An introduction to stochastic emulation

Andrew Parnell
andrew.parnell@mu.ie

Maynooth University
National University of Ireland Maynooth

https://andrewcparnell.github.io/intro_emulators

Outline

- What are emulators?
- Some jargon and notation
- A simple example
- A reminder on Gaussian Processes
- A more complex example: emulating an SEIR model
- Other complications

What are emulators?

- Suppose we are in a situation where we have a complicated system from which we can simulate
- The system will have input and output variables
- Suppose that the simulations are very slow
- An emulator is a statistical short-cut to the system which produces estimated values of the outputs for a given set of inputs
- Examples include: climate models, power plants, bombs, biological systems, etc

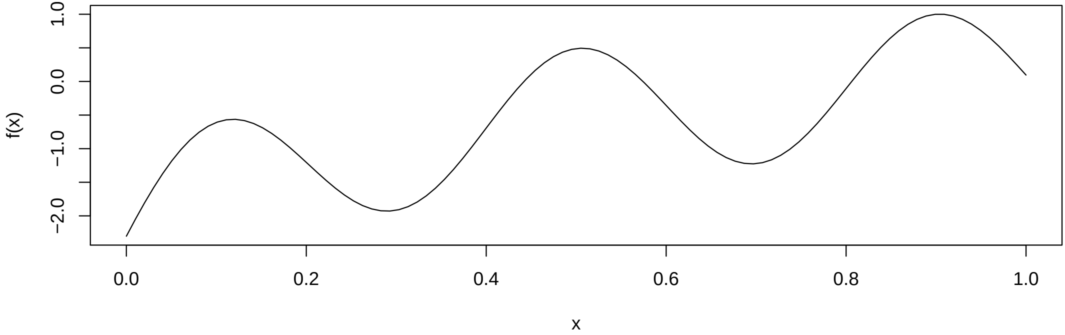
Some jargon and notation

- The complicated system is called the *simulator*
- The statistical short-cut is called the *emulator*
- Let the inputs to the simulator be x, the outputs y, and the simulator f
- Usually the simulator is deterministic so $y = f(x)$ with no noise
- The emulator is $\hat{f}$
- You mission is to find $\hat{f}$ given that it's very expensive to call f

A simple example

Suppose our simulator looked like this:

```r
x = seq(0, 1, length = 100)
f = function(x) log(x+0.1)+sin(5*pi*x)
plot(x, f(x), type = 'l')
```



Building a simple emulator

The usual approach is:

1. Decide on how many runs you can afford
2. Specify a few design points x^* at which to run f. Obtain $y^* = f(x^*)$
3. Fit a *Gaussian Process* to the outputs
4. Use the Gaussian Process to predict where the biggest uncertainties are to specify your next set of design points
5. Repeat from 3 until you have used up all your runs

The final Gaussian Process can be used as the emulator and the simulator can be thrown away!

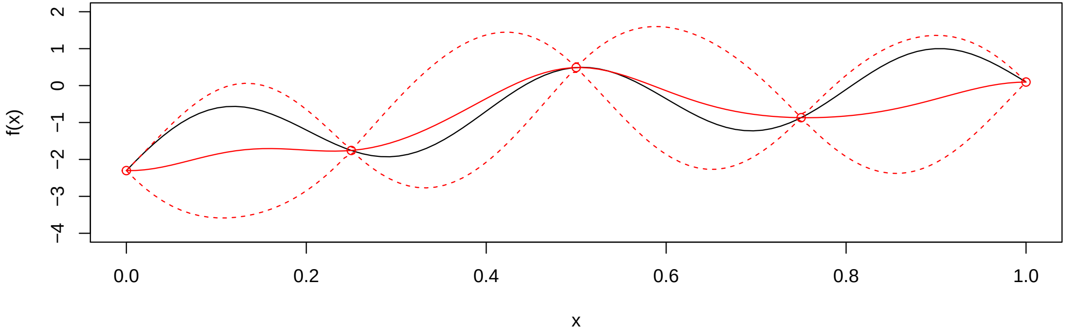
Back to the example

- Suppose we decided that we have 10 points at which to run the emulator, and we would start with 5 runs

```
x_star = seq(0, 1, length = 5)
y_star = f(x_star)
library(GPfit)
f_hat = GP_fit(x_star, y_star)
x_new = seq(0, 1, length = 100)
pred = predict(f_hat ,x_new)
```

Plot

```
plot(x, f(x), type= 'l', ylim = c(-4, 2))
points(x_star, y_star, col = 'red')
lines(x_new, pred$Y_hat, col = 'red')
lines(x_new, pred$Y_hat - 2*sqrt(pred$MSE), lty = 2, col = 'red')
lines(x_new, pred$Y_hat + 2*sqrt(pred$MSE), lty = 2, col = 'red')
```



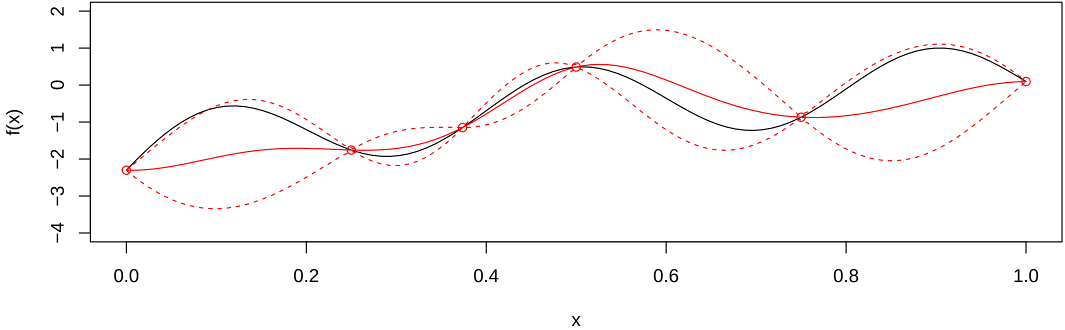
Step 2

- Now find the place (or places) where the simulator has done badly and re-run

```
x_star = c(x_star, x_new[which.max(pred$MSE)])
y_star = c(y_star, f(x_star[6]))
f_hat = GP_fit(x_star, y_star)
x_new = seq(0, 1, length = 100)
pred = predict(f_hat ,x_new)
```

Plot 2

```
plot(x, f(x), type= 'l', ylim = c(-4, 2)); points(x_star, y_star, col = 're
lines(x_new, pred$Y_hat, col = 'red')
lines(x_new, pred$Y_hat - 2*sqrt(pred$MSE), lty = 2, col = 'red')
lines(x_new, pred$Y_hat + 2*sqrt(pred$MSE), lty = 2, col = 'red')
```



. . . and repeat

What is going on in the background?

- The `GPfit` package is fitting a Gaussian Process
- This is the model:

$$y|x \sim MVN(\mu 1, \Sigma);\ \Sigma_{ij} = \tau^2 \rho_\phi (x_i - x_j)^2$$

- So there are 3 parameters: μ, ϕ, τ
- The parameter τ^2 controls the variance of the Gaussian process (bigger values have more uncertainty)
- The parameter ϕ controls how smooth the curve is
- The function ρ controls the correlation function; how the correlation between the y values decreases as x gets further away

Gaussian process predictions

- The GP has a wonderful formula for prediction:

$$\hat{y}^*|y \sim MVN(\mu 1 + \Sigma^* \Sigma^{-1}(y - \mu 1), \Sigma^{**} - \Sigma^* \Sigma^{-1} (\Sigma^*)^T)$$

- Here Σ^* and Σ^{**} are the covariance matrix of the prediction points and their variance respectively
- This means that you can get predicted means and uncertainties from every point

Why Gaussian processes?

- There is nothing special about the fact that it's a Gaussian Process used here. Any statistical model that can produce predictions with quantified uncertainties should be OK
- The nice thing about GPs is that they are smooth which often matches the differential equations underlying the simulator
- The bad thing about them is that they can be slow to fit - we need to solve the covariance matrix when optimising the parameters and predicting

A more complicated example

- Suppose we now want to emulate a more complicated model
- Example: an SEIR infectious disease model that predicts the time to extinction of a disease
- The inputs are the basic reproduction number R_0, the initial number of exposed individuals E, the number of infected individuals I, and the number of recovered individuals so far R
- The output is a set of quantiles for the length of time before the virus is extinct
- The model takes a long time to run

Set up

- I'm willing to run the simulator over 24 hours (maybe 500 runs if well coded)
- I need good values to start the simulator off
- In 4 input dimensions I need the starting values to cover the space well
- Use a Latin hypercube design
- (NB: the `GP_fit` function requires all input values to be scaled between 0 and 1)
- There are other input parameters too but these are fixed values

Building the emulator

1. File `run_simulator.R`
2. File `build_emulator_*.R`
3. File `out_lt1.txt`
4. File `fit_emulator.R`
5. File `run_emulator.R`
6. File `app.R`

Other issues

- Discontinuities in the simulator
- Design of experiments for input space (and adaptive design)
- Priors on input space
- Multivariate responses
- Emulating time series data
- Emulating stochastic systems