Calibration of computer experiments
Problem 1

Description of the problem

The aim of this problem is to implement the models of Sections 1 and 3 in the lecture slides (calibration without model error and Gaussian process model for the model error, both with a linear approximation of the code). We address here a one-dimensional problem, in order to conveniently plot and interpret the results.

We work on $D = [0, 1]$ and the physical system is, for $x \in D$,

$$\phi(x) = -\sin(\pi x/(1.3)).$$

We consider the linear code function

$$f(x, \boldsymbol{\beta}) = \beta_0 + \beta_1 x,$$

so that $p = 2$. We have, for the prior distribution on $\boldsymbol{\beta}$,

$$\boldsymbol{\beta}_{prior} = \begin{pmatrix} -0.6 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \boldsymbol{Q}_{prior} = \begin{pmatrix} 0.36 & 0 \\ 0 & 0.36 \end{pmatrix}.$$

The choice of the nominal $\boldsymbol{\beta}_{nom}$ is here arbitrary since the code is linear with respect to $\boldsymbol{\beta}$.

We consider $n = 10$ equi-spaced observations, with noise variance $\sigma_m^2 = 0.1^2$.

Part a)

(R code refers here to `Problem_1a.R` unless stated otherwise.)

In this Part a), we only address the model

$$\phi(x) = \sum_{i=1}^{p} \boldsymbol{\beta}_{0,i} h_i(x)$$

of Section 1.

1. Complete `fct_H` in the R code.
2. Complete `y=` in the R code.
3. Plot the physical system function and the code function parameterized by $\boldsymbol{\beta}_{prior}$.
4. Complete `hat_sigma_m=` in the R code.
5. Complete `fct_beta_post` in the R code `functions.R`.
6. Add to the plot the code function parameterized by $\boldsymbol{\beta}_{post}$.
7. Complete `fct_Q_post` in the R code `functions.R`.
8. Complete `cond_var_cont=` in the R code.
9. Add the curve of the 95% confidence intervals for the value of $\phi(x)$, conditionally to $\boldsymbol{y}$ for $x \in [0, 1]$. These confidence intervals are of the form

$$\boldsymbol{h}(x)^t \boldsymbol{\beta}_{post} \pm 1.96 \sqrt{\boldsymbol{h}(x)^t \boldsymbol{Q}_{post} \boldsymbol{h}(x)}.$$

10. Comment the final plot
11. Redo the plot with $n = 50$ and re-comment.

Part b)

(R code refers here to `Problem_1b.R` unless stated otherwise.)

In this Part b), we only address the model

$$\phi(x) = \sum_{i=1}^{p} \boldsymbol{\beta}_{0,i} h_i(x) + Z(x)$$

of Section 3.

We work with the Gaussian covariance function (slide 30) with fixed parameters $\sigma^2 = 1$ and $\ell = 0.5$.

1. Complete `fct_H` in the R code.
2. Complete `y=` in the R code.
3. Plot the physical system function and the code function parameterized by $\boldsymbol{\beta}_{prior}$.
4. Complete `fct_cov_gauss` in the R code `functions.R`.
5. Calculate $\boldsymbol{\beta}_{post}$ and $\boldsymbol{Q}_{post}$ (slide 71). Compare the value of $\boldsymbol{Q}_{post}$ here and the value of $\boldsymbol{Q}_{post}$ in Part a). Redo this comparison with $n = 50$. Comment this in relation with the identifiability of $\boldsymbol{\beta}_0$ in the models in Sections 1 and 3.
6. Add to the plot the code function parameterized by $\boldsymbol{\beta}_{post}$.
7. Complete `fct_hat_phi` and `fct_hat_sigma_2` in the R code `functions.R`.
8. For 100 equi-spaced values of $x_0 \in D$, compute $\hat{\phi}(x_0)$ and $\hat{\sigma}^2(x_0)$, cf slide 73.
9. Add to the plot the curves of $\hat{\phi}(x_0)$ and of the confidence intervals

$$\hat{\phi}(x_0) \pm 1.96\hat{\sigma}(x_0).$$

10. Comment the final plot.
11. Redo the plot with $n = 50$ and re-comment.

Other venues for implementation

With this one-dimensional model, one can consider the following, additionally to the above questions.

1. Changing the simulation parameters.
2. Estimating the covariance parameters by restricted maximum likelihood.
3. Working with a non-linear computer model, and observing what happens graphically.