# Code Compendium: Multivariate and Functional Output Emulation

Suppmental Material for Adventures in Space-Time Modeling with Maike and Dave

Maike Holthuijzen (*maikeh@vt.edu*) Dave M. Higdon (*dhigdon@vt.edu*)

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## Contents

# A Simple Example

We begin by constructing the functional model depicted in Figure 2 of the Chapter 7. Next, we source the required R files from GitHub, which provide several utility functions used in the analysis. Finally, we define the two-dimensional input space over which the model (Eq 7.1) is evaluated.

```
source("Cov_functions.R")
source("Estimation_1D.R")
source("Estimation_Basis.R")

nc = 10 # Number of input settings
s = 11  # Number of vector values produced by f(x)

# Creates a grid of points where x[,2] represents x and x[,1] represents t
t1 = seq(0,1, length = s)
x1 = seq(0,1, length = nc)
x = expand.grid(t1,x1)

# Input grid points into the deterministic function to be emulated
f = (x[,2]+1)*cos(pi*x[,1]) + 0.03*(exp(x[,2]))
```

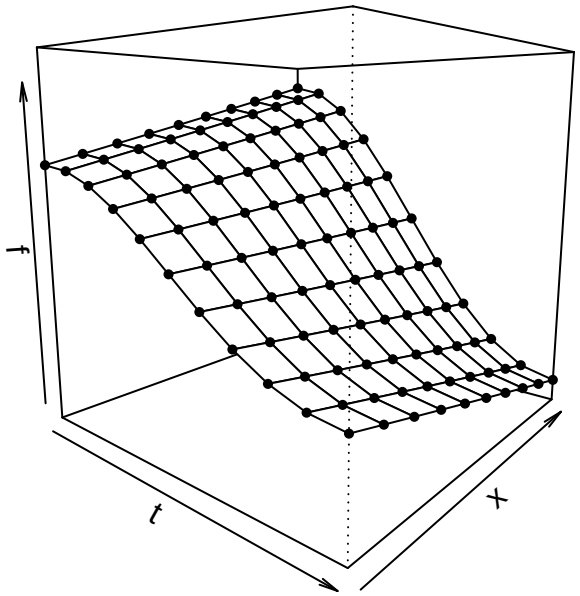



Figure 1: A simple functional model to be emulated

We assume the function $f$ can be modeled as a zero-mean Gaussian Process (GP) with a covariance structure given by the Kronecker product of spatial and temporal covariance matrices. From Section 0.1, we can model $\text{vec}(\text{Y}) = f$ using a Kronecker representation for the correlation

$$f \sim N(0, \sigma^2(R_x \otimes R_t) + \nu I). \tag{1}$$

## 1.1 Estimating Parameters

We assume the prior for $f$ is given by Equation 1 and aim to derive the posterior distribution, $f|D_n$ where $D_n$ is the data. We estimate the parameters, $\phi_x, \phi_y, \sigma^2, \nu$, using the functions in `Estimation_1D.R`.

The likelihood function, derived from the matrix normal distribution with an added nugget term, is given by

(Stegle et al., 2011):

$$L(\mathbf{y_c}; \nu, \sigma^2, \phi) \propto |\sigma^2 S_x \otimes S_t + \nu I|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\text{vec}\left(U_t^T Y U_x\right)^T \left(\sigma^2 s_x \otimes S_t + \nu I\right)^{-1} \text{vec}\left(U_t^T Y U_x\right)\right\},$$

given the eigendecomposition $R_x = U_x S_x U_x^T$ and $R_t = U_t S_t U_t^T$, where $UU^T = I$. Fortunately, it is not necessary to explicitly compute the Kronecker products when evaluating the likelihood. Notably, the matrix $(S_x \otimes S_t + \nu I)^{-1} = \nu^{-\mathbf{1}}$ is diagonal, allowing both its inverse and the log-determinant to be computed efficiently. In particular, the log-determinant simplifies to $\log\left|\sigma^2 R_x(\phi) \otimes R_t(\phi) + \nu I\right| = \mathbf{1}^T \log(\nu)$. The remaining quantity of interest, the sum of squares, can also be evaluated efficiently. A summary of these calculations is provided in Table 0.1 of Chapter 7, and pseudocode in Section 1.1.1 outlines how the log-determinant and sum of squares are efficiently computed and implemented in the parameter estimation functions found in `Estimation_1D.R`.

Estimates for the covariance parameters of $R_x$ and $R_t$ can be obtained via maximum likelihood. However, the maximum likelihood estimates (MLEs) of the marginal variance $\sigma^2$ and lengthscale $\phi$ are not consistent; that is, their accuracy does not improve as the sample size increases. As a first step, we compute the pairwise distance matrices for the input dimensions $x$ and $t$ using the `get_distmat` function from `Cov_function.R`:

```
Tdist = get_distmat(t1, t1) # 11 x 11 matrix
Xdist = get_distmat(x1, x1) # 10 x 10 matrix
```

We then estimate the covariance parameters using the functions provided in `Estimation_1D.R`. Optimization is performed using the `nmkb` function from the `dfoptim` R package which implements the Nelder-Mead algorithm for derivative-free optimization. The function `Estimate_params` takes the following arguments:

- `distC` and `distR`: the first and second distance matrices in the Kronecker product (order matters)
- `z`: the vector of computer model output to be emulated

takes as arguments `distC` and `distR`,

The `nkmb` function returns the parameters estimates in the following order:

1. scale estimate for the first covariance, $R_x$, matrix $\phi_x$,
2. scale estimate for the second covariance, $R_t$, matrix $\phi_y$,
3. nugget $\nu$,
4. marginal variance,$\sigma^2$.

Sensible upper and lower bounds for the optimization procedure are also specified below:

```
# Function assumes the Kronecker product: kronecker(C, R), so order matters
params = nmkb(c(0.5, .5, .0001, .5),
              Estimate_params, distC = Xdist, distR = Tdist, z=f,
              lower = c(0.1, 0.1, 1e-6, .1), upper = c(100, 100, 100, 100))
```

The parameter estimates and associated R code to print the values are:

| Parameter | $\phi_x$ | $\phi_y$ | $\nu$ | $\sigma^2$ |
|---|---|---|---|---|
| Estimates | 12.1517375 | 1.1269516 | $10^{-6}$ | 99.999987 |
| R Code | `params$par[1]` | `params$par[2]` | `params$par[3]` | `params$par[4]` |

### 1.1.1 Efficiently caluculating the sum of squares and log determinant

In Chapter 7, Table 0.1, we present the fundamental calculations for exploiting the Kronecker structure in a multivariate emulator. The following *pseudocode* demonstrates how the log-determinant and sum of squares are computed efficiently and subsequently used in the parameter estimation functions in `Estimation_1D.R`. The process begins by performing singular value decomposition (SVD) on $R_x$ and $R_t$ to obtain their respective

components. Specifically, we perform **eigen-decomposition** on $R_x = U_x S_x U_x^T$ and $R_y = U_y S_y U_y^T$, as shown in Table 0.1

```
svdx = svd(Rx) # Eigendecomposition of Rx
# Obtaining components from Eigendecompsition
Ux = svdx$u
Sx = svdx$d
Ux_t = t(svdx$v)

svdt = svd(Rt) # Eigendecomposition of Rt
# Obtaining components from Eigendecompsition
Ut = svdt$u
St = svdt$d
Ut_t = t(svdt$v)
```

In Table 0.1, we under the variance and inverse label we note that $(S_x \otimes S_t + \nu I)^{-1} = \text{diag}(\mathbf{v}^{-1}) = \text{diag}(\lambda)$ which is a diagonal matrix that we compute as follows:

```
nu = params$par[3]                    # obtaining the nu estimate
v = sigma2 * kronecker(Sx, St) + nu # compute v
lambda = 1/v
```

In Table 0.1, we perform multiplication of $\left(U_x^T \otimes U_t^T\right) \mathbf{y_c} = \text{vec}\left(U_t^T Y U_x\right)$ where $Y = \text{matrix}\left(\mathbf{y_c}, \text{nrow} = s, \text{ncol} = n_c\right)$. In this context, $\mathbf{y_c}$ is represented by $f$.

```
Ymat = matrix(f, nrow = nc, ncol = s)  # Construct the matrix Y
Yvec = as.vector(Ut_t %*% Ymat %*% Ux) # Performing Multiplication in Table 0.1
```

Lastly, we put the various elements together to evaluate the sums of squares and the log log-determinant efficiently using the Kronecker products.

```
ssqKronecker = (Yvec)^2 %*% lambda # Sums of Squares calculation
LogDet = sum(log(lambda))          # log determinant calculation in Table 0.1
```

## 1.2 Computing the conditional mean and covariance

In this section, we use the parameter estimates from the previous section to obtain the (posterior) conditional mean and covariance. In other words, we obtain the posterior predictive distribution $f|D_n$, which is also multivariate normal distribution where $D_n$ represents the data.

First, we build $R_x$ and $R_t$ using estimates for $\phi_x$ and $\phi_t$ . Note that we assume Gaussian covariance functions throughout.

```
scaleX = params$par[1]
scalet = params$par[2]

Rt = exp( -(Tdist / scalet)^2 )
Rx = exp( -(Xdist / scaleX)^2 )
```

Next, we set up a prediction grid for new $x$ locations ($x_{new}$). We also construct an augmented $x$ input space, where $x^* = [x, x_{new}]$ and construct the cross covariance matrix $R_{x^*,x}$. Next, we perform an eigendomposition of $R_x$, $R_t$ and $R_{x^*,x}$ which is necessary for efficient computation of the conditional mean (see book chapter). Note that for this example, we only vary $x$, not $t$.

```
s = 11

# prediction grid of new locations, xnew
xnew = c(.135, .72, .97)
```

```
# make the augmented x grid
xstar_grid = c(x1, xnew)

# build covariance matrix, R_x*,x*
dist_xstar_xstar = get_distmat(xstar_grid, xstar_grid)
R_xstar_xstar = exp( -(dist_xstar_xstar / scaleX)^2 )

# build cross covariance matrix, R_x*,x
dist_xstar_x = get_distmat(xstar_grid, x1)

R_xstar_x = exp( -(dist_xstar_x / scaleX)^2 )
```

For the calculation of the conditional mean, we perform an eigendecomposition of $R_x$ and $R_t$

```
svdx = svd(Rx)
svdt = svd(Rt)

Ux = svdx$u
Sx = svdx$d
Ux_t = t(svdx$v)

Ut = svdt$u
St = svdt$d
Ut_t = t(svdt$v)
```

Now, we can efficiently obtain the conditional mean using Kronecker product properties (see Table 0.1 in the book chapter).

```
nu = params$par[3]
sig2 = params$par[4]

# calculate kronecker product of singular values Sx and St
lambda = diag(1 / (sig2*kronecker(Sx, St) + nu))

# reshape the response to be s * nc
f_reshape = matrix(f, nrow = s, ncol = nc)

res1 = lambda %*% as.vector(Ut_t %*% f_reshape %*% Ux)

resmat = matrix(res1, nrow = s, ncol = nc)

cond_mean = sig2 * as.vector(Rt %*% Ut %*% resmat %*% Ux_t %*% t(R_xstar_x) )
```

Now we can plot the conditional mean. In the code below, we only plot at test locations ($x_{new}$).

```
# grid for plotting
# train locations in black; test locations in red

plot_grid_train = expand.grid(t1, x1)
plot_grid = expand.grid(t1, xnew)

# this is for differentiating train/test indices
train_idx = 1:length(x1)
train_idx_kron = 1:(length(train_idx) * length(t1))
test_idx_kron = (train_idx_kron[length(train_idx_kron)] + 1): (length(xstar_grid) * s)
```

Now we can inspect the predicted mean on the grid of training points.

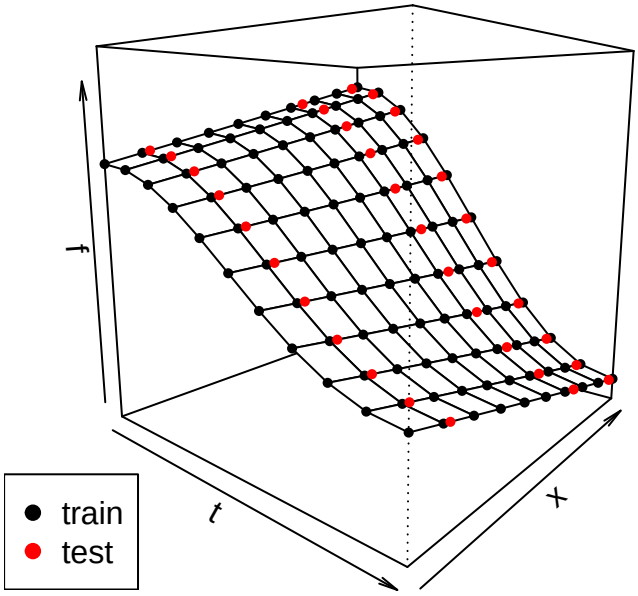



Figure 2: Conditional mean predictions (red) on the grid of training points (black)

**Generating conditional realizations**

For large $n$, obtaining the conditional variance may not be computationally feasible. However, as stated in the book chapter, we can use a technique described in \citep{nychka2002multiresolution} to generate realizations from the conditional predictive distribution.

Before we delve into details, it is instructive to recall the matrix-normal distribution. The matrix-normal distribution (with error) [**?**] is related to the multivariate normal distribution as follows:

$$\mathbf{X} \sim \mathcal{MN}_{n\times p}(\mathbf{M}, \mathbf{U}, \mathbf{V}),$$

if and only if

$$\text{vec}(\mathbf{X}) \sim \mathcal{MVN}_{np}(\text{vec}(\mathbf{M}), \mathbf{V} \otimes \mathbf{U}). \tag{2}$$

The probability distribution function (PDF) of the matrix-normal distribution is given by:

$$P(\mathbf{X}|\mathbf{M}, \mathbf{U}, \mathbf{V}) = \frac{\exp(\text{tr}([\mathbf{V^{-1}}(\mathbf{X}-\mathbf{M})^{\mathbf{T}}\mathbf{U^{-1}}(\mathbf{X}-\mathbf{M})])}{(2\pi)^{np/2}|\mathbf{V}|^{\mathbf{n/2}}|\mathbf{U}|^{\mathbf{p/2}}}$$
$$\mathbf{M} = n \times p$$
$$\mathbf{U} = n \times n$$
$$\mathbf{V} = p \times p.$$

Suppose $\mathbf{Y}$ has a matrix normal distribution with mean matrix $Z = \mathbf{0}_{n\times p}$ and covariance matrices $\mathbf{U}$ and $\mathbf{V}$. Then for a mean matrix $\mathbf{M}$ and linear transformations $\mathbf{L}$ and $\mathbf{R}$, $\mathbf{Y}$ can be expressed as:

$$\mathbf{Y} = \mathbf{M} + \mathbf{LZR}, \tag{3}$$

where $\mathbf{Y}$ has a matrix-normal distribution with parameters $\mathbf{M}, \mathbf{LL^T}, \mathbf{R^TR}$. In (3), Cholesky decomposition is used to construct the matrices $\mathbf{L}$ and $\mathbf{R}$, the Cholesky factors of $\mathbf{U}$ and $\mathbf{V}$, respectively. If an eigendecomposition is used, then $\mathbf{LL^T} = \mathbf{U_u D_u^{1/2} D_u^{1/2} U_u^T}$ is the eigendecomposition of $\mathbf{U}$ and $\mathbf{R^TR} = \mathbf{U_v D_v^{1/2} D_v^{1/2} U_v^T}$

is the eigendecomposition of $\mathbf{V}$. This, in turn implies that (3) can be used to generate MVN variates with $\mathbf{L} = \mathbf{U_u D_u^{1/2}}$ and $\mathbf{R} = \mathbf{D_v^{1/2} U_v^T}$

To efficiently sample from a MVN distribution with mean vector $m$ and covariance matrix $V \otimes U$, only a few steps are needed. We begin by expressing $m$ as a matrix $\mathbf{M}$ of size $n \times p$. The matrix of $N(0,1)$ random variates $\mathbf{Z}$ must also be of size $n \times p$. We use either Cholesky or an eigendecomposition to obtain $\mathbf{L}$ and $\mathbf{R}$ in (3). We prefer the eigendecomposition, as it is more stable.

To carry out the generation of realizations, we begin by performing eigendecompositions of $R_t$, $R_x$ and $R_{x^*,x^*}$:

```
svdR_xstar_xstar = svd(R_xstar_xstar)
Rstst_U = svdR_xstar_xstar$u
Rststd = svdR_xstar_xstar$d

svdt = svd(Rt)
Ut = svdt$u
Ut_t = t(svdt$v)
St = svdt$d

svdx = svd(Rx)
Sx = svdx$d
Ux = svdx$u
Ux_t = t(svdx$v)
```

The function below carries out the calculation ($U_t \tilde{Z} U_x^T$) from table 0.1.

```
pre_process_svd = function(z, s, Ut, St, Rstst_U, Rststd){
  nc_prime = length(Rststd)
  # need to take square roots!!
  eigs = kronecker(sqrt(Rststd), sqrt(St))
  ztilde = eigs*z
  mysim = as.vector(Ut %*% matrix(ztilde, nrow = s, ncol = nc_prime) %*% t(Rstst_U))
}
```

Now we can carry out steps to generate realizations (steps are listed in Table 0.1 in the chapter). We generate a matrix of N(0,1) random variates and collect them into an appropriately sized matrix:

```
nreals = 100
nc_prime = length(Rststd)

# generate a matrix of N(0,1)'s
allZs = matrix(rnorm(s*nc_prime*nreals), nrow=s*nc_prime)
```

Here we set up an incidence matrix to make it easier to extract $\mathbf{u}$.

```
kmat = matrix(0, nrow = length(train_idx_kron), ncol = s*nc_prime)
kmat[train_idx_kron, train_idx_kron] = diag(1, nrow= length(train_idx_kron))
```

The function below will enable us to efficiently calculate the *psuedo conditional mean* ($\mathbf{w}^*$ from Table 0.1).

```
get_cond_mean = function(svdt, svdx, R_xstar_x, y_tilde, nu, sig2){

  Ut = svdt$u
  Ut_t = t(svdt$v)
  St = svdt$d

  Sx = svdx$d
  Ux = svdx$u
```

```
  Ux_t = t(svdx$v)

  # carry out conditional mean calculation for each
  # column of y_tilde, where each col of y_tilde is a single y_tilde as in Table .01
  # if we do it this way, we can vectorize calculation steps as much as possible
  # except for this one for loop....
  lambda = diag(1 / (sig2*kronecker(Sx, St) + nu))

  cond_mean_mat = matrix(nrow = nrow(R_xstar_x)*length(St), ncol = ncol(y_tilde))
  for (i in 1:ncol(y_tilde)){
    y_star_samp = y_tilde[, i]
  # reshape to be s * nc
  zreshape = matrix(y_star_samp, nrow = s, ncol = nc)

  res1 = lambda %*% as.vector(Ut_t %*% zreshape %*% Ux)

  resmat = matrix(res1, nrow = s, ncol = nc)

  cond_mean_samp = sig2 * as.vector(Rt %*% Ut %*% resmat %*% Ux_t %*% t(R_xstar_x) )
  cond_mean_mat[,i] = cond_mean_samp
  }
  return(cond_mean_mat)
}
```

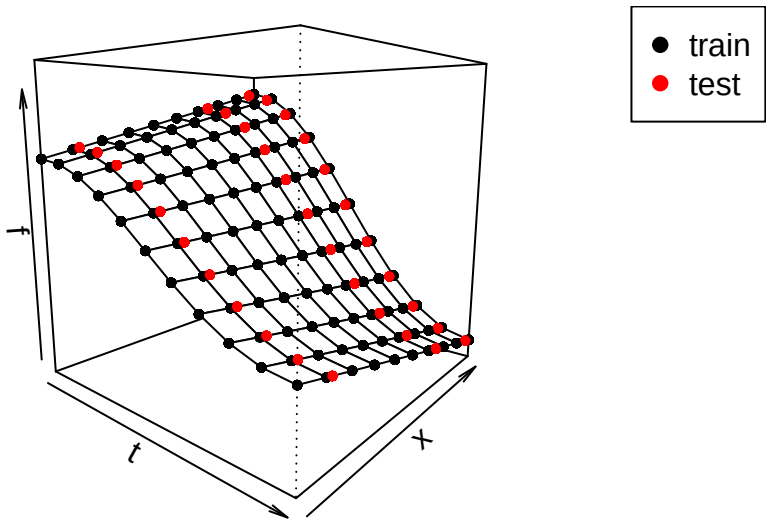
Here are all the steps (the function `rmultnorm` is located in `Cov_functions.R`):

```
# generate epsilon ~ MVN(0, nu)
epsilon = t(rmultnorm(nreals, rep(0, s*nc), diag(nu, nrow = s*nc)))

# use the pre_process_svd() function to get u and collect into a matrix
umat = apply(allZs,2, function(x) pre_process_svd(z=x, s=s,
            Ut = Ut, St = St, Rstst_U = Rstst_U, Rststd = Rststd))
# get y_tilde
y_tilde = kmat %*% umat + epsilon
# get w_star
w_star = get_cond_mean(svdt, svdx, R_xstar_x, y_tilde, nu, sig2)
ustar = umat - w_star
# we calculated cond_mean previously
conditional_samps = as.vector(cond_mean) + ustar
```

We can plot results as before and inspect the realizations.

```
persp(t1, x1,
      matrix(cond_mean[train_idx_kron], nrow = s),
      theta = 130-90,
      phi = 10,
      xlab = 't', ylab = 'x', zlab = 'f',
      zlim = c(-2.2, 2.4)) -> res
for (i in 1:nreals){
  points(trans3d(plot_grid_train[,1],
                 plot_grid_train[,2],
                 conditional_samps[train_idx_kron, i],
                 pmat = res),
         col = 'black',
         pch = 16,
```

```
        cex = 0.7)

  points(trans3d(plot_grid[, 1],
                 plot_grid[, 2],
                 conditional_samps[test_idx_kron, i],
                 pmat = res),
         col = 'red',
         pch = 16,
         cex = 0.7)
}
legend("topright", legend = c("train", "test"), col = c("black", "red"), pch=19)
```




## Parameter estimation: output basis strategies? Idk what to call this

In this section we show how covariance parameters can be estimated for the case when basis strategies is used for handling multivariate computer model output. Here, we choose to use bases based on singular value decomposition (see section 0.3.2.1 in the book chapter).

A common choice of basis functions are estimated empirically from the existing ensemble of model outputs held in the $s \times n_c$ matrix $Y_c$ using empirical orthogonal functions (EOFs) \cite{ramsay2005principal}; \cite{hannachi2007empirical}. We use the simple example shown in Figure 2. The goal of the optimization is to minimize the negative of the (log) likelihood shown in (7) in the book chapter. We highly recommend reviewing the optimization functions in `Estimation_Basis.R`.

```
s = 11          # size of output space
nc = 10         # number of computer model runs

t1 = seq(0,1,length = s)
x1 = seq(0,1,length = nc)
x = expand.grid(t1, x1)

# function to emulate
f = (x[, 2]+1)*cos(pi*x[, 1]) + .03*(exp(x[, 2]))
```

The optimization function `ML_pcEMU()` only requires three parameters: a vector of computer model output `fn`, computer model inputs `x`, and `q`, the number of bases used in representing computer model output. The

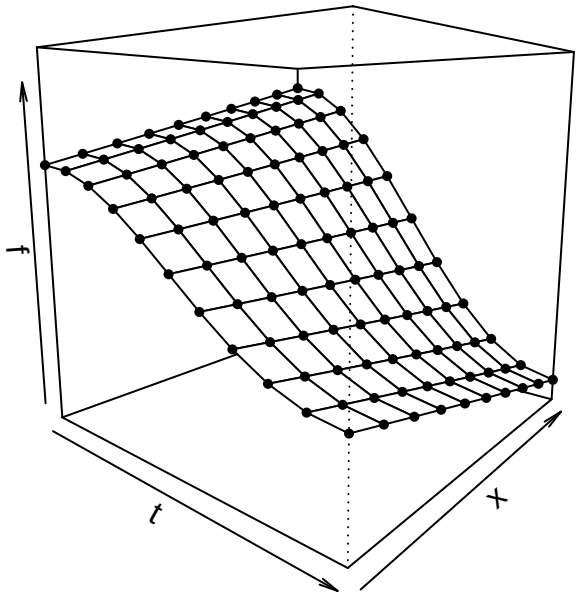



Figure 3: A simple functional model to be emulated

parameter $\nu$ is not estimated here and is fixed at a value of 1e-5.

```
# carry out optimization
params = ML_pcEMU(fn = f, x = x1, q = 2)
print(params)
```

```
## [[1]]
##       phi   sigma^2
## 6.7395563 0.7710988
##
## [[2]]
##       phi   sigma^2
## 7.3470944 0.8953043
```

## Conditional mean and realizations

Here is a function that returns the predictive mean and covariance matrix of $\mathbf{w}_j^*$ for new input locations `xnew`.

```
# f =  function output at train points
# xnew = vector of new locations
# nc = number of computer runs
# q = number of bases
# x1 = original x train locations
# params = object you get from the basis estimation function
get_wstar_distr_preds = function(f, xnew, nc, q, x1,t1, params){

  nc_new = length(xnew)

  fmat = matrix(f, ncol=nc)

  xdist_aug = as.matrix(dist( c(x1, xnew)) )

  # subtract means of rows
```

```
  meanf = apply(fmat, 1, mean)
  fmat0 = fmat - meanf

  # do svd
  fsvd = svd(fmat0)

  # make K
  K = fsvd$u[,1:q] %*% diag(fsvd$d[1:q]) / sqrt(nc)

  s = nrow(K)
  wlist = list()

  preds = rep(0, length(t1)*nc_new)
  for (i in 1:q){
    phi = params[[i]][1]
    sig2 = params[[i]][2]

    nu = 1e-6

    kj = K[, i]

    Rcov = sig2*exp(-(phi*xdist_aug)^2)
    nug = nu / sum(kj^2)

    # get the parts of V
    sigma11 = nug * diag(1, nrow = nc, ncol = nc) +  Rcov[1:nc, 1:nc]
    sigma12 = Rcov[1:nc,(nc+1):(nc+nc_new) ]
    sigma22 = Rcov[(nc+1):(nc+nc_new), (nc+1):(nc+nc_new) ]
    sigma21 = t(sigma12)

    sig11_inv = solve(sigma11)

    what_j = fsvd$v[ ,i] * sqrt(nc)

    wmean = sigma21 %*% sig11_inv %*% what_j

    wcov = sigma22 - sigma21 %*%  sig11_inv %*% sigma12
    sublist = list(wmean = wmean, wcov = wcov)
    wlist[[i]] = sublist

  }

  return(list(wlist = wlist, K = K, meanf = meanf, fmat0 = fmat0))

}
```

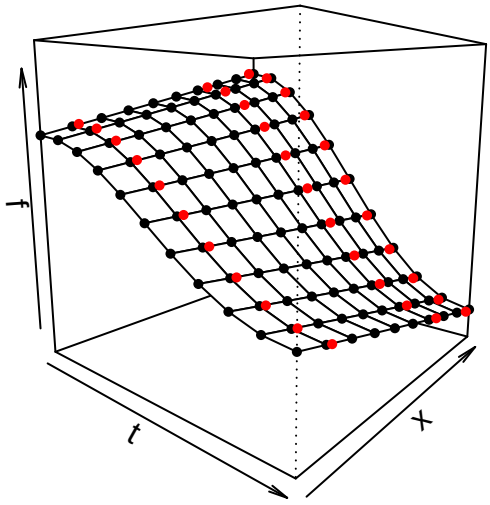
Now, we can use our previous results to generate predictions using the function `get_wstar_distr_preds()`. Note that the function also returns the mean and covariance for $w^*$, which can be used to generate realizations.

```
w_stuff = get_wstar_distr_preds(f=f,xnew = xnew, nc=nc,q=2, x1=x1, t1=t1, params=params)
# get predictive mean of w_1 and w_2
w1 = as.vector( w_stuff$wlist[[1]]$wmean)
w2 = as.vector( w_stuff$wlist[[2]]$wmean)
```

```
# grab the K matrix
K = w_stuff$K

# mean of f (f is demeaned prior to parameter estimation)
meanf = w_stuff$meanf

# make w's into a q x nc matrix
w_all = rbind(w1, w2)

# get predictions, add mean back
basis_preds = K %*% w_all
basis_preds = as.vector(basis_preds + meanf)
```

Let's plot just the predictions (not realizations) to see if they look ok.

```
persp(t1, x1,
      matrix(f, nrow = s),
      theta = 130-90,
      phi = 10,
      xlab = 't', ylab = 'x', zlab = 'f',
      zlim = c(-2.4, 2.4)) -> res

points(trans3d(x[, 1], x[, 2],
               f,
               pmat = res),
       col = 'black',
       pch = 16,
       cex = 0.7)

points(trans3d(plot_grid[, 1],
                 plot_grid[, 2],
                 basis_preds,
                 pmat = res),
         col = 'red',
         pch = 16,
         cex = 0.7)
```




We can also generate realizations.

```r
# get covariance matrices for w's
w1cov = w_stuff$wlist[[1]]$wcov
w2cov = w_stuff$wlist[[2]]$wcov

w1reals = rmultnorm(200, mu = w1, sigma = w1cov)
w2reals = rmultnorm(200, mu = w2, sigma = w2cov)

reals_matrix = matrix(nrow = 200, ncol = length(basis_preds))
for (i in 1:200){
  w_all = rbind(w1reals[i,], w2reals[i, ])
  bpreds = as.vector(K %*% w_all + meanf)
  reals_matrix[i, ] = bpreds
}
```