CUED - Engineering Tripos Part IIB 2019-2020 **Module Coursework**

Module	**4M24**	Title of report	**High-Dimensional MCMC**
Date submitted: **10/12/2020**		Assessment for this module is ☐ 100% / ☑ **25% coursework** of which this assignment forms **100** %	

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Feedback to the student

☐ **See also comments in the text**

		Very good	**Good**	Needs improvmt
CONTENT	**Completeness, quantity of content:** Has the report covered all aspects of the lab? Has the analysis been carried out thoroughly?			
	Correctness, quality of content Is the data correct? Is the analysis of the data correct? Are the conclusions correct?			
	Depth of understanding, quality of discussion Does the report show a good technical understanding? Have all the relevant conclusions been drawn?			
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PRESENTATION	**Attention to detail, typesetting and typographical errors** Is the report free of typographical errors? Are the figures/tables/references presented professionally?			
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Overall assessment (circle grade)		A*	**A**	B	C	D
Guideline standard		>75%	**65-75%**	55-65%	40-55%	<40%
Penalty for lateness:		*20% of marks per week or part week that the work is late.*				

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4M24 CW - High-Dimensional MCMC

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Abstract

This report outlines the result of the 4M24 coursework on high-dimensional Markov Chain Monte Carlo (MCMC).

Contents

1 Introduction

2 Simulation

a Sampling from a Gaussian Process

We begin with a Gaussian Process (GP) defined on a 2D domain $\boldsymbol{x} \in [0,1]^2$. The realisations from this process are denoted $\boldsymbol{u} \sim \mathcal{N}(0, C)$ where $C_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$ and k is the Squared Exponential (SE) covariance function with length parameter l:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(\frac{-||\boldsymbol{x} - \boldsymbol{x}'||^2}{2l^2}\right) \tag{1}$$

If we specify the latent variables $\{\boldsymbol{x}_i\}_{i=1}^N$, then we can compute C and hence fully specify the prior on u. We choose to place $\{x_i\}_{i=1}^N$ on a $D \times D$ grid with equal spacing, starting at $(0,0)$ and ending at $(1,1)$. Obviously, we require $N = D^2$.

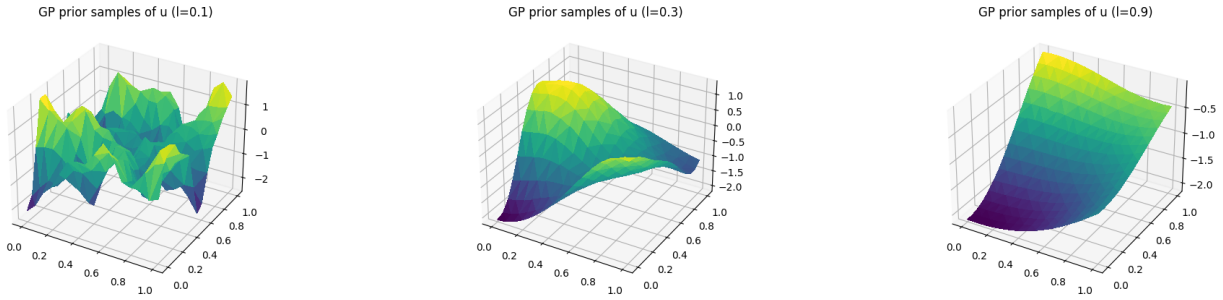
We can now plot the u-surface atop this grid by ensuring that for each $i \in \{1 \dots N\}$, u_i denotes the Z-position and $\boldsymbol{x}_i$ the X-Y-position. We can then investigate the effect of varying the length-scale parameter l. Three settings of l and the associated plots are given in figure 1 for $D = 16$.

We now proceed to make M random draws (denoted by the $M \times 1$ vector $\boldsymbol{v}$) from these samples $\boldsymbol{u}$ with additive Gaussian noise $\boldsymbol{\epsilon} \sim \mathcal{N}(0, I)$. The subsampling factor f is defined as $f \coloneqq N/M$. The draws can be computed as follows:

$$\boldsymbol{v} = G\boldsymbol{u} + \boldsymbol{\epsilon} \tag{2}$$

Where G is an $M \times N$ matrix with a single one in each row in a random location (without repetition) and rest zeros. The result is that the observations $\boldsymbol{v}$ are a jumbled subsample of $\boldsymbol{u}$ with additive noise $\boldsymbol{\epsilon}$. We can plot the data overlaid on the original prior samples by simply matching each entry of $\boldsymbol{v}$ back to the coordinate it was selected from. The result is plotted on figure 2.

We observe $M = N/f = 16^2/4 = 64$ samples contained in the $\boldsymbol{v}$ vector. These are equally likely to appear above or below the $\boldsymbol{u}$-surface as the noise has zero mean. The noise variance for each data-point is of similar magnitude to the variation in



(a) Small $l = 0.1$ (b) Medium $l = 0.3$ (c) Large $l = 0.9$

Figure 1: Samples from GP prior for varying length scales ($D = 16$)

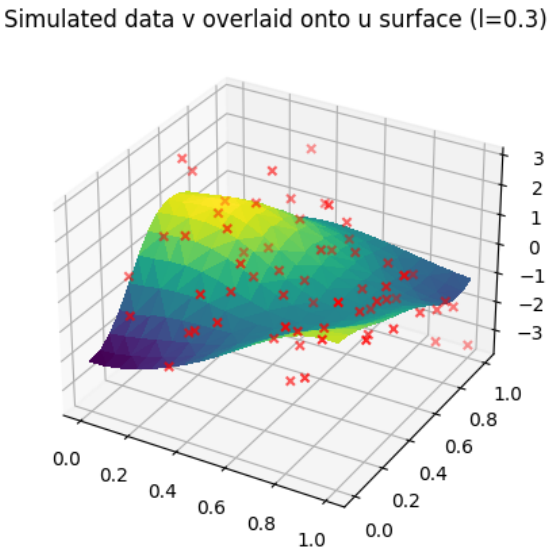


Figure 2: $\boldsymbol{v}$ (red crosses) overlaid on $\boldsymbol{u}$-surface ($f = 4, D = 16, l = 0.3$)

the surface ($\sigma^2 = 1$) so some crosses appear relatively far away from the surface. Moreover, as the subsampling is random, the $\boldsymbol{v}$-points appear at randomly chosen (but distinct) locations X-Y plane.

b Log probabilities and MCMC

We assume that we have realised a set of observations $\boldsymbol{v}$ and it is now our job to determine probability distributions for $\boldsymbol{u}$ based on this information. As a matter of notation, we define the prior function $\pi(\cdot) \coloneqq p(\boldsymbol{u} = \cdot)$ and likelihood function $\lambda(\cdot) \coloneqq \ln p(\boldsymbol{v}|\boldsymbol{u} = \cdot)$. Likewise, we define the posterior $\rho(\cdot) \coloneqq p(\boldsymbol{u} = \cdot|\boldsymbol{v})$.

The log prior can be calculated simply, through manipulation of the Gaussian pdf:

$$\begin{aligned}\ln \pi(\boldsymbol{w}) &= \ln \mathcal{N}(\boldsymbol{w}; 0, C) \\ &= \ln \frac{1}{(2\pi)^{N/2}|C|^{1/2}} \exp\left(-\frac{1}{2}\boldsymbol{w}^T C^{-1}\boldsymbol{w}\right) \\ &= -\left(\frac{N}{2}\ln 2\pi + \frac{1}{2}\ln|C| + \frac{1}{2}\boldsymbol{w}^T C^{-1}\boldsymbol{w}\right)\end{aligned} \tag{3}$$

Likewise, $\boldsymbol{v}|\boldsymbol{u}$ is also a Gaussian such that $\boldsymbol{v}|\boldsymbol{u} \sim \mathcal{N}(G\boldsymbol{u}, I)$ (see equation 2). By comparison with the form of equation 3, we can jump straight to the log-likelihood, noting that $\ln|I| = 0$:

$$\ln \lambda(\boldsymbol{w}) = -\left(\frac{M}{2}\ln 2\pi + \frac{1}{2}(\boldsymbol{v} - G\boldsymbol{w})^T(\boldsymbol{v} - G\boldsymbol{w})\right) \tag{4}$$

From these it is trivial to determine the log-posterior from Bayes' rule:

$$\begin{aligned} \rho(\boldsymbol{w}) &\propto \pi(\boldsymbol{w}) \cdot \lambda(\boldsymbol{w}) \\ \therefore \ln \rho(\boldsymbol{w}) &= \ln \pi(\boldsymbol{w}) + \ln \lambda(\boldsymbol{w}) + \text{const} \end{aligned} \tag{5}$$

It is important to note that, $\boldsymbol{w}$ is simply a dummy variable. We can simplify this notation further by defining $\mathcal{P} \coloneqq \ln \rho + \text{const}$, $\Pi \coloneqq \ln \pi$ and $\Lambda \coloneqq \ln \lambda$. The constant can be chosen to give us:

$$\mathcal{P}(\boldsymbol{\omega}) = \Pi(\boldsymbol{\omega}) + \Lambda(\boldsymbol{\omega}) \tag{6}$$

b.1 Gaussian Random Walk - Metropolis Hastings (GRW-MH)

Armed with the log-posterior (equation 6), observations $\boldsymbol{v}$ and observation matrix G, we can now apply the Gaussian Random Walk Metropolis-Hastings algorithm to draw samples of $\boldsymbol{u}$ from the posterior. We start with an initial estimate drawn from the prior $\boldsymbol{u}^{(0)} \sim p(\boldsymbol{u}) = \mathcal{N}(\boldsymbol{u}; 0, C)$. For simplicity we use the symbol $\boldsymbol{\zeta}^*$ to denote a fresh sample drawn from the prior $\pi \sim \mathcal{N}(0, C)$. It is computed by applying a Cholesky decomposition to the covariance matrix C and multiplying a standard Gaussian vector $\boldsymbol{z} \sim \mathcal{N}(0, I)$. As such:

$$\boldsymbol{\zeta}^* = C^{1/2}\boldsymbol{z} \tag{7}$$

To emphasise, every time $\boldsymbol{\zeta}^*$ appears in an equation we draw a fresh sample according to equation 7. We then pick a symmetric proposal distribution to sequentially generate samples. Given a sample $\boldsymbol{u}^t$ we generate a proposal $\boldsymbol{w}^{(t)}$ as follows:

$$\boldsymbol{w}^{(t)} \coloneqq \boldsymbol{u}^{(t)} + \beta\boldsymbol{\zeta}^* \tag{8}$$

Where β is a hyperparameter that controls the step-size of each iteration. As our proposal distribution is symmetric, the acceptance probability $\alpha^{(t)} \coloneqq \alpha(\boldsymbol{u}^{(t)}, \boldsymbol{w}^{(t)})$ simplifies to the ratio of posteriors (with an upper bound of 1):

$$\alpha(\boldsymbol{u}, \boldsymbol{w}) \coloneqq \min\left(\frac{\rho(\boldsymbol{w})}{\rho(\boldsymbol{u})}, 1\right) \tag{9}$$

It may be more natural to deal in log of this value:

$$\ln \alpha^{(t)} = \min\Big(\mathcal{P}(\boldsymbol{w}^{(t)}) - \mathcal{P}(\boldsymbol{u}^{(t)}), 0\Big) \tag{10}$$

Note that the constant term in the $\mathcal{P}$ definition cancels. Naturally, we can sample a uniform random variable $U \sim \mathcal{U}(0, 1)$ and compare to $\alpha^{(t)}$:

$$\begin{aligned} p(U < \alpha) &= \alpha \\ \therefore p(\ln U < \ln \alpha) &= \alpha \end{aligned} \tag{11}$$

As such the algorithm goes as follows:

Algorithm 1 Gaussian Random Walk - Metropolis Hastings

$\boldsymbol{u}^{(0)} \leftarrow \boldsymbol{\zeta}^*$
for $t \in \{0, 1 \cdots T-1\}$ **do**
  $\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{u}^{(t)} + \beta\boldsymbol{\zeta}^*$ ▷ Generate proposal
  $\ln \alpha^{(t)} \leftarrow \min\big(\mathcal{P}(\boldsymbol{w}^{(t)}) - \mathcal{P}(\boldsymbol{u}^{(t)}), 0\big)$
  $U^{(t)} \leftarrow\sim \mathcal{U}(0, 1)$

  if $\ln U^{(t)} \leq \ln \alpha^{(t)}$ **then**
    $\boldsymbol{u}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)}$ ▷ Proposal accepted
  else
    $\boldsymbol{u}^{(t+1)} \leftarrow \boldsymbol{u}^{(t)}$ ▷ Proposal rejected
  end if
end for

As our algorithm depends only on the difference of the posteriors, there is no need to compute the constant term. This massively speeds up computation.

b.2 Preconditioned Crank-Nicholson (pCN)

Preconditioned Crank-Nicholson is rather similar, except we choose a subtly different proposal distribution:

$$\boldsymbol{\omega}^{(t)} \coloneqq \sqrt{1-\beta^2}\boldsymbol{u}^{(t)} + \beta\boldsymbol{\zeta}^* \tag{12}$$

This changes the form of our acceptance probability subtly by exchanging the log-posterior $\mathcal{P}$ for the log-likelihood Λ. The rest of the algorithm is broadly unchanged:

Algorithm 2 preconditioned Crank-Nicholsons

$\boldsymbol{u}^{(0)} \leftarrow \boldsymbol{\zeta}^*$
for $t \in \{0, 1 \cdots T-1\}$ **do**
  $\boldsymbol{w}^{(t)} \leftarrow \sqrt{1-\beta^2}\boldsymbol{u}^{(t)} + \beta\boldsymbol{\zeta}^*$ ▷ Generate proposal
  $\ln \alpha^{(t)} \leftarrow \min\left(\Lambda(\boldsymbol{w}^{(t)}) - \Lambda(\boldsymbol{u}^{(t)}), 0\right)$
  $U^{(t)} \leftarrow\sim \mathcal{U}(0,1)$

  if $\ln U^{(t)} \leq \ln \alpha^{(t)}$ **then**
    $\boldsymbol{u}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)}$ ▷ Proposal accepted
  else
    $\boldsymbol{u}^{(t+1)} \leftarrow \boldsymbol{u}^{(t)}$ ▷ Proposal rejected
  end if
end for

One advantage is that we do not need to compute the prior probability for each proposal, speeding up computation.

c Probit classification

The model is now extended to work on a probit classification problem. The data $\boldsymbol{v}$ is put through a sign function to give the vector $\boldsymbol{t}$, such that $t_i \coloneqq \text{sign}(v_i)$. As such the likelihood has the following form:

$$\begin{aligned} p(t_i = 1|\boldsymbol{u}) &= p(v_i > 0|\boldsymbol{u}) \\ &= p([G\boldsymbol{u}]_i + \epsilon_i > 0) \\ &= p(-\epsilon_i < [G\boldsymbol{u}]_i) \\ &= \Phi([G\boldsymbol{u}]_i) \end{aligned} \tag{13}$$

Where $\Phi(\cdot)$ is the standard Gaussian CDF (as $-\epsilon_i \sim \epsilon_i \sim \mathcal{N}(0,1)$). Conversely, for the case $t_i = -1$ the likelihood is given by:

$$\begin{aligned} p(t_i = -1|\boldsymbol{u}) &= 1 - p(t_i = 1|\boldsymbol{u}) \\ &= 1 - \Phi([G\boldsymbol{u}]_i) \\ &= \Phi(-1 \cdot [G\boldsymbol{u}]_i) \end{aligned} \tag{14}$$

This means we can simplify the expression for $t_i \in -1, 1$, leading to:

$$p(t_i|\boldsymbol{u}_i) = \Phi(t_i \cdot [G\boldsymbol{u}]_i) \tag{15}$$

We can extend this easily to find the likelihood $\lambda(\cdot)$[1] of the latent variables $\boldsymbol{u}$ given the whole vector of observations $\boldsymbol{t}$:

$$\begin{aligned} \lambda(\boldsymbol{u}) &= p(\boldsymbol{t}|\boldsymbol{u}) \\ &= \prod_{i=1}^{M} p(t_i|\boldsymbol{u}) \\ &= \prod_{i=1}^{M} \Phi(t_i \cdot [G\boldsymbol{u}]_i) \end{aligned} \tag{16}$$

[1]Note that for simplicity we are not changing notation and all previous symbols in the $\boldsymbol{v}$ problem will retain their meaning for the $\boldsymbol{t}$ problem

The second line arises from the fact that $t_i \perp\!\!\!\perp t_j | \boldsymbol{u}$ or more specifically given $G\boldsymbol{u}$. This a direct result of equation 2 as the noise terms ϵ_i are mutually independent. However, instead we find it easier to deal with the log-likelihood $\Lambda(\cdot) \coloneqq \ln \lambda(\cdot)$ as this turns the multiplication into a summation:

$$\begin{aligned} \Lambda(\boldsymbol{u}) &= \sum_{i=1}^{M} \ln \Phi(t_i \cdot [G\boldsymbol{u}]_i) \\ &= \mathbf{1}^T \left[\ln \Phi(\boldsymbol{t} \odot G\boldsymbol{u})\right] \end{aligned} \tag{17}$$

Where $\odot$ denotes element-wise multiplication of vectors, ln and Φ are extended to operate element-wise also and $\mathbf{1}$ is simply the vector of all-ones. This form in equation 17 is very easy to implement using numpy as it is vectorised.

d Length scale inference

3 Spatial Data

a Poisson Likelihood

b Monte Carlo Estimation

Words: XX