Engineering Tripos Part IIB FOURTH YEAR

Coursework 4M24: High-Dimensional MCMC

The performance of MCMC algorithms for high-dimensional problems is analysed in this coursework. The methods seen in the lecture notes: Gaussian random walk Metropolis Hastings (GRW-MH) and the preconditioned Crank-Nicolson (pCN) method) are compared, when sampling latent variables on a 2D domain. Code for the coursework supplied in `functions.py` contains useful functions for generating matrices, plotting, and skeleton code to be completed. The files `simulation.py` and `spatial.py` contain the code to set up the problem and relevant plotting examples.

Part I - Simulation

A Gaussian Process is defined on a 2D domain $\mathbf{x} \in [0,1] \times [0,1]$, and the latent variables are defined as $\mathbf{u} \sim \mathcal{N}(0, K)$, where $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$ and k is a Gaussian covariance function parametrised by a length-scale l.

$$k(\mathbf{x}, \mathbf{x}^{'}) = \exp\left(\frac{-\|\mathbf{x} - \mathbf{x}^{'}\|^2}{2l^2}\right)$$

The coordinates of the latent variables $\{\mathbf{x}_i\}_{i=1}^N$ define the GP prior, and are placed on a regular $D \times D$ grid. We generate the data by observing a subsample of the latent variables, with added observation noise. The task will then be to use the noisy data $\mathbf{v}$ to infer the values of all the latent variables $\mathbf{u}$.

$$\mathbf{v} = G\mathbf{u} + \boldsymbol{\epsilon}$$

Where the matrix G is generated based on the latent variable coordinate locations that are chosen to be observed through random subsampling - the function `get_G` generates this matrix from the subsampling indexes given by the function `subsample`. The observation noise is given by $\boldsymbol{\epsilon} \sim \mathcal{N}(0, I)$.

(a) Sample from the GP prior, and then the observation noise to simulate the data $\mathbf{v}$ - set the parameters $D = 16, l = 0.3$, `subsample_factor` $= 4$. Use the function `plot_3D`, comment on the effect of varying the length-scale parameter on the GP surface. Visualise the prior sample with the data overlaid using `plot_result`.

(b) Complete the functions `log_prior` and `log_continuous_likelihood`, which should return $\ln p(\mathbf{u})$ and $\ln p(\mathbf{v}|\mathbf{u})$ respectively. Complete the TODO sections in the skeleton functions `grw` and `pcn`, which are the GRW-MH and pCN algorithms - see Lectures 5 & 11 for details. Sample from $p(\mathbf{u}|\mathbf{v})$ using both these algorithms (use $n = 10000, \beta = 0.2$), and plot the mean of the inferred $\mathbf{u}$ alongside the data. Visualise the absolute error field between the original $\mathbf{u}$ and the inferred $\mathbf{u}$, comparing the performance of the two algorithms. Comment on the GRW-MH and pCN acceptance rate for low and high-dimensional latent variable spaces (try $D = 4$ and $D = 16$). Vary the parameter β between 0 and 1 - comment on the effect on the acceptance rate. What adverse affect would a very small β have on the samples?

Extension: Demonstrate the robustness of the pCN method to 'mesh refinement' [1] *by increasing the latent dimension size N for a fixed dataset (i.e. refine the mesh), and comparing the acceptance rate to the GRW.*

[1] See Fig 1 from Cotter's paper - https://arxiv.org/abs/1202.0709

Now the model is extended to work on a probit classification problem. The data $\mathbf{v}$ is put through a probit transform to give the vector $\mathbf{t}$, where the i^{th} component is given below. This gives the following form of the likelihood, where Φ is the standard normal CDF.

$$t_i = \begin{cases} 0 & \text{if } v_i \leq 0 \\ 1 & \text{otherwise} \end{cases} \quad , \qquad p(t_i = 1|\mathbf{u}) = \Phi([G\mathbf{u}]_i)$$

(c) Derive the full log-likelihood for the probit classification problem, and use this to complete the function
`log_probit_likelihood` to return $p(\mathbf{t}|\mathbf{u})$. Generate samples from the posterior $p(\mathbf{u}|\mathbf{t})$ using the pCN method. Predict the true class assignments $\mathbf{t}_{\text{true}} = \texttt{probit}(\mathbf{u})$, using a MC (Monte-Carlo) estimate of the predictive distribution (Complete the function `predict_t`). Visualise these simply using the `plot_2D` function, comparing the true assignments to the predictive probabilities.

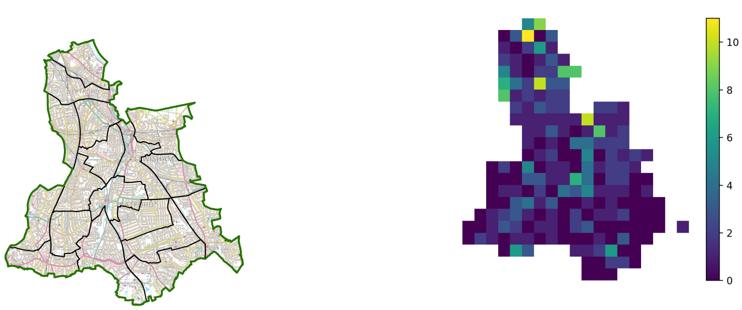
Hint: The predictive distribution is given below, use the samples from the posterior to form a MC estimate of this distribution.

$$p(t^* = 1|\mathbf{t}) = \int p(t^* = 1, \mathbf{u}|\mathbf{t}) d\mathbf{u} = \int p(t^* = 1|\mathbf{u}) p(\mathbf{u}|\mathbf{t}) d\mathbf{u}$$

(d) Now make hard assignments by thresholding the predicted class assignments at $p(t^* = 1|\mathbf{t}) = 0.5$. This can be compared to the true class assignments to give a mean prediction error. Up until now, the true length-scale parameter has been given to the model - you will now attempt to find the parameter through optimisation. Minimise the prediction error with respect to the length-scale parameter, by performing a simple 1D grid-search between $l = 0.01, l = 10$ and plotting the error. Compare this to the true value of l used to generate the data - can the length scale be inferred?

Part II - Spatial Data

This section looks at predicting the number of bike thefts in Lewisham borough (Figure 1a) [2] over 2015. The dataset given in `data.csv` contains a lists of x, y locations of $400m^2$ cells and the corresponding number of bike thefts in that location in 2015. The task is to subsample this count data, then infer the field $\mathbf{u}$ on the original coordinates given this data, and evaluate performance based on predictions of the original data.



(a) Map of Lewisham Borough

(b) Bike theft dataset

Figure 1

[2] https://www.lgbce.org.uk/_flysystem/s3/2018-07/lewisham_0.jpg

The likelihood needed here is the Poisson likelihood. The field $\mathbf{u}$ is mapped to $\mathbb{R}^+$ using the exponential function for positivity, giving $\theta_i = \exp([G\mathbf{u}]_i)$, which is used as the Poisson rate for each data point location. We denote the subsampled count data by the vector $\mathbf{c}$, and the likelihood of $\mathbf{c}$ given the rate parameters at the subsampled locations $\boldsymbol{\theta}$ is shown below:

$$p(\mathbf{c}|\boldsymbol{\theta}) = \prod_{i=1}^{M} f(c_i|\theta_i) = \prod_{i=1}^{M} \frac{e^{-\theta_i}\theta_i^{c_i}}{c_i!}$$

(e) Derive the full Poisson log-likelihood , and use this to complete the function `log_poisson_likelihood` to return $p(\mathbf{c}|\mathbf{u})$. Generate samples from the posterior $p(\mathbf{u}|\mathbf{c})$ using the pCN method.

The inferred expected counts are given by:

$$\mathbb{E}_{p(c^*|\mathbf{c})}[c^*] = \sum_{k=0}^{\infty} k p(c^* = k|\mathbf{c})$$

We have samples from $p(\mathbf{u}|\mathbf{c})$, so using the predictive distribution of bike theft counts at a test location:

$$p(c^* = k|\mathbf{c}) = \int p(c^* = k, \mathbf{u}|\mathbf{c}) d\mathbf{u} = \int p(c^* = k|\mathbf{u}) p(\mathbf{u}|\mathbf{c}) d\mathbf{u}$$

(f) Show that the expectation can be approximated using the MC estimate below, using the fact that $\mathbb{E}_{f(c^\star|\theta^\star)}[c^\star] = \theta^\star$, where $c^\star$ is the count of a test location $\mathbf{x}^\star$, and $\theta^\star$ the respective transformed field value $u^\star$:

$$\mathbb{E}_{p(c^\star|\mathbf{c})}[c^\star] \simeq \frac{1}{n}\sum_{j=1}^{n} \theta^{\star(j)} = \frac{1}{n}\sum_{j=1}^{n} \exp\left(u^{\star(j)}\right)$$

Use this to infer the expected counts and compare these to the bike theft counts from the original dataset. Visualise four plots - the original count data, the subsampled data, the inferred counts, and the error field. Run the model using extreme length-scale parameter values (low and high), and comment on the predicted counts. Suggest a reasonable length-scale value.