Exercises 06: Bayesian Optimization

Kevin Heubacher (15329079), Akshay Chikhalkar (15489036),
John Paul Semakula (15487087)

22.11.2022

1 Problem

With this exercise, we aim to make the algorithm more efficient so that it requires fewer steps to find an optimal degree of polynomial features. Bayesian optimization is a sequential design strategy for the global optimization of black-box functions that does not assume any functional forms. It is usually employed to optimize expensive-to-evaluate functions.

2 Formalization

The process of optimization is based on a real-valued objective function defined on a domain X; $f : X \mapsto \mathbb{R}$. Optimization aims to systematically search for the point x^* in the domain X to find the global maximum or minimum value f^*: $f^* = \max f(x) = f(x^*)$.

3 Algorithm

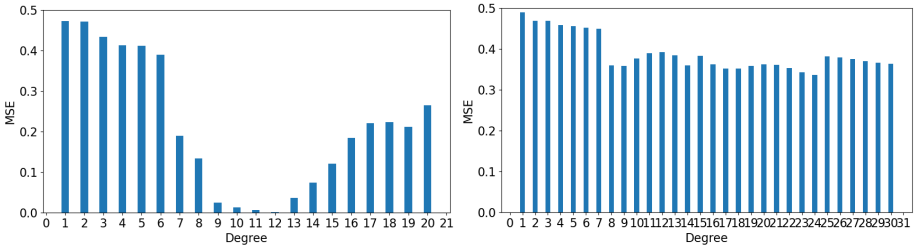
Algorithm 1: Sequential Optimization

Input: Initial sample set **S**
Output: Sample set **S**

repeat
  $x \leftarrow Policy(\mathbf{S})$; `/* Choose next point based on EI */`
  $y \leftarrow Observe(x)$; `/* Observe f(x) */`
  $\mathbf{S} \leftarrow \mathbf{S} \cup \{(x, y)\}$; `/* Join S with new sample */`
until *termination criterion reached*;
return S

4 Results

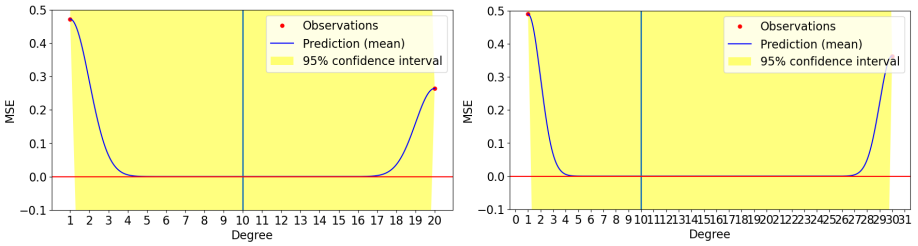
We have taken 2 different values of x_min and x_max.



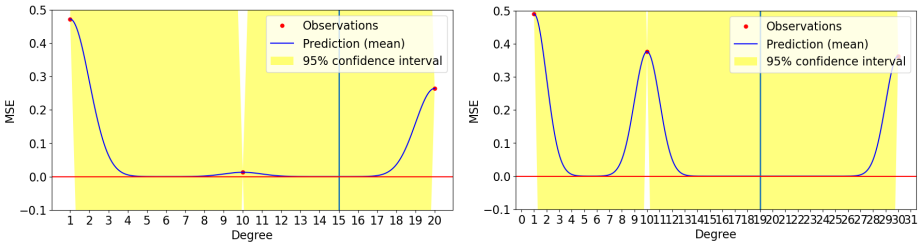
(a) $x\_min = 1$, $x\_max = 20$ (b) $x\_min = 1$, $x\_max = 30$

Figure 1: Bar plots from unoptimised code section

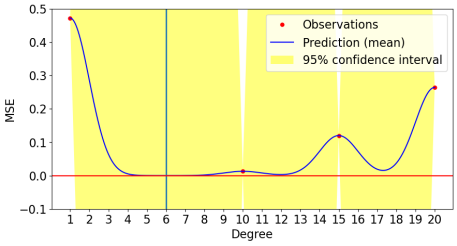
The unoptimised ($x\_min = 1$, $x\_max = 20$) script takes 18 steps and the optimised script ($x\_min = 1$, $x\_max = 20$) with termination criterion $MSE = 0.01$) takes 4 steps to perform Bayesian Optimization.



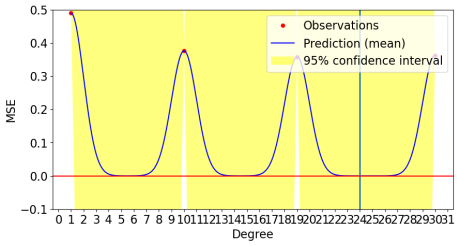
(a) $x\_min = 1$,$x\_max = 20$, $MSE = 0.01$ (b) $x\_min = 1$, $x\_max = 30$,$MSE = 0.35$



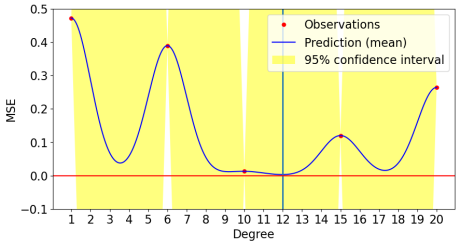
(a) $x\_min = 1$, $x\_max = 20$, $MSE = 0.01$ (b) $x\_min = 1$, $x\_max = 30$, $MSE = 0.35$



(a) $x\_min = 1$, $x\_max = 20$, $MSE = 0.01$



(b) $x\_min = 1$, $x\_max = 30$, $MSE = 0.35$



(c) $x\_min = 1$, $x\_max = 20$, $MSE = 0.35$

5 Conclusion

By applying the exit termination criterion we are able to minimise the number of iterations to find a low mean square value. This results in a reduction in processing costs.