distribution of $z(\theta^{(new)})$ is normal with mean

$$E[z(\theta^{(new)})|z_{\text{known}}] = \mu(\theta^{(new)}) + \sigma^2_{GP}r'V^{-1}(z_{\text{known}} - M) \tag{5}$$

and variance

$$Var[z(\theta^{(new)})|z_{\text{known}}] = \sigma^2_{\text{GP}} + \sigma^2_e - \sigma^4_{GP}r'V^{-1}r.$$

For more details, see Santner *et al.* (2003).

2.2 Maximum likelihood estimation

We first need some additional notation. Mean functions that are constant or linear in design parameters have the form $\mu(\theta) = x(\theta)F$, where $x(\theta)$ is a row vector of regression parameters, and F is a column vector of regression coefficients. Note that for a constant mean function, $x(\cdot) \equiv 1$ and F is a single value corresponding to the constant mean. The mean matrix M defined in equation (2) has the form $M = XF$, where the ith row of X is equal to $x(\theta^{(i)})$.

Let us also rewrite the variance-covariance matrix V from equation (4) to be

$$V \equiv \sigma^2_{\text{GP}}(C(\beta) + \sigma^2_{e*}I) \equiv \sigma^2_{\text{GP}}W(\beta, \sigma^2_{e*}), \tag{6}$$

where $\sigma^2_{e*} = \sigma^2_e/\sigma^2_{\text{GP}}$, and the matrix W depends on the correlation parameters $\beta = [\beta_1, \ldots, \beta_p]$ and the scaled nugget term σ^2_{e*}.

When the matrix W is fully specified, maximum likelihood estimates of the mean regression parameters and σ^2_{GP} exist in closed form and are

$$\hat{F} = (X^TW^{-1}X)^{-1}X^TW^{-1}z_{\text{known}} \tag{7}$$

and

$$\hat{\sigma}^2_{\text{GP}} = \frac{1}{m}(z_{\text{known}} - \hat{M})^TW^{-1}(z_{\text{known}} - \hat{M}), \tag{8}$$

where $\hat{M} = X\hat{F}$.

The package *mlegp* uses numerical methods in conjunction with equations (7) and (8) to find maximum likelihood estimates of all GP parameters.

2.3 Diagnostics

The cross-validated prediction $z_{-i}(\theta^{(i)})$ is the predicted response obtained using equation (5) after removing all responses at design point $\theta^{(i)}$ from z_{known}. Note that it is possible for multiple $\theta^{(i)}$'s, for various i's, to be identical, in which case all corresponding observations are removed. The cross-validated residual for this observations is

$$\frac{z(\theta^{(i)}) - z_{-i}(\theta^{(i)})}{\text{se}(z_{-i}(\theta^{(i)})}, \tag{9}$$

where $\text{se}(z_{-i}(\theta^{(i)}))$ is the standard error of $z_{-i}(\theta^{(i)})$

2.4 What does *mlegp* do?

The package *mlegp* extends the Gaussian process model of (3) by allowing the user to replace the identity matrix I in equations (3) and (4) with a diagonal matrix N, thereby specifying the *nugget matrix* up to a multiplicative constant. This extension provides some flexibility for modeling heteroscedastic responses. The user also has the option of fitting a GP with a constant mean (i.e., $\mu(\theta) \equiv \mu_0$) or mean functions that are linear regression functions in all elements of θ (plus an intercept term). For multi-dimensional output, the user has the option of fitting independent GPs to each dimension (i.e., each type of observation), or to the most important principle component weights following singular value decomposition. The latter is ideal for data rich situations, such as functional output, and is explained further in Section (5). GP accuracy is analyzed through diagnostic plots of cross-validated predictions and cross-validated residuals, which were described in Section (2.3). Sensitivity analysis tools including FANOVA decomposition, and plotting of main and two-way factor interactions are described in Section (4).

3 Examples: Gaussian process fitting and diagnostics

3.1 A simple example

The function *mlegp* is used to fit Gaussian processes (GPs) to a vector or matrix of responses observed under the same set of design parameters. Data can be input from within R or read from a text file using the command *read.table* (type '?read.table' from within R for more information). The example below shows how to fit multiple Gaussian processes to multiple outputs $z1$ and $z2$ for the design matrix x. Diagnostic plots are obtained using the *plot* function, which graphs observed values vs. cross-validated predicted values for each GP. The plot obtained from the code below appears in Figure (1).

```
> x = -5:5
> z1 = 10 - 5 * x + rnorm(length(x))
> z2 = 7 * sin(x) + rnorm(length(x))
> fitMulti = mlegp(x, cbind(z1, z2))
> plot(fitMulti)
```

After the GPs are fit, simply typing the name of the object (e.g., $fitMulti$) will return basic summary information.

```
> fitMulti

num GPs: 2
Total observations (per GP): 11
Dimensions: 1
```

We can also access individual Gaussian processes by specifying the index. The code below, for examples, displays summary information for the first Gaussian process, including diagnostic statistics of cross-validated root mean squared error (CV RMSE) and cross-validated root max squared error (CV RMaxSE), where squared error corresponds to the squared difference between cross-validated predictions and observed values.

```
> fitMulti[[1]]

Total observations = 11
Dimensions = 1

mu = 10.49854
sig2:          191.4983
nugget:          0
```
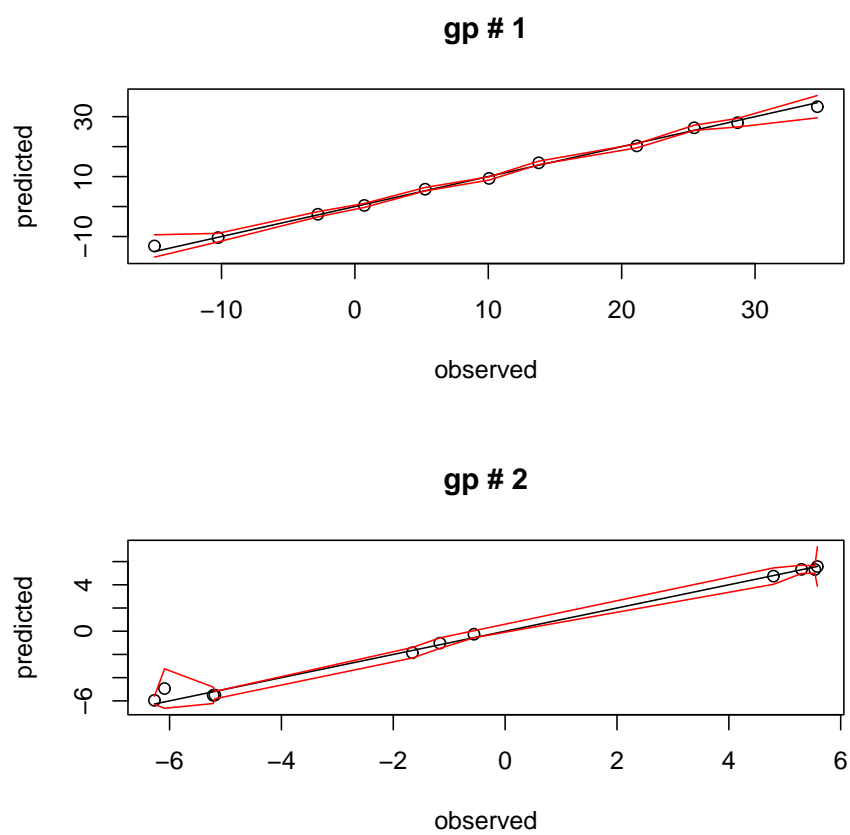
Figure 1: Gaussian process diagnostic plots. Open circles, cross-validated predictions; solid black lines, observed values; solid red lines, confidence bands corresponding to cross-validated predictions ± standard deviation.

```
Correlation parameters:

        beta a
1 0.2030227 2

Log likelihood = -33.34552

CV RMSE: 0.8953252
CV RMaxSE: 3.509689
```

3.2   Heteroscedastic responses and the nugget matrix

In cases where the responses are heteroscedastic (have non-constant variance), it is possible to
specify the diagonal nugget matrix up to a multiplicative constant. Future versions of *mlegp* will
allow more complicated forms of the nugget matrix; currently, we recommend specifying the nugget
matrix based on sample variances for replicate design points (which is easily obtained using the
function *varPerReps*), or the use of prior information. In the example below, we demonstrate how
to fit a Gaussian process with a constant nugget term and a Gaussian process where the diagonal
nugget matrix is specified up to a multiplicative constant. First we generate heteroscedastic data,
with variance related to the design parameter.

```
> x = seq(1, 10, by = 0.15)
> z = sin(x) + rnorm(length(x), sd = 0.2 * x)
```

By default, a nugget term is automatically estimated if there are replicates in the design matrix,
and is not estimated otherwise. However, one can estimate a nugget term by specifying an initial
scalar value for the 'nugget' argument during the call to *mlegp*. This is done in the code below.

```
> fit1 = mlegp(x, z, nugget = mean((0.2 * x)^2))
```

Alternatively, one can set 'nugget' equal to a vector corresponding to the diagonal nugget matrix
as described in Section (2.4). This allows the nugget matrix to be specified up to a multiplicative
constant, and is demonstrated in the code below.

```
> fit2 = mlegp(x, z, nugget = (0.2 * x)^2)
```

It is also possible to force a constant nugget term or the diagonal elements of the nugget matrix
to have a minimum value by setting the argument 'min.nugget'. This is especially important when
the responses are noiseless, and is useful insituations when the variance-covariance matrix of the
GP is not stable.

Finally, we demonstrate the advantage of using a diagonal nugget matrix by comparing the
correlations between the true response and predictions from each fitted GP, and providing diag-
nostic plots, whose output is displayed in Figure 2). Importantly, predictions are biased when a
constant nugget term is assumed.

```
> cor(sin(x), predict(fit1))

          [,1]
[1,] 0.8251486

> cor(sin(x), predict(fit2))

          [,1]
[1,] 0.937518
```

```
> par(mfrow = c(1, 2))
> plot(fit1, type = 1)
> lines(sin(x), sin(x), col = "blue")
> plot(fit2, type = 1)
> lines(sin(x), sin(x), col = "blue")
```
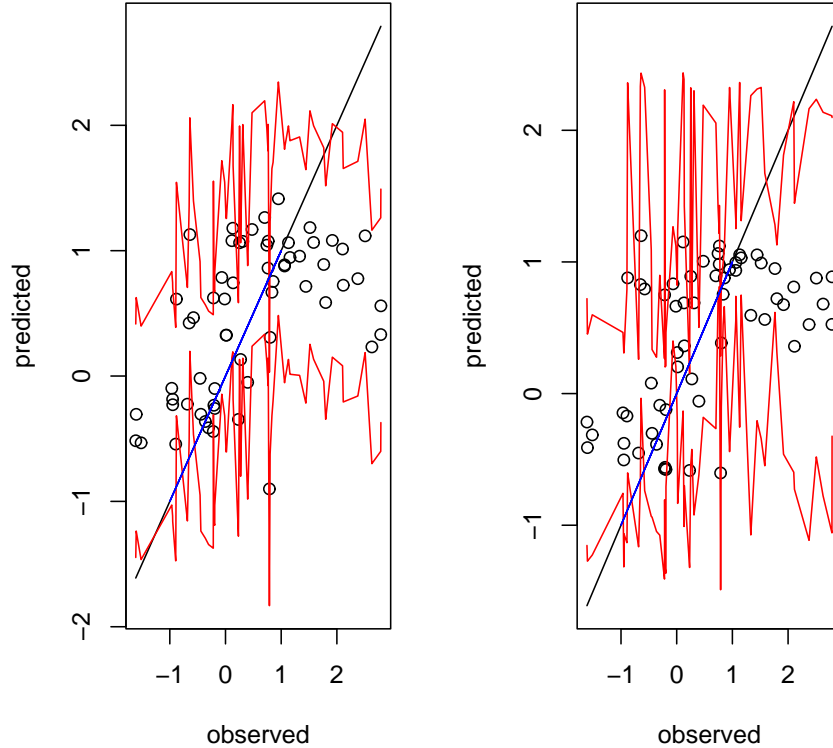

Figure 2: Diagnostic plots for Gaussian processes with constant nugget term (left) and diagonal nugget matrix (right). Open circles, cross-validated predictions; solid black lines, observed response; solid blue line, true (noiseless) response; solid red lines, confidence bands.

4 Sensitivity Analysis

4.1 Background

For a response $y = f(x)$, where x can be multidimensional, sensitivity analysis (SA) is used to (a) quantify the extent in which uncertainty in the response y can be attributed to uncertainty in the design parameters x, and (b) characterize how the response changes as one or more design parameters are varied. General SA methods can be found in Saltelli *et al.* (2000). We briefly describe SA using Gaussian process models, which is described in Schonlau and Welch (2006).

For independent marginal priors on the components of θ, the total variance of the GP predictor can be decomposed into variance contributions from main and higher order interaction effects, a technique known as Functional Analysis of Variance (FANOVA) decomposition. The percentage

of the total functional variance accounted for by a particular effect provides a measure of the importance of that effect.

The main effect of parameter θ_k, defined as $E[z(\theta)|z_{\text{known}}, \theta_k]$, predicts output for a fixed value of θ_k, averaged over the remaining parameters according to a prior (or weight function) $\pi(\theta_{-k})$ on all components of θ except for the kth. The two-way interaction effect for parameters θ_k and θ_l, defined as $E[z(\theta)|z_{\text{known}}, \theta_k, \theta_l]$, predicts output for jointly fixed values of θ_k and θ_l, averaged over the remaining parameters according to a prior $\pi(\theta_{-k,-l})$. Main effects plots and contour plots conveniently illustrate main effects and two-factor interactions.

In *mlegp*, we implement FANOVA decomposition and the plotting of main and two-way factor interactions using indepedent uniform priors on all components of θ. By default, the range of each component is taken to be the range of that component in the design matrix, but these ranges can be overwritten via the arguments 'lower' and 'upper'.

4.2 Examples

4.2.1 FANOVA decomposition

The function *FANOVADecomposition* is used to perform FANOVA decomposition on a single Gaussian processes, or on (a subset) of all Gaussian processes in a list. The function returns a table that reports the % contribution of each effect to the total functional variance of the Gaussian process predictor (or each Gaussian process predictor, in the case of a list). The code below demonstrates the use of the *FANOVADecomposition* function on a Gaussian process with two design parameters.

```
> x1 = kronecker(seq(0, 1, by = 0.25), rep(1, 5))
> x2 = rep(seq(0, 1, by = 0.25), 5)
> y = 4 * x1 - 2 * x2 + x1 * x2 + rnorm(length(x1), sd = 0.001)
> fit = mlegp(cbind(x1, x2), y, param.names = c("x1", "x2"))

> FANOVADecomposition(fit, verbose = F)

  param % contribution
1    x1       90.1388705
2    x2        9.4930923
3 x1:x2        0.3740572
```

4.2.2 Graphical plots for main and interaction effects

The function *plotMainEffects* is a generic function for plotting multiple main effects for a single Gaussian process; comparing a main effect across multiple Gaussian processes; and visualizing main effects of a single parameter on functional output. The first two uses of *plotMainEffects* are demonstrated below; an example of the latter can be found in Section (5).

First, we use *plotMainEffects* to plot the main effects for all input parameters on the Gaussian process created above. By default, all main effects are plotted, but a subset of effects can be specified by either name or number through the argument 'effects'. Setting 'FANOVA = TRUE' will calculate, for each main effect, the percentage contribution of that effect to the total functional variance of the GP predictor, and this will be reported in the legend. The function *plotInteractionEffect* is used to create a contour plot which visualizes interaction effects, and this is also demonstrated below. Output from the code can be seen in Figure (3).

```
> par(mfrow = c(1, 2))
> plotMainEffects(fit, graphStyle = 1, FANOVA = TRUE)
> plotInteractionEffect(fit, effects = c(1, 2))
```

It is also possible to use *plotMainEffects* to compare a main effect of a single parameter across multiple responses. We first create a Gaussian process list object that contains three GPs, each
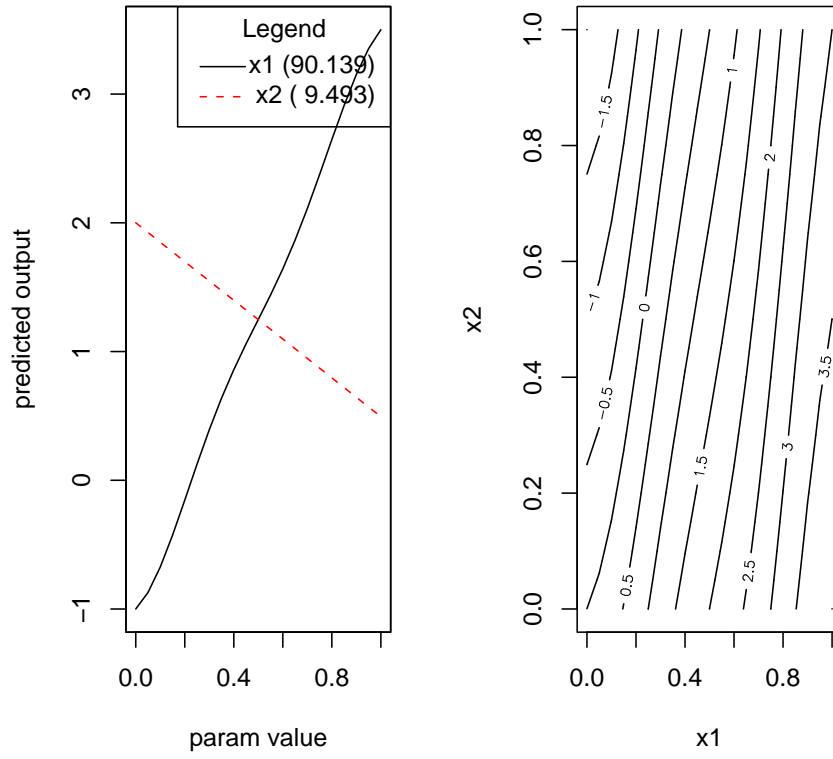
Figure 3: Main and Two-Way Interaction Effect Plots. For each main effect, the percent contribution of that effect to the total functional variance of the Gaussian process is also reported.

with the design parameter x. We then plot the main effect of x on the three GPs. This example also illustrates how the main effect can be referred to by name instead of by number. The main effects plot produced by the code is displayed in Figure (4).

```
> x = -5:5
> z1 = 10 - 5 * x + rnorm(length(x))
> z2 = 4 - 5 * x + rnorm(length(x))
> z3 = 7 * sin(x) + rnorm(length(x))
> fitMulti = mlegp(x, cbind(z1, z2, z3), param.names = "x")


> plotMainEffects(fitMulti, effects = "x", graphStyle = 1)
```
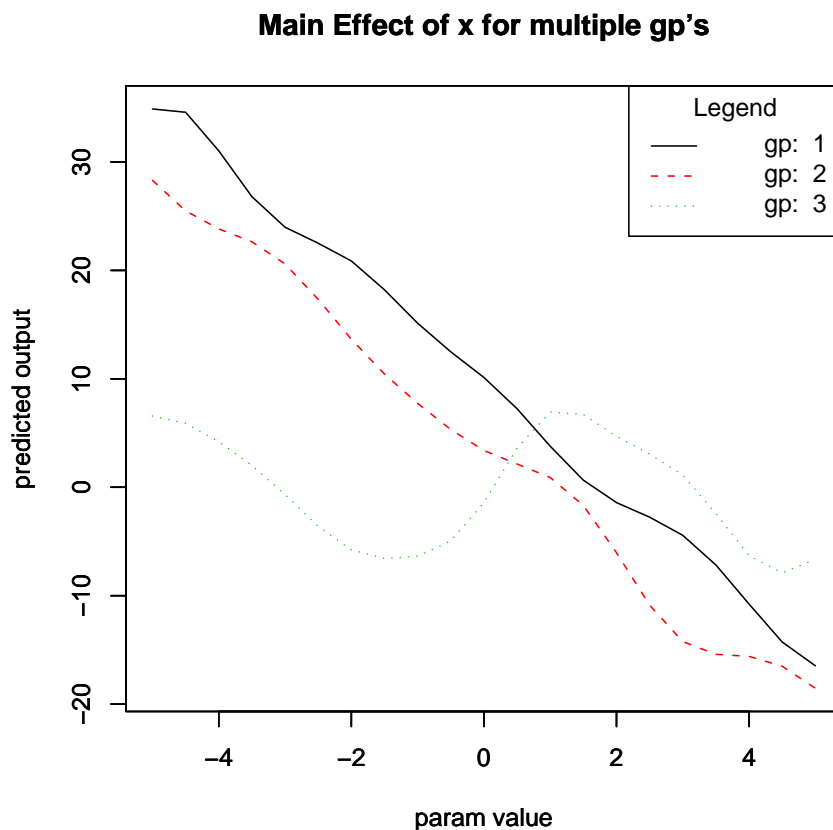
Main Effect of x for multiple gp's

Figure 4: Main effects of the parameter x on a Gaussian process list that models three responses.

5   Multivariate Output and Dimension Reduction

5.1   Background

For multivariate or functional output, singular value decomposition can be used to reduce the dimensionality of the response (Heitmann *et al.*, 2006). Let $[z]_{i,j}$, $i = 1, \ldots, k$, $j = 1, \ldots, m$ be a matrix of m multivariate responses, where column j of the matrix contains the k-dimensional

output of the response corresponding to the input parameter $\theta^{(j)}$. Also let $r = \min(k, m)$. Using singular value decomposition,

$$[z]_{i,j} = [U_{kxr}D_{rxr}V'_{rxm}]_{i,j} = \sum_{p=1}^{r} \lambda_p \{\alpha_p\}_i \{w_p(\theta)\}_j, \quad (10)$$

where λ_p is the pth singluar value, α_p is the pth column of U, and $w_p(\theta)$ is the pth row of V'. We will refer to the jth column of V', which contains the elements $\{w_p(\theta)\}_j$, $p = 1, \ldots, r$, as a vector of *principle component weights* corresponding to the jth observation. The output z is approximated by keeping the $l < r$ most important principle component weights, corresponding to the l largest singular values. For a response matrix z as described above, *mlegp* fits independent Gaussian processes to the most important principle component weights. The number of principle component weights to be kept is specified through the argument 'PC.num'; alternatively, setting the argument 'PC.percent' will keep the most important principle component weights that account for 'PC.percent' of the variation in the response.

5.2   Examples

5.2.1   Basics: Modeling functional output

The first example demonstrates the use of *mlegp* to fit GPs to principle component weights in order to model functional output. The functional responses are sinusoidal, consisting of 161 points, with a vertical offset determined by the design parameter p. We first create the functional responses and plot them. This output is displayed in Figure (5).

```
> x = seq(-4, 4, by = 0.05)
> p = 1:10
> y = matrix(0, length(p), length(x))
> for (i in 1:length(p)) {
+     y[i, ] = sin(x) + 0.2 * i + rnorm(length(x), sd = 0.01)
+ }

> for (i in p) {
+     plot(x, y[i, ], type = "l", col = i, ylim = c(min(y), max(y)))
+     par(new = TRUE)
+ }
```

For functional output such as this, it is possible to fit separate GPs to each dimension. However, with 161 dimensions, this is not reasonable. In the code below, we first use the function *singularValueImportance* and see that the two most important principle component weights explain more than 99.99% of the variation in the response. Then, we fit the GPs to these two principle component weights. Note that in the call to *mlegp* we take the transpose of the response matrix, so that columns correspond to the functional responses.

```
> numPCs = 2
> singularValueImportance(t(y))[numPCs]

[1] 99.996

> fitPC = mlegp(p, t(y), PC.num = numPCs)
```

The GPs, which model principle component weights, can now be used to predict and analyze the functional response, based on the UDV' matrix of equation (10). The UD matrix corresponding to the principle component weights that are kept is saved as a component of the Gaussian process list object. The R code below demonstrates use of the *predict* method to reconstruct (approximately) the original functional output.
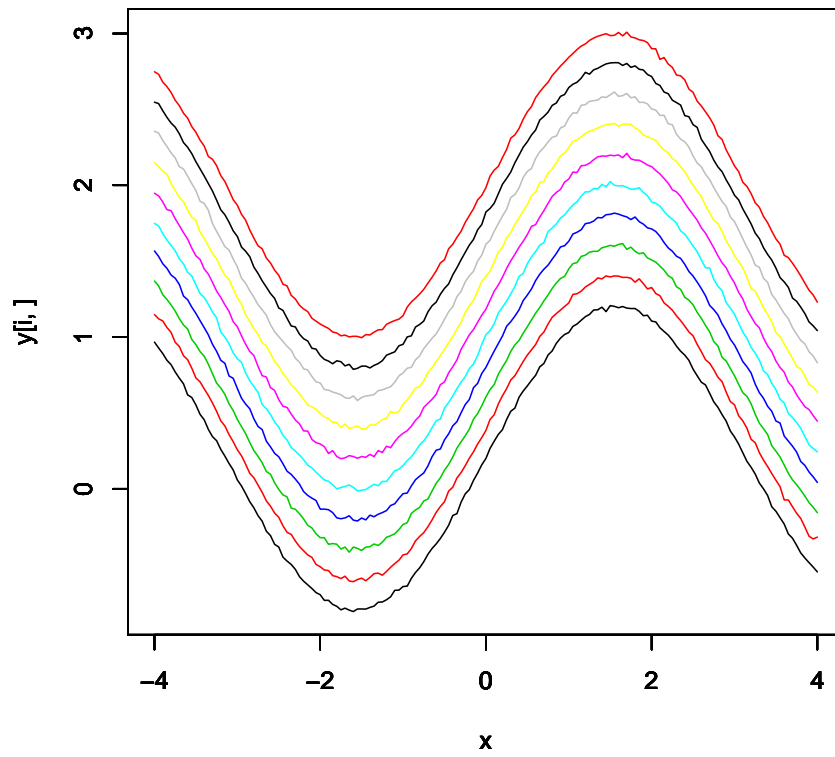
Figure 5: An example of functional responses where the design parameter determines the vertical offset

```
> Vprime = matrix(0, numPCs, length(p))
> Vprime[1, ] = predict(fitPC[[1]])
> Vprime[2, ] = predict(fitPC[[2]])
> predY = fitPC$UD %*% Vprime
```

5.2.2   Calculating main effects

The function *plotMainEffects* visualizes main effects of design parameters on functional output for GPs fit to principle component weights. This is demonstrated below, for the Gaussian processes that were fit above. The graphical plot is displayed in Figure (6).

```
> plotMainEffects(fitPC, effect = 1, graphStyle = 1)
```
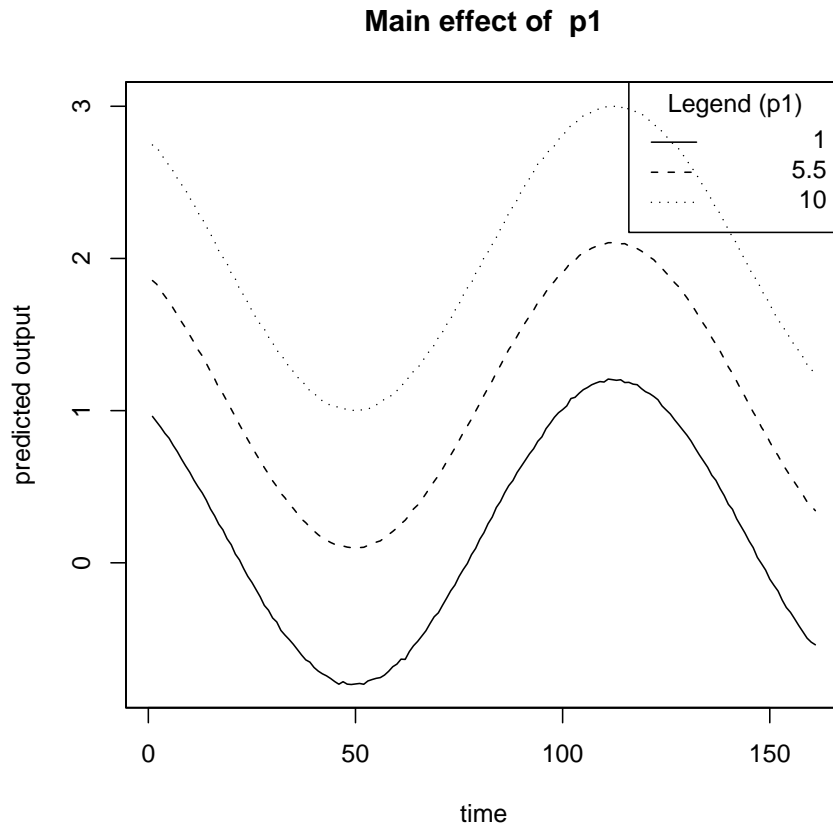
Main effect of p1

Figure 6: Main effect of $p1$ on functional output, based on Gaussian process modeling of the two most important principle component weights.

5.2.3   Modeling high dimensional (and not necessarily functional) data

Although the above example involves functional output, the singular value decomposition technique can applied generally to any multi-dimensional response. One can also use *mlegp* to analyze non-functional data of high-dimension, as well as multiple functional responses, by manipulating the output of *predict* and calling *plotMainEffects* functions with 'no.plot'= 'TRUE', which returns the main effects without plotting them. In our final example, we consider *two* sets of functional

outputs: the sinusoidal response $y1$ and the linear response $y2$. Both responses depend on the design parameter p. After combining the output vectors $y1$ and $y2$, we fit Gaussian processes to the most important principle component weights that explain at least 99.999% of the variation in output.

```
> p = 1:10
> x1 = seq(-4, 4, by = 0.05)
> x2 = 1:5
> y1 = matrix(0, length(p), length(x1))
> y2 = matrix(0, length(p), length(x2))
> for (i in 1:length(p)) {
+     y1[i, ] = sin(x1) + 0.2 * p[i] + rnorm(length(x1), sd = 0.01)
+     y2[i, ] = 0.1 * p[i] + x2 + rnorm(length(x2), sd = 0.01)
+ }
> y = cbind(y1, y2)
> fitPC = mlegp(p, t(y), PC.percent = 99.999)
```

Plotting main effects for the different types of responses is now a matter of retrieving all of the main effects from *plotMainEffects*, and breaking this predicted effect into the separate main effects for the two responses of interest. Main effects for both responses are displayed in Figure (7).

```
> main = plotMainEffects(fitPC, effect = 1, no.plot = TRUE)
> preds = main$preds
> beg1 = 1
> end1 = length(x1)
> beg2 = end1 + 1
> end2 = beg2 + length(x2) - 1
> par(mfrow = c(1, 2))
> for (i in 1:dim(preds)[1]) {
+     plot(x1, preds[i, beg1:end1], ylim = c(min(preds[, beg1:end1]),
+         max(preds[, beg1:end1])), type = "l", col = i, xlab = "x1",
+         ylab = "y1", main = "main effect on y1")
+     par(new = TRUE)
+ }
> par(new = FALSE)
> for (i in 1:dim(preds)[1]) {
+     plot(x2, preds[i, beg2:end2], ylim = c(min(preds[, beg2:end2]),
+         max(preds[, beg2:end2])), type = "l", col = i, xlab = "x2",
+         ylab = "y2", main = "main effect on y2")
+     par(new = TRUE)
+ }
```
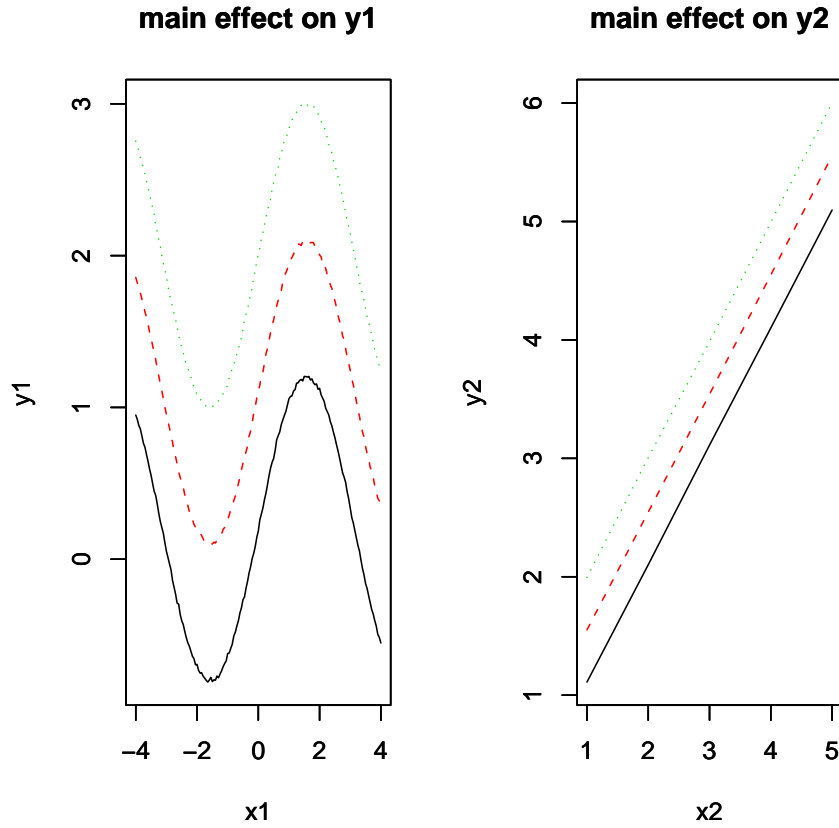
Figure 7: Main effects of the parameter p on functional responses $y1$ (left) and $y2$ (right). Values of p are 1 (black solid lines), 5.5 (red dashed lines), and 10 (green dotted lines).

References

Heitmann, K., Higdon, D., Nakhleh, C., Habib, S., 2006. Cosmic Calibrat ion, *The Astrophysical Journal*, **646**, 2, L1-L4.

Saltelli, A., Chan, K., Scott, E.M., 2000. Sensitivity analysis. (Chichester; New York: Wiley).

Santner, T.J., Williams, B.J., Notz, W., 2003. The Design and Analysis of Computer Experiments (New York: Springer).

Schonlau, M. and Welch, W., 2006. Screening the Input Variables to a Comp uter Model Via Analysis of Variance and Visualization, in Screening: Methods for Experimentation in Industry, Drug Discovery, and Genetics. A. Dean and S. Lewis, eds. (New York: Springer).

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