Uncertainty Quantification course
Homework assignment 11

November 29, 2023

This homework assignment will be graded. Please submit one report (in pdf) per team by email **before** 6 December, in other words send it on 5 December 23:59h at the latest, to `D.T.Crommelin@uva.nl`. Reports sent in after that time will not be considered, instead the minimum grade will be given to the team. Put the names of the team members who were involved in making the assignment on the report.

Reports can have 3 pages maximal length, including figures. Please add a print-out of your Matlab or Python code (with some inline comments) as an appendix to your report, this print-out will not count towards the 3-page maximum.

You are given the following set of data points:

$$\begin{aligned} d &= \{(x_i, y_i) \mid i = 1, 2, \cdots, n = 6\} \\ &= \{(0., 0.), (0.2, 0.59), (0.4, -0.95), (0.6.0.95), (0.8, -0.59), (1., 0)\} \end{aligned}$$

Use the function-space view to construct a Gaussian Process trained on this data set. The data comes from a function which is periodic over $x \in [0, 1]$. Select therefore the following periodic kernel function:

$$k(x, x') = \sigma_f^2 \exp\left[-\frac{2}{l^2}\sin^2\left(\pi\frac{|x - x'|}{T}\right)\right]$$

Here σ_f, l, T are the amplitude, correlation length and period respectively. Use $\sigma_f = 1$, $l = 1$ and $T = 0.5$. Make a 2D contour plot of this kernel.

Draw a small number of prior samples $\mathbf{f}_* = f(\mathbf{x}_*)$ from the prior

$$\mathbf{f} \sim \mathcal{N}(0, K(X_*, X_*)),$$

where $\mathbf{x}_*$ is a vector of 100 equidistant points between 0 and 1. Plot these random samples and verify that they are indeed periodic, and that their pattern is repeated twice (a consequence of $T = 1/2$).

Next, write down the expression for the posterior predictive distribution of $\mathbf{f}_* \mid \mathbf{y}, X, X_*$, and draw 1000 random samples from it, using the same 100-dimensional input vector $\mathbf{x}_*$ that you used for the prior. To do so, use

$$\mathrm{cov}(y_i, y_j) = k(x_i, x_j) + \sigma^2\delta_{ij}$$

for the covariance of the data. Here δ_{ij} is the Kronecker delta and use the nugget $\sigma = 0.01$. Plot the 1000 samples together with the posterior predictive mean, and make another contour plot for the posterior (100×100) covariance matrix.

Finally, make a separate plot with just the posterior mean $\pm$ 2 posterior standard deviations. Use the algorithm based on the Cholesky decomposition, described on page 19 of the book by Rasmussen. Note that this algorithm is point-wise, so you have to compute the scalar mean $\overline{f}_*$ and variance $V[f_*]$ 100 times, once for every point in the vector $\mathbf{x}_*$. Can you show that these expressions based on the Cholesky decomposition are indeed equal to the posterior mean and variance (i.e. equal to Eqs. 2.25 and 2.26 of the book)?