

Computer Lab 1 - GP Regression and Classification

The labs are the only examination, so you should do the labs **individually**.
You can use any programming language you prefer, but do **submit the code**.
Submit a readable report in **PDF** (no Word documents!) or a **JuPyteR notebook**

1. *Heteroscedastic GP regression*

- (a) Consider the following heteroscedastic GP regression

$$\begin{aligned}y_i &= f(\mathbf{x}_i) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma_{n,i}^2) \\f(\mathbf{x}) &\sim \text{GP}(0, k(\mathbf{x}, \mathbf{x}')) \\ \log \sigma_{n,i}^2 &= w_0 + \mathbf{w}_1^T \mathbf{x}\end{aligned}$$

Let \mathbf{X}_* be a matrix of test inputs and \mathbf{f}_* the corresponding mean function values. Implement an algorithm that samples from the joint posterior

$$p(\mathbf{f}_*, w_0, \mathbf{w}_1 | \mathbf{y}, \mathbf{X}, \mathbf{X}_*) = p(\mathbf{f}_* | w_0, \mathbf{w}_1, \mathbf{y}, \mathbf{X}, \mathbf{X}_*) p(w_0, \mathbf{w}_1 | \mathbf{y}, \mathbf{X}, \mathbf{X}_*).$$

Use the prior $(w_0, \mathbf{w}_1)^T \sim N(0, \tau^2 I)$, independent of f .

[Hint: $p(\mathbf{f}_* | w_0, \mathbf{w}_1, \mathbf{y}, \mathbf{X}, \mathbf{X}_*)$ is really close to the formulas (2.22) to (2.24) in the GPML book. The distribution $p(w_0, \mathbf{w}_1 | \mathbf{y}, \mathbf{X}, \mathbf{X}_*)$ is available in closed form and its expression is close to an expression in the GPML book (if you think a little ...). However, $p(w_0, \mathbf{w}_1 | \mathbf{y}, \mathbf{X}, \mathbf{X}_*)$ is not a standard (known) distribution, and you need to use MCMC or HMC, or something else, to simulate from it. It is OK to use a package for MCMC and HMC.]

- (b) Use your code in 1a) to analyze the Lidar data (available on the course web page) with the **Distance** variable as the only covariate/feature in both the mean and variance. Use a squared exponential kernel for f . Set the prior hyperparameters σ_f , ℓ and τ^2 to reasonable values.

2. Poisson GP regression.

- (a) Consider the following Poisson GP regression for count data:

$$y_1, \dots, y_n | f \stackrel{iid}{\sim} \text{Pois}(\exp(f(\mathbf{x})))$$

$$f(\mathbf{x}) \sim \text{GP}(0, k_\theta(\mathbf{x}, \mathbf{x}'))$$

Derive the Laplace approximation of the posterior of f on the training data $\mathbf{f} = \mathbf{f}(\mathbf{X})$.

- (b) Derive the (saddlepoint) approximation of the log marginal likelihood for this model.

3. BONUS QUESTION, ONLY IF YOU HAVE THE TIME AND ENERGY. A more general heteroscedastic GP regression can be of the form

$$y_i = f(\mathbf{x}_i) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \exp(g(\mathbf{x}_i)))$$

$$f(\mathbf{x}) \sim \text{GP}(0, k_{\theta_f}(\mathbf{x}, \mathbf{x}'))$$

$$g(\mathbf{x}) \sim \text{GP}(0, k_{\theta_g}(\mathbf{x}, \mathbf{x}'))$$

where θ_f are kernel hyperparameter for the mean function $f(\mathbf{x})$ and θ_g are hyperparameters for the (log) variance function $g(\mathbf{x})$. Note that noise is heteroscedastic and modelled nonparametrically using an additional GP. Let \mathbf{X}_* be a matrix of test inputs and \mathbf{f}_* the corresponding mean function values, just as in the GPML book. Moreover, let \mathbf{g}_* be the corresponding (log) variances at the test inputs, and finally let \mathbf{g} be the vector of (log) variances at the training inputs. Derive the joint posterior distribution of \mathbf{f}_* , \mathbf{g}_* and \mathbf{g} given some training data \mathbf{y} and \mathbf{X} in the form of the following decomposition

$$p(\mathbf{f}_*, \mathbf{g}_*, \mathbf{g} | \mathbf{X}, \mathbf{y}, \mathbf{X}_*) = p(\mathbf{f}_* | \mathbf{g}_*, \mathbf{g}, \mathbf{X}, \mathbf{y}, \mathbf{X}_*) p(\mathbf{g}_* | \mathbf{g}, \mathbf{X}, \mathbf{y}, \mathbf{X}_*) p(\mathbf{g} | \mathbf{X}, \mathbf{y}, \mathbf{X}_*).$$

[Hint: $p(\mathbf{f}_* | \mathbf{g}_*, \mathbf{g}, \mathbf{X}, \mathbf{y}, \mathbf{X}_*)$ is a standard distribution, and so is $p(\mathbf{g}_* | \mathbf{g}, \mathbf{X}, \mathbf{y}, \mathbf{X}_*)$. The last factor, $p(\mathbf{g} | \mathbf{X}, \mathbf{y}, \mathbf{X}_*)$ can be derived in closed form, but will not be a standard distribution].

HAVE FUN!