BOSS Demo 1
Analytic 1D Function

1 Problem

A one dimensional problem is the simplest case to solve with BOSS. By looking at the plotted GP models step-by-step, it is transparent what is going on in BOSS. Studying a 1D case is also often a part of solving a bigger optimization problem, as short 1D searches of each simulation variable separately gives important insight on how to set up the large problem. In this demo the target function is

$$f(x) = sin(x) + 1.5 * exp[-(x - 4.3)^2], \quad x \in [0, 7]. \tag{1}$$

There is a Gaussian added to a sine wave, which makes up a fairly simple but not trivial non-periodic 1D function. The domain of the variable x is $[0, 7]$ by definition, and because of the sine, the values of $f(x)$ are known to be roughly within $[-1, 1]$. Figure 1 shows the target function, which is easy to construct in the case of an analytic function.

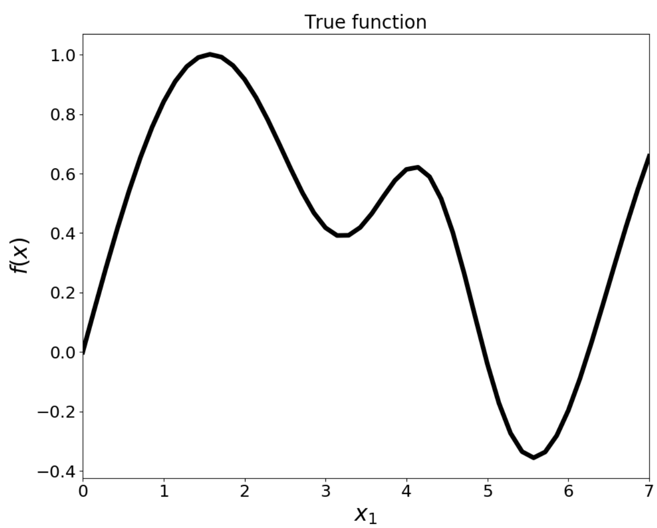


Figure 1: Target function

2 Run instructions

This demo involves BOSS optimization and post-processing starting from scratch. The analytic target function is calculated directly in the python user function script, making it unnecessary to code any external scripts related to evaluating the user function. After following the instructions in this demo, you can compare your BOSS results with the enclosed output files.

Run tasks

1. Read the input file in `templates/` (or build your own) and check the BOSS manual for the meaning of any keywords you do not understand. In this case the input file has been made to include only the most important keywords apart from post-processing.

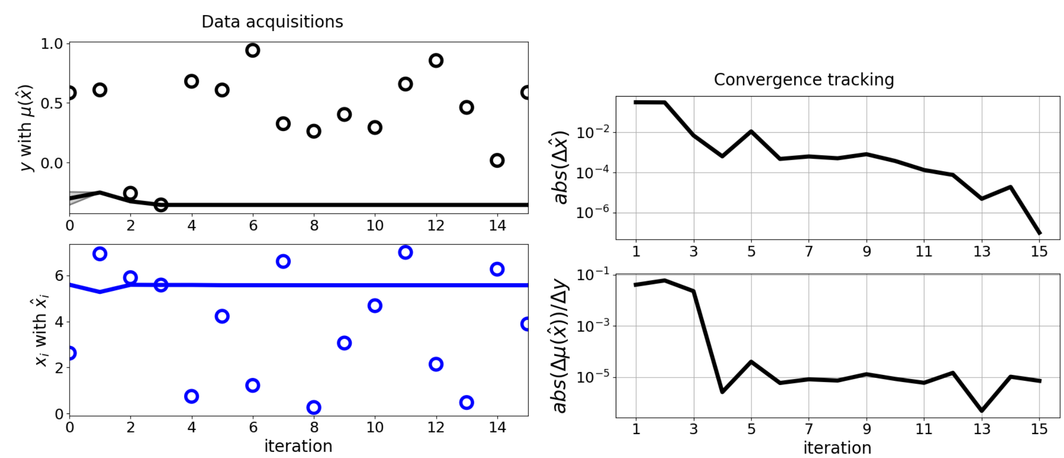
2. Consider the variable boundary and estimated target function values range (keyword `yrange`). Are they set properly? The kernel type should be chosen to be the non-periodic `rbf` (why?).

3. Check also the user function script, although it is very short and simple. Note how the first (and only) variable is accessed with $x[0][0]$.
4. Run boss optimization with post-processing on the input file. Check the produced boss.out and pay attention to the subtitles corresponding to initpts and iterpts, which were defined in the input file. Make sure you have a basic understanding of the quantities printed out for every iteration. Is the global minimum prediction getting closer to what we know it should be based on looking at the target function?
5. Check the figures in the postprocessing directory. Can you determine whether the global minimum prediction has converged, and how many target function evaluations does that roughly take? How about the quality of the model prediction away from the global minimum? Compare your results with the analysis in section 3.
6. Change the verbosity of output (keyword verbosity), and see how it affects the produced boss.out file.

3 Results and Analysis

The convergence of GP model global minimum prediction can be seen from the plots in figure 2. 2a shows the acquisition locations and obtained values with respect to the current global minimum prediction. It is only on iterations 2 and 3, that data is acquired very near the global minimum prediction. After those evaluations, that location is known so well that the sampling method BOSS uses favors exploration for the rest of the run. Thus the global minimum prediction remains almost unchanged since iteration 3, which can be seen in figure 2b as both location and value of minimum prediction change being within 10^{-3} or lower.

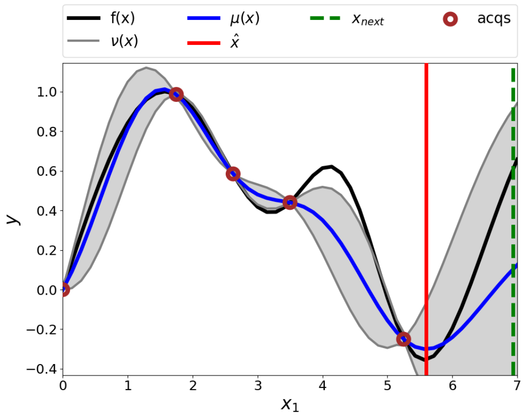
As the target function is 1D and very fast to calculate, it is easy to compare the refined GP model to the target function step-by-step, and make qualitative conclusions about BOSS prediction convergence based on the plots. Looking at figure 3, we can see that the global minimum (indicated by red vertical line) is found on iteration 2, whereas the entire target function is predicted correctly at iteration 5. It is also noteworthy how next sampling points (indicated by green vertical dashed line) are sometimes chosen near the predicted global minimum and sometimes at high uncertainty locations.



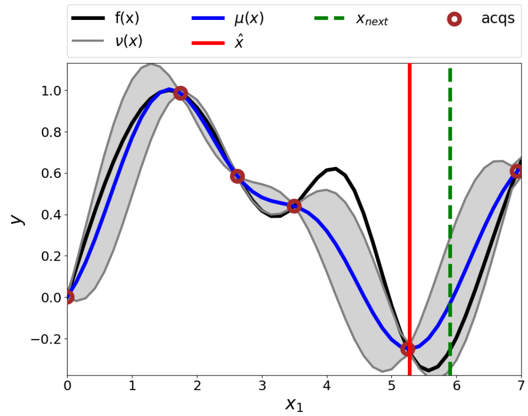
(a) Data acquisitions

(b) Global minimum prediction change

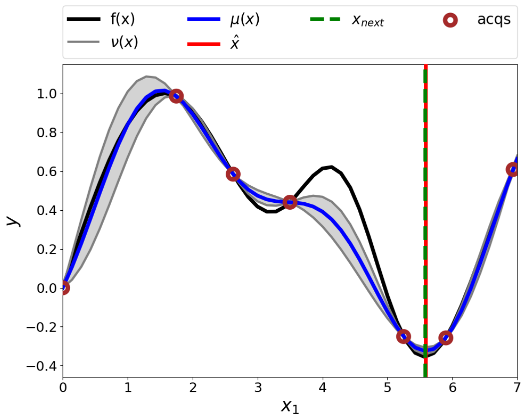
Figure 2: Quantitative analysis graphs of global minimum prediction convergence. (a) shows locations and values of acquisitions compared to global minimum predictions. (b) shows the change in global minimum prediction location and value.



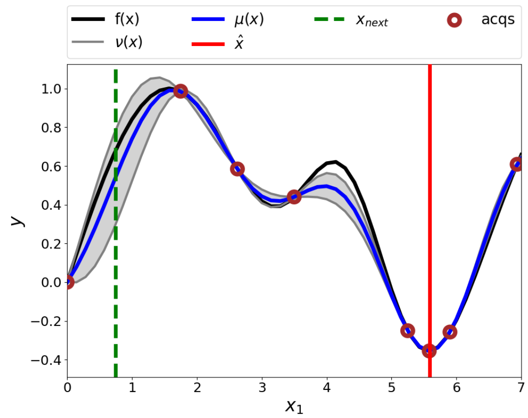
(a) iteration 0



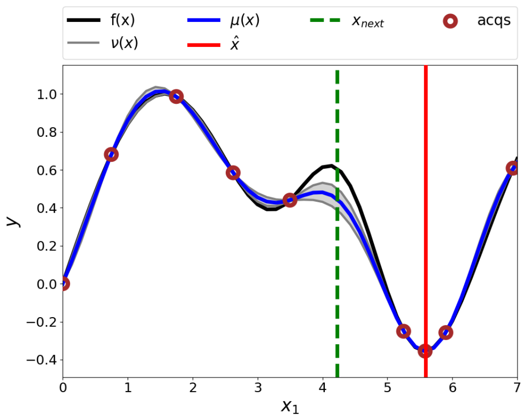
(b) iteration 1



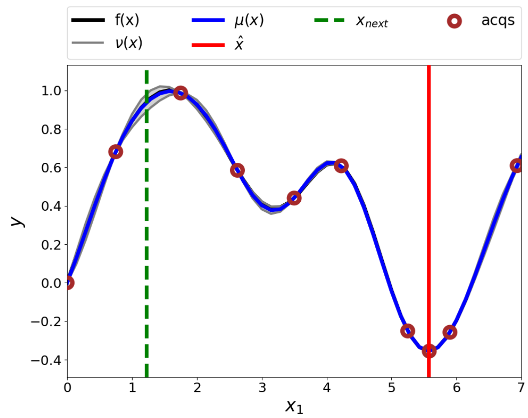
(c) iteration 2



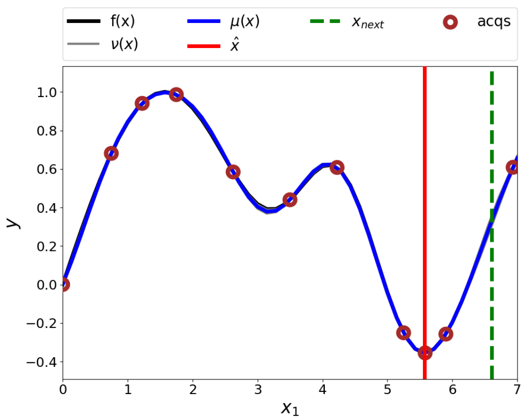
(d) iteration 3



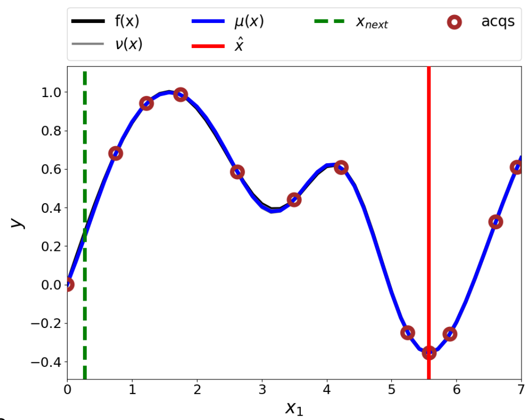
(e) iteration 4



(f) iteration 5



(g) iteration 6



(h) iteration 7

Figure 3: Iterative evolution of the GP model