

4M24 CW - High-Dimensional MCMC

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1 Simulation

a Gaussian Process Prior

Our prior is a Gaussian Process has zero mean and a squared exponential covariance kernel, $k(\mathbf{x}, \mathbf{x}')$, with length scale ℓ . The coordinates, $\{\mathbf{x}_n\}_{n=1}^N$, of our samples are placed on a regular $D \times D$ grid in $[0, 1]^2$.

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2}\right) \quad (1)$$

Our samples, \mathbf{u} , collected into an $N \times 1$ vector and is distributed $\mathbf{u} \sim \mathcal{N}(\mathbf{0}, C)$, where C is the $N \times N$ covariance matrix with entries $C_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$.

Samples from this prior are shown in Figure 1 for 3 values of ℓ . Larger values result in a smoother surface with more correlation between nearby points.

We subsample the grid with M uniform random draws and apply independent Gaussian measurement noise, ϵ , to the observations. This subsampling can be captured by the $M \times N$ matrix G with entries $G_{ij} = 1$ if the i th observation is at the j th grid point and 0 otherwise. The observations, \mathbf{v} . We also define the subsampling factor $f := N/M$.

$$\mathbf{v} = G\mathbf{u} + \epsilon \quad \epsilon \sim \mathcal{N}(\mathbf{0}, I) \quad (2)$$

One sample is produced from this model with $D = 16$, $f = 4$ and $\ell = 0.3$ to be used as our dataset for the analysis within this section. Figure 2 shows the latent surface, \mathbf{u} , and $M = \frac{N}{f} = 64$ noisy observations, \mathbf{v} .

b Likelihoods and MCMC

We now proceed to infer the latent surface, \mathbf{u} , from the noisy observations, \mathbf{v} , using MCMC. To compute our posterior we need to evaluate the likelihood, $p(\mathbf{v}|\mathbf{u})$, and the prior, $p(\mathbf{u})$. The form of the prior was given previously

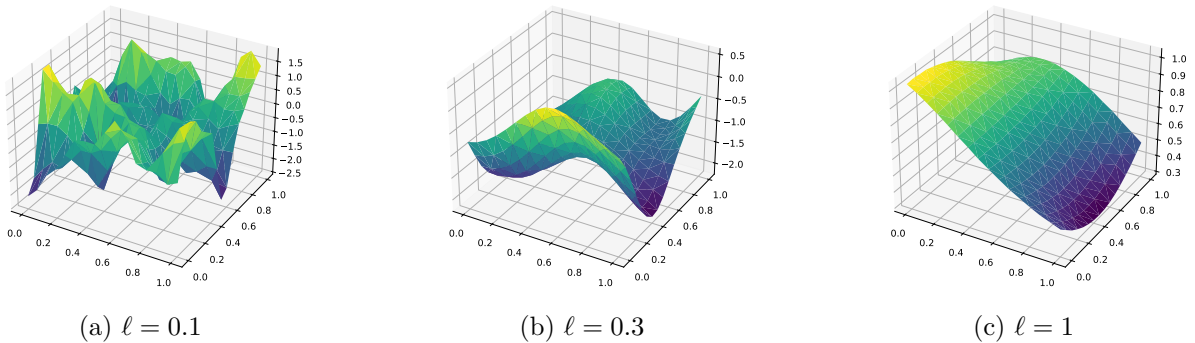


Figure 1: Samples from the Gaussian Process Prior

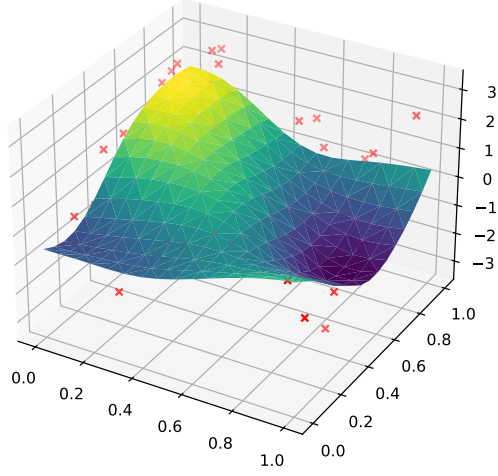


Figure 2: Simulated dataset: \mathbf{v} - red crosses, \mathbf{u} - surface

but is repeated below and its logarithm can be computed with simple algebraic manipulation.

$$\begin{aligned}
 \mathbf{u} &\sim \mathcal{N}(\mathbf{0}, K) \\
 \ln p(\mathbf{u}) &= -\frac{N}{2} \ln(2\pi) - \frac{1}{2} \ln(|K|) - \frac{1}{2} \mathbf{v}^T K^{-1} \mathbf{v} \\
 &= -\frac{1}{2} \mathbf{v}^T K^{-1} \mathbf{v} + \text{const}
 \end{aligned} \tag{3}$$

Likewise the likelihood is given below.

$$\begin{aligned}
 \mathbf{v}|\mathbf{u} &\sim \mathcal{N}(G\mathbf{u}, I) \\
 \ln p(\mathbf{v}|\mathbf{u}) &= -\frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln(|I|) - \frac{1}{2} (\mathbf{v} - G\mathbf{u})^T (\mathbf{v} - G\mathbf{u}) \\
 &= -\frac{1}{2} (\mathbf{v} - G\mathbf{u})^T (\mathbf{v} - G\mathbf{u}) + \text{const}
 \end{aligned} \tag{4}$$

Computation of the posterior is straightforward using Baye's rule. Note that we only need to compute the log-prior and log-likelihood up to a constant which greatly saves on computation.

$$p(\mathbf{u}|\mathbf{v}) \propto p(\mathbf{v}|\mathbf{u})p(\mathbf{u}) \therefore \ln p(\mathbf{u}|\mathbf{v}) = \ln p(\mathbf{v}|\mathbf{u}) + \ln p(\mathbf{u}) + \text{const} \tag{5}$$

We now consider two MCMC algorithms for generating samples from the posterior.

b.1 Gaussian random walk Metropolis-Hastings