Calibration of computer experiments
Problem 2

Description of the problem

The aim of this problem is to implement the model of Section 4 in the lecture slides (Gaussian process model for the model error, with a linear approximation of the code, with an iterative linear approximation of the code and without linear approximation of the code). We address here a three-dimensional problem, where we do not plot results but provide predictions indicators (RMSE in slide 65).

We work on $D = [0,1]^3$ (d=3) and the physical system is, for $x \in D$,

$$\phi(\boldsymbol{x}) = x_1 + x_2^2 + (1+x_3)^{0.1+0.6^2} + 1.5(1+x_1)(0.3x_2) - \frac{1.5}{1+x_3^2}.$$

We consider the non-linear code function

$$f(\boldsymbol{x}, \boldsymbol{\beta}) = \beta_1 x_1 + \beta_2^2 x_2^2 + (1+x_3)^{0.1+\beta_3^2}$$

so that $p = 3$. We have, for the prior distribution on $\boldsymbol{\beta}$,

$$\boldsymbol{\beta}_{prior} = \begin{pmatrix} 1 \\ 1 \\ 0.6 \end{pmatrix} \qquad \text{and} \qquad \boldsymbol{Q}_{prior} = \begin{pmatrix} 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{pmatrix}.$$

The nominal code parameter is $\boldsymbol{\beta}_{nom} = \boldsymbol{\beta}_{prior}$.

We consider $n = 50$ observation points independently and uniformly distributed on D, with noise variance $\sigma_m^2 = 0.1^2$.

Questions

(R code refers here to `Problem_2.R` unless stated otherwise.)

We address the model

$$\phi(x) = f(\boldsymbol{x}, \boldsymbol{\beta}_0) + Z(x)$$

of Section 4.

We work with the Matérn 3/2 covariance function (slide 30) with fixed parameters $\sigma^2 = 1$ and $\boldsymbol{\ell} = (0.6, 0.6, 0.6)^t$.

1. Complete `y=` in the R code.
2. Complete `fct_cov_matern_3_2` in the R code `functions.R`.
3. Calculate the RMSE when predicting the physical system for 500 new inputs (uniformly distributed on D) with only the code function calibrated by $\boldsymbol{\beta}_{prior}$.
4. Implement the iterative linearization method of slide 72, with 5 iterations starting at $\boldsymbol{\beta}_{nom}$ above. Comment the convergence.
5. For the 5 $\boldsymbol{\beta}_{nom,i}$ of Question 4, compute the RMSE when predicting the physical system for the 500 new inputs with only the code function calibrated by $\boldsymbol{\beta}_{nom,i}$.
6. For the 5 $\boldsymbol{\beta}_{nom,i}$ of Question 4, compute the Gaussian process prediction $\hat{\phi}(\boldsymbol{x}_0)$ (slide 73) for the 500 new inputs of the physical system above. Compute the 5 corresponding RMSE. Comment on the convergence of the prediction RMSE, along the 5 iterated $\boldsymbol{\beta}_{nom}$.
7. Compute $\boldsymbol{Q}_{post}$ for $\boldsymbol{\beta}_{nom,5}$ obtained at the end of question 4.

8. We now address the exact non-linear calibration and prediction of Section 4. For numerical reasons, when computing pdf, we work with logarithms and substract the largest logarithm to each pdf. More precisely, let (cf slides 74, 75, 76, 77)

$$\bar{p}(\boldsymbol{\beta}_i) = \exp\left(\ln(p(\boldsymbol{\beta}_i)) - \max_{j=1,\dots,N} \ln(p(\boldsymbol{\beta}_j))\right)$$

and

$$\bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i) = \exp\left(\ln(p(\boldsymbol{y}|\boldsymbol{\beta}_i)) - \max_{j=1,\dots,N} \ln(p(\boldsymbol{y}|\boldsymbol{\beta}_j))\right).$$

The we have

$$\tilde{\mathbb{E}}(\boldsymbol{\beta}_0|\boldsymbol{y}) = \frac{\sum_{i=1}^N \boldsymbol{\beta}_i \bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i)\bar{p}(\boldsymbol{\beta}_i)}{\sum_{i=1}^N \bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i)\bar{p}(\boldsymbol{\beta}_i)},$$

$$\tilde{cov}(\boldsymbol{\beta}_0|\boldsymbol{y}) = \frac{\sum_{i=1}^N \boldsymbol{\beta}_i \boldsymbol{\beta}_i^t \bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i)\bar{p}(\boldsymbol{\beta}_i)}{\sum_{i=1}^N \bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i)\bar{p}(\boldsymbol{\beta}_i)} - \tilde{\mathbb{E}}(\boldsymbol{\beta}_0|\boldsymbol{y})\tilde{\mathbb{E}}(\boldsymbol{\beta}_0|\boldsymbol{y})^t$$

and

$$\tilde{\mathbb{E}}(\phi(x_0)|\boldsymbol{y}) = \frac{\sum_{i=1}^N \mathbb{E}(\phi(x_0)|\boldsymbol{y}, \boldsymbol{\beta}_i)\bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i)\bar{p}(\boldsymbol{\beta}_i)}{\sum_{i=1}^N \bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i)\bar{p}(\boldsymbol{\beta}_i)}.$$

Calculate the $\bar{p}(\boldsymbol{\beta}_i)$ and $\bar{p}(\boldsymbol{y}|\boldsymbol{\beta}_i)$ for $N = 10000$ $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_N$ uniformly distributed on $[-1, 2]^3$.

9. Compute $\tilde{\mathbb{E}}(\boldsymbol{\beta}_0|\boldsymbol{y})$ and the diagonal of the matrix $\tilde{cov}(\boldsymbol{\beta}_0|\boldsymbol{y})$.

10. Compare the two previous quantities with those of Questions 4 and 7.

11. Compute $\tilde{\mathbb{E}}(\phi(x_0)|\boldsymbol{y})$ for the N values of x_0. Calculate the resulting RMSE for predicting the physical system at the 500 new input points.

12. Discuss the differences of RMSE between the Gaussian process models with and without the linear approximation of the code.

Other venues for implementation

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

- Changing the simulation parameters.
- Estimating the covariance parameters by restricted maximum likelihood.
- Trying to limit the number of calls to the computer model by building a Kriging model for it.