

# Creating a simple emulator case study from scratch: a cookbook

Robin K. S. Hankin  
University of Stirling

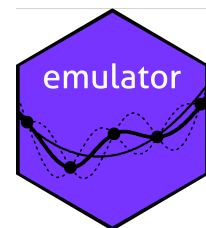
---

## Abstract

This document constructs a minimal working example of a simple application of the **emulator** package, step by step. Datasets and functions have a `.vig` suffix, representing “vignette”.

*Keywords:* emulator, BACCO, R.

---



## 1. Introduction

Package **emulator** of bundle **BACCO** performs Bayesian emulation of computer models. This document constructs a minimal working example of a simple problem, step by step. Datasets and functions have a `.vig` suffix, representing “vignette”.

This document is not a substitute for [Kennedy and O’Hagan \(2001a\)](#) or [Kennedy and O’Hagan \(2001b\)](#) or [Hankin \(2005\)](#) or the online help files in **BACCO**. It is not intended to stand alone: for example, the notation used here is that of [Kennedy and O’Hagan \(2001a,b\)](#), and the user is expected to consult the online help in the **BACCO** package when appropriate.

This document is primarily didactic, although it is informal.

Nevertheless, many of the points raised here are duplicated in the **BACCO** helpfiles.

The author would be delighted to know of any improvements or suggestions. Email me at [hankin.robin@gmail.com](mailto:hankin.robin@gmail.com).

## 2. List of objects that the user needs to supply

The user needs to supply three objects:

- A design matrix, here `val.vig` (rows of this show where the code has been evaluated)
- Basis functions. Here `basis.vig()`. This shows the basis functions used for fitting the

prior

- Data, here `z.vig`. This shows the data obtained from evaluating the various levels of code at the points given by the design matrix and the subsets object.

Each of these is discussed in a separate subsection below.

But the first thing we need to do is install the library:

```
> val.vig <- as.matrix(read.table("val.txt",header=TRUE))
```

## 2.1. Design matrix: USER TO SUPPLY

In these sections I show the objects that the user needs to supply, under a heading like the one above. In the case of the `emulator` we need a design matrix and a vector of outputs.

The first thing needed is the design matrix `val.vig`, ie the points in parameter space at which the lowest-level code is executed. The example here has just two parameters, `a` and `b`:

```
> head(val.vig)
```

```

          V1          V2
1 0.7500000 0.08333333
2 0.7166667 0.25000000
3 0.5833333 0.61666667
4 0.7833333 0.01666667
5 0.1833333 0.81666667
6 0.4166667 0.11666667
```

```
> nrow(val.vig)
```

```
[1] 30
```

Notes

- Each row is a point in parameter space, here two dimensional.
- The parameters are labelled `a` and `b`

## 2.2. Basis functions: USER TO SUPPLY

Now we need to choose a basis function. Do this by copying `basis.toy()` but fiddling with it:

```
> basis.vig <- function (x){
+   out <- c(1, x , x[1]*x[2])
+   names(out) <- c("const", LETTERS[1:2], "interaction")
+   return(out)
+ }
```

Notes

- This is shamelessly ripped off from `basis.toy()`, except that I've changed the basis to be `c(1,a,b,ab)`.
- in the function, `out` is a vector of length four: `c(1,x[1],x[2], x[1]*x[2])`.

### 2.3. Data: USER TO SUPPLY

The data we have for the `.vig` example is a vector whose elements are the output of the code at the points specified in `val.vig`:

```
> z.vig <- scan("z.txt")
> head(z.vig)

[1] 1.91 2.74 5.31 1.88 3.64 1.13

> summary(z.vig)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
 0.610  1.980   3.955   3.811   5.285   7.650
```

NB: object `z.vig` was created using the precepts of the Gaussian process; the details are given in this vignette but output is suppressed.

## 3. Data analysis

The previous section showed what data and functions the user needs to supply. These all have a `.vig` suffix. This section shows the data being analyzed.

First we will estimate the scales to use:

```
> os <- optimal.scales(val=val.vig, scales.start=c(10,10), d=z.vig, func=basis.vig)
> os

[1] 3.599552 10.857590
```

So we can estimate the coefficients. But first we have to calculate the variance matrix and invert it:

```
> A.os <- corr.matrix(xold=val.vig,scales=REAL.SCALES)
> Ainv.os <- solve(A)
```

Given this, use `betahat.fun()` to get the coeffs:

```
> betahat.fun(xold=val.vig, d=z.vig, Ainv=solve(A),func=basis.vig)
```

const	A	B	interaction
0.3091892	2.5153772	3.4313162	4.1637763

The central function is interpolant:

```
> interpolant(x=c(0.5,0.5), d=z.vig, Ainv=Ainv.os, scales=os,
+ xold=val.vig, func=basis.vig, give.full.list=TRUE)
```

\$betahat

const	A	B	interaction
0.3091892	2.5153772	3.4313162	4.1637763

\$prior

```
      [,1]
[1,] 4.32348
```

\$beta.var

	const	A	B	interaction
const	0.9465417	-0.8806066	-1.029046	1.094054
A	-0.8806066	1.6814999	1.061171	-2.090084
B	-1.0290457	1.0611710	2.286147	-2.503974
interaction	1.0940537	-2.0900839	-2.503974	4.990196

\$beta.marginal.sd

const	A	B	interaction
0.9729038	1.2967266	1.5120011	2.2338747

\$sigmahat.square

```
[1] 1.376784
```

\$mstar.star

```
      [,1]
[1,] 6.284112
```

\$cstar

```
[1] -0.4962515
```

\$cstar.star

```
[1] -0.4776302
```

\$Z

```
[1] 0.8109215
```

And that's it, really.

## References

Hankin RKS (2005). “Introducing **BACCO**, an R bundle for Bayesian analysis of computer code output.” *Journal of Statistical Software*, **14**(16).

Kennedy MC, O’Hagan A (2001a). “Bayesian calibration of computer models.” *Journal of the Royal Statistical Society, Series B*, **63**(3), 425–464.

Kennedy MC, O’Hagan A (2001b). “Supplementary details on Bayesian calibration of computer models.” Internal Report.

## A. Data generation

The data used in this study were created by directly sampling from the appropriate multivariate Gaussian:

```
> REAL.BETA <- 1:4
> REAL.SCALES <- c(3,6)
> REAL.SIGMASQUARED <- 0.3
> A <- corr.matrix(xold=val.vig,scales=REAL.SCALES)
> z.vig.synthetic <-
+ as.vector(rmvnorm(n=1,mean=crossprod(REAL.BETA,apply(val.vig,1,basis.vig)),sigma=A*REAL.
```

### Affiliation:

Robin K. S. Hankin  
University of Stirling  
Scotland  
E-mail: [hankin.robin@gmail.com](mailto:hankin.robin@gmail.com)