

# Part III Astrostatistics: Example Sheet 4

## Example Class: Tuesday, 30 April 2019, 12pm in MR13

So far includes solutions to problem 1, 2, 3, 4.1 & 5.

### 1 Warm-Up

Prove that the product of  $m$  multivariate Gaussian densities in random  $d$ -dimensional vector  $\mathbf{x}$ :

$$I(\mathbf{x}) = \prod_{i=1}^m N(\mathbf{x} | \boldsymbol{\mu}_i, \mathbf{C}_i) \quad (1)$$

is proportional to a single Gaussian density in  $\mathbf{x}$ . Here the  $\{\boldsymbol{\mu}_i\}$  and  $\{\mathbf{C}_i\}$  are  $m$  pairs of constant mean  $d$ -vectors and  $d \times d$  covariance matrices. Find the mean and covariance matrix of the single resulting Gaussian.

**Solution: First, we derive a vectorial “complete the square” lemma:**

$$\begin{aligned} \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{x}^T \mathbf{b} + c &= (\mathbf{x} - \mathbf{d})^T \mathbf{A} (\mathbf{x} - \mathbf{d}) + e = \mathbf{x}^T \mathbf{A} \mathbf{x} - \mathbf{d}^T \mathbf{A} \mathbf{x} - \mathbf{x}^T \mathbf{A} \mathbf{d} + \mathbf{d}^T \mathbf{A} \mathbf{d} + e \\ &= \mathbf{x}^T \mathbf{A} \mathbf{x} - 2\mathbf{d}^T \mathbf{A} \mathbf{x} + \mathbf{d}^T \mathbf{A} \mathbf{d} + e \end{aligned}$$

Therefore,  $\mathbf{d} = -\frac{1}{2} \mathbf{A}^{-1} \mathbf{b}$  and  $e = c - \mathbf{d}^T \mathbf{A} \mathbf{d} = c - \frac{1}{4} \mathbf{b}^T \mathbf{A}^{-1} \mathbf{b}$ .

Now, by definition,

$$\begin{aligned} I(\mathbf{x}) &= \prod_{i=1}^m |2\pi \mathbf{C}_i|^{-\frac{1}{2}} \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_i)^T \mathbf{C}_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i) \right] \\ -2 \log I(\mathbf{x}) &= \text{const} + \sum_{i=1}^m \mathbf{x}^T \mathbf{C}_i^{-1} \mathbf{x} - \mathbf{x}^T \mathbf{C}_i^{-1} \boldsymbol{\mu}_i - \boldsymbol{\mu}_i^T \mathbf{C}_i^{-1} \mathbf{x} + \boldsymbol{\mu}_i^T \mathbf{C}_i^{-1} \boldsymbol{\mu}_i \\ &= \text{const} + \mathbf{x}^T \left[ \sum_{i=1}^m \mathbf{C}_i^{-1} \right] \mathbf{x} - 2\mathbf{x}^T \sum_{i=1}^m \mathbf{C}_i^{-1} \boldsymbol{\mu}_i \end{aligned}$$

Let  $\mathbf{A} = \sum_{i=1}^m \mathbf{C}_i^{-1}$  and  $\mathbf{b} = -2 \sum_{i=1}^m \mathbf{C}_i^{-1} \boldsymbol{\mu}_i$ . We have

$$I(\mathbf{x}) \propto \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_x)^T \mathbf{C}_x^{-1} (\mathbf{x} - \boldsymbol{\mu}_x) \right] \propto N(\mathbf{x} | \boldsymbol{\mu}_x, \boldsymbol{\Sigma}_x)$$

where the resulting precision matrix is the sum of the individual precision matrices,

$$\boldsymbol{\Sigma}_x^{-1} \equiv \sum_{i=1}^m \mathbf{C}_i^{-1}$$

and the resulting mean is the precision-weighted mean of the individual means,

$$\mu_x \equiv \Sigma_x \sum_{i=1}^m C_i^{-1} \mu_i = \left[ \sum_{i=1}^m C_i^{-1} \right]^{-1} \sum_{i=1}^m C_i^{-1} \mu_i$$

## 2 A Hierarchical Bayesian Model for Supernovae and Dust

Consider the following hierarchical Bayesian generative model for supernova colours. The latent intrinsic colour of a supernova  $s$  is  $C_s$  and is drawn from a Gaussian distribution with mean colour  $\mu_C$  and variance  $\sigma_{\text{int}}^2$ :  $C_s \sim N(\mu_C, \sigma_{\text{int}}^2)$ . The latent reddening due to interstellar dust in the supernova's galaxy is  $E_s$ , and is drawn from an exponential distribution with mean  $\tau$ :  $E_s \sim \text{Expon}(\tau)$ , i.e.,

$$P(E_s | \tau) = \tau^{-1} \exp(-E_s/\tau) \times H(E_s), \quad (2)$$

where  $H(x)$  is the Heaviside step function:

$$H(x) = \begin{cases} 1, & x > 0, \\ 0, & x \leq 0. \end{cases} \quad (3)$$

Because the presence of interstellar dust can only redden the colours, the probability density is only positive for  $E_s > 0$ . The measured, observed colour  $\hat{O}_s$  results from the sum of the intrinsic colour, reddening, and measurement error with known variance  $\sigma_{O,s}^2$ :  $\hat{O}_s | E_s, C_s \sim N(C_s + E_s, \sigma_{O,s}^2)$ . There are  $s = 1, \dots, N$  independent supernovae in our sample. For hyperpriors, you may use the improper, noninformative  $P(\mu_C) \propto 1$ ,  $P(\tau) \propto H(\tau)$ , and  $P(\sigma_{\text{int}}^2) \propto H(\sigma_{\text{int}}^2)$ .

1. Write down the joint probability distribution of the observed data  $\{\hat{O}_s\}$ , latent variables  $\{C_s, E_s\}$ , and hyperparameters  $\mu_C, \sigma_{\text{int}}^2, \tau$  for the sample of  $N$  supernovae.

**Solution:** Let us change notation slightly to save typing:  $\mu = \mu_C$ ,  $\sigma^2 \equiv \sigma_{\text{int}}^2$ . The joint probability density is:

$$\begin{aligned} P(\{\hat{O}_s, E_s, C_s\}, \mu, \sigma^2, \tau) \\ = \left[ \prod_{s=1}^N N(\hat{O}_s | C_s + E_s, \sigma_{O,s}^2) N(C_s | \mu, \sigma^2) \text{Expon}(E_s | \tau) \right] \times P(\mu) P(\sigma^2) P(\tau) \end{aligned}$$

For positive  $\tau, \sigma^2$ , this is

$$\begin{aligned} P(\{\hat{O}_s, E_s, C_s\}, \mu, \sigma^2, \tau) \\ = \left[ \prod_{s=1}^N N(\hat{O}_s | C_s + E_s, \sigma_{O,s}^2) N(C_s | \mu, \sigma^2) \text{Expon}(E_s | \tau) \right] \end{aligned}$$

and zero otherwise. QED.

2. Draw a probabilistic graphical model or directed acyclic graph representing this joint distribution. **Solution:** See Figure 1 below.

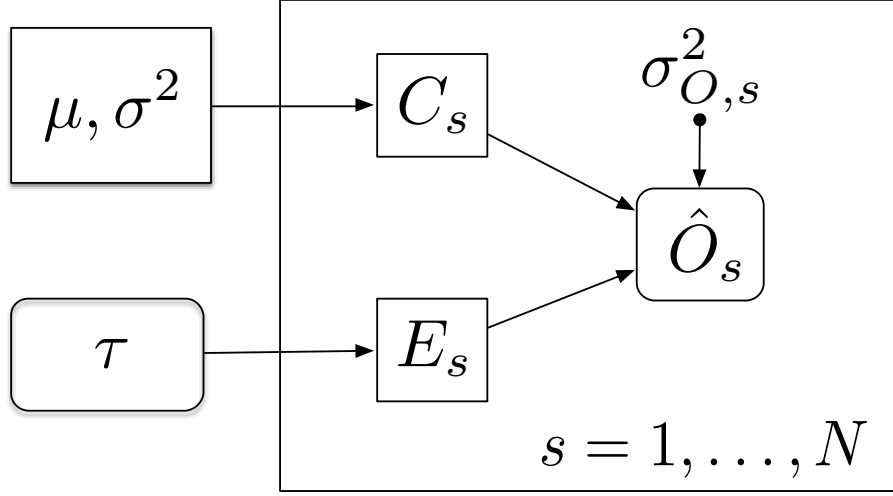


Figure 1: Probabilistic Graphical Model for the Gaussian-Exponential hierarchical Bayesian model for supernovae and dust.

3. Construct a Gibbs sampler that generates an MCMC to sample the joint posterior probability density of the unknown latent variables and hyperparameters given the observed colours,  $P(\{C_s, E_s\}, \mu_C, \sigma^2, \tau | \{\hat{O}_s\})$ , by deriving the  $2N+3$  conditional posterior densities that one can directly sample from. You may assume that you have access to algorithms that allow you to directly sample random variates from the following probability densities:

- Gaussian  $N(x | \mu, \sigma^2)$ .
- truncated Gaussian  $\propto H(x) \times N(x | \mu, \sigma^2)$ .
- Inverse gamma:  $\text{Inv-Gamma}(x | a, b) \propto x^{-(a+1)} \exp(-b/x)$ ,  $x > 0$ .

Briefly describe how you would implement the sampler, and analyse and assess the convergence of the MCMC.

**Solution:** There are several valid Gibbs samplers, and we will present one solution. We will derive the following conditionals from the full joint posterior density:  $P(\{E_s, C_s\}, \mu, \sigma^2, \tau | \mathcal{D})$ , where the data are the measurements  $\mathcal{D} = \{\hat{O}_s\}$ .

- (a)  $P(C_s | \dots; \mathcal{D})$
- (b)  $P(E_s | \dots; \mathcal{D})$
- (c)  $P(\mu, \sigma^2 | \dots, \mathcal{D})$
- (d)  $P(\tau | \dots, \mathcal{D})$ .

We then construct a Gibbs sampler by sampling from each conditional in a sequence.

- (a)  $P(C_s | \dots; \mathcal{D})$ : By inspecting the graph, or the full posterior density, for conditional independence, we see that the posterior conditional for  $C_s$  given

everything else, depends only on  $E_s, \mu, \sigma^2$  and  $\hat{O}_s$ .

$$\begin{aligned}
P(C_s | \dots; \mathcal{D}) &= P(C_s | E_s, \mu, \sigma^2, \hat{O}_s) \\
&\propto N(\hat{O}_s | C_s + E_s, \sigma_{O,s}^2) \times N(C_s | \mu, \sigma^2) \\
&\propto N(C_s | \hat{O}_s - E_s, \sigma_{O,s}^2) \times N(C_s | \mu, \sigma^2) \\
&= N\left(C_s \left| \frac{(\hat{O}_s - E_s)\sigma_{O,s}^{-2} + \mu\sigma^{-2}}{\sigma_{O,s}^{-2} + \sigma^{-2}}, (\sigma_{O,s}^{-2} + \sigma^{-2})^{-1} \right.\right)
\end{aligned}$$

- (b)  $P(E_s | \dots; \mathcal{D})$ : We inspect the graph for conditional independence, or identify the factors in the full posterior that depend on  $E_s$ . We find that the conditional posterior of  $E_s$  only depends on  $C_s, \tau$ , and  $\hat{O}_s$ .

$$\begin{aligned}
P(E_s | \dots; \mathcal{D}) &= P(E_s | C_s; \tau; \hat{O}_s) \\
&\propto N(\hat{O}_s | C_s + E_s, \sigma_{O,s}^2) \times \text{Exponen}(E_s | \tau) \\
&\propto N(E_s | \hat{O}_s - C_s, \sigma_{O,s}^2) \times \tau^{-1} \exp(-E_s/\tau) H(E_s)
\end{aligned}$$

At this step, we expand and combine the exponents of the Gaussian and exponential, express the result as a quadratic in  $E_s$  then “complete the square” to find that the density is proportional to a truncated Gaussian:

$$P(E_s | C_s; \tau; \hat{O}_s) \propto N(E_s | \hat{O}_s - C_s - \sigma_{O,s}^2/\tau, \sigma_{O,s}^2) \times H(E_s)$$

- (c)  $P(\mu, \sigma^2 | \dots, \mathcal{D})$ : Again, by inspection of the graph or the posterior density, we find that this conditional only depends on  $\{C_s\}$ . For  $\sigma^2 > 0$ ,

$$P(\mu, \sigma^2 | \dots, \mathcal{D}) = P(\mu, \sigma^2 | \{C_s\}) \propto \left[ \prod_{s=1}^N N(C_s | \mu, \sigma^2) \right]$$

(and zero otherwise).

$$P(\mu, \sigma^2 | \{C_s\}) \propto (\sigma^2)^{-N/2} \exp\left(-\frac{1}{2\sigma^2} \sum_{s=1}^N (C_s - \mu)^2\right)$$

We perform the trick of adding and subtracting  $\bar{C} = N^{-1} \sum_{s=1}^N C_s$  inside the exponent.

$$\begin{aligned}
P(\mu, \sigma^2 | \{C_s\}) &\propto (\sigma^2)^{-N/2} \exp\left(-\frac{1}{2\sigma^2} \sum_{s=1}^N (C_s - \bar{C} + \bar{C} - \mu)^2\right) \\
&= (\sigma^2)^{-N/2} \exp\left(-\frac{1}{2\sigma^2} [N(\bar{C} - \mu)^2 + (N-1)S^2]\right)
\end{aligned}$$

where  $S^2 = (N-1)^{-1} \sum_{s=1}^N (C_s - \bar{C})^2$ . We can factor this expression into:

$$P(\mu, \sigma^2 | \{C_s\}) = P(\mu | \sigma^2, \{C_s\}) P(\sigma^2 | \{C_s\})$$

where

$$\begin{aligned}
P(\mu | \sigma^2 | \{C_s\}) &\propto \exp\left(-\frac{N}{2\sigma^2} (\bar{C} - \mu)^2\right) \\
&= N(\mu | \bar{C}, \sigma^2/N)
\end{aligned}$$

and  $P(\sigma^2 | \{C_s\}) = \int d\mu P(\mu, \sigma^2 | \{C_s\})$ :

$$\begin{aligned}
P(\sigma^2 | \{C_s\}) &\propto (\sigma^2)^{-N/2} \exp\left(-\frac{N-1}{2\sigma^2} S^2\right) \int d\mu \exp\left(-\frac{N}{2\sigma^2} (\bar{C} - \mu)^2\right) \\
&\propto (\sigma^2)^{-N/2} \exp\left(-\frac{N-1}{2\sigma^2} S^2\right) \sqrt{2\pi\sigma^2/N} \\
&\propto (\sigma^2)^{-(N-1)/2} \exp\left(-\frac{N-1}{2\sigma^2} S^2\right) \\
&= \text{Inv-Gamma}(\sigma^2 | a = (N-3)/2, b = (N-1)S^2/2)
\end{aligned}$$

Thus a draw of  $\mu, \sigma^2 \sim P(\mu, \sigma^2 | \{C_s\})$  is accomplished by first drawing  $\sigma^2 \sim P(\sigma^2 | \{C_s\}) = \text{Inv-Gamma}(\sigma^2 | a, b)$ , then  $\mu | \sigma^2 \sim N(\mu | \bar{C}, \sigma^2/N)$ .

(d) We find  $P(\tau | \dots, \mathcal{D}) = P(\tau | \{E_s\})$ . For  $\tau > 0$

$$\begin{aligned}
P(\tau | \{E_s\}) &\propto \prod_{s=1}^N \tau^{-1} \exp(E_s/\tau) \\
&\propto \tau^{-N} \exp\left(-\sum_{s=1}^N E_s/\tau\right) \\
&= \text{Inv-Gamma}(\tau | a = N-1, b = \sum_{s=1}^N E_s)
\end{aligned}$$

(and zero otherwise).

We build our Gibbs sampler by running through this sequence of steps.

For every  $s = 1, \dots, N$  we draw

$C_s \sim P(C_s | \dots; \mathcal{D})$ , which is a Gaussian draw.

$E_s \sim P(E_s | \dots; \mathcal{D})$ , which is a draw from a truncated Gaussian.

Then we update the hyperparameters  $\mu, \sigma^2$ :

$\sigma^2 \sim P(\sigma^2 | \{C_s\})$  and  $\mu | \sigma^2 \sim P(\mu | \sigma^2, \{C_s\})$ , which are inverse gamma and Gaussian draws, respectively.

Then we update the hyperparameter  $\tau$ :  $\tau \sim P(\tau | \dots, \mathcal{D})$  which is an inverse gamma draw.

This sequence of draws defines a single Gibbs cycle, and we repeat this cycle through convergence of the MCMC until we get a sufficient effective sample size of samples from the posterior.

To run the chain, first we would initialise each chain with randomised, but reasonable starting values near the mode of the posterior. For this model, we could analytically derive the marginal  $P(\mu, \sigma^2, \tau | \mathcal{D})$  and then numerically optimise it to find the mode, and reasonable starting values for the hyperparameters. To diagnose convergence, we run 4 – 8 independent chains from different initial values. We can assess the convergence and mixing of the chains by comparing within-chain variance to between-chain variance using the Gelman-Rubin ratio. The G-R ratio helps us ascertain the initial “burn-in” of each of the chains that needs to be discarded (the chains after removing the burn-in should have

a G-R close to 1). We plot the sample autocorrelation function of the chains in each parameter-dimension to determine the thinning and effective sample size. We find the slowest-mixing parameter by finding the slowest-decaying autocorrelation function. We find the lag (number of Gibbs cycles) after which the samples in this parameter are close to uncorrelated, and choose this as the thinning factor  $t$ . We can use this to compute the Effective Sample Size. We can then thin the chains in all the parameters by only keeping every  $t$ th sample (where a sample is a  $2N + 3$  dimensional vector). If we have sufficient Effective Sample Size, we combine all the chains for analysis to, for example, compute sample posterior expectations and variances in each parameter, or compute histograms or 2D density plots of the joint posterior samples.

4. Apply your sampler to analyse the data from the Table 3 dataset from Jha, Riess & Kirshner. (2007), “Improved Distances to Type Ia Supernovae with Multicolor Light-Curve Shapes: MLCS2k2.” Compute posterior summaries of the hyperparameters  $\mu_C, \sigma_{\text{int}}^2, \tau$  and the latent variables  $\{C_s, E_s\}$ . The data is provided online.

**Solution: Implementing this for  $10^4$  steps, I find the following posterior mean and standard deviation estimates of the hyperparameters.**

$$\hat{\mu} = 1.057 \pm 0.017 \text{ mag}$$

$$\hat{\sigma} = 0.057 \pm 0.017 \text{ mag}$$

$$\hat{\tau} = 0.139 \pm 0.022 \text{ mag}$$

**QED.**

### 3 Harmonic Mean Estimator for Bayesian Evidence

Consider a general Bayesian inference problem with data  $y$ , parameter  $\theta$ , likelihood function  $P(y|\theta)$  and a proper prior  $P(\theta)$ . We wish to compute the evidence or marginal likelihood  $Z \equiv P(y) = \int P(y|\theta) P(\theta) d\theta$ .

1. Suppose you have  $i = 1, \dots, m$  independent, random samples from the posterior distribution,  $\theta_i \sim P(\theta|y)$ . Consider the estimator

$$\hat{I} \equiv \frac{1}{m} \sum_{i=1}^m P(y|\theta_i)^{-1}. \quad (4)$$

Show that  $\mathbb{E}_{\theta|y}[\hat{I}] = Z^{-1}$ , where the expectation is taken with respect to the posterior density  $P(\theta|y)$ . Thus, by LLN, as  $m \rightarrow \infty$ , this converges to the inverse of the evidence.

**Solution: From Bayes’ Theorem, the posterior density is:**

$$P(\theta|y) = \frac{P(y|\theta)P(\theta)}{Z}$$

**Thus, the expectation with respect to the posterior density is:**

$$\begin{aligned} \mathbb{E}_{\theta|y}[\hat{I}] &= \frac{1}{m} \sum_{i=1}^m \mathbb{E}_{\theta|y}[P(y|\theta)^{-1}] \\ &= \frac{1}{m} \sum_{i=1}^m \int \frac{P(y|\theta)P(\theta)}{P(y|\theta)Z} d\theta \\ &= Z^{-1} \int P(\theta) d\theta = Z^{-1} \end{aligned}$$

since the prior is proper and normalised. **QED.**

2. Suppose the sampling distribution of the data is  $y \sim N(\theta, \sigma^2)$  and the proper prior is  $\theta \sim N(0, \tau^2)$ . The measurement variance  $\sigma^2$  and the prior variance  $\tau^2$  are known, and  $\tau \gg \sigma$ .

- (a) What is the posterior density  $P(\theta|y)$ ? **Solution:**

$$\begin{aligned} P(\theta|y) &\propto P(y|\theta)P(\theta) \\ &\propto N(y|\theta, \sigma^2) \times N(\theta|0, \tau^2) \\ &= N(\theta|\tilde{\theta}, \sigma_{\tilde{\theta}}^2), \end{aligned}$$

where  $\sigma_{\tilde{\theta}}^{-2} = \sigma^{-2} + \tau^{-2}$  and  $\tilde{\theta} = \sigma_{\tilde{\theta}}^2(\sigma^{-2}y)$ .

- (b) What is the exact evidence  $Z$ ? **Solution:**

$$Z = P(y) = \int P(y|\theta)P(\theta) d\theta = \int N(y|\theta, \sigma^2) N(\theta|0, \tau^2) d\theta = N(y|0, \sigma^2 + \tau^2)$$

- (c) What is the expectation of the estimator  $\mathbb{E}_{\theta|y}[\hat{I}]$ ? **Solution:**

$$\mathbb{E}_{\theta|y}[\hat{I}] = N(y|0, \sigma^2 + \tau^2)^{-1}$$

- (d) What is the variance of the estimator  $\text{Var}_{\theta|y}[\hat{I}]$ ? **Solution:**

$$\text{Var}_{\theta|y}[\hat{I}] = \text{Var}\left[\frac{1}{m} \sum_{i=1}^m P(y|\theta_i)^{-1}\right] = \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m \text{Cov}[P(y|\theta_i)^{-1}, P(y|\theta_j)^{-1}] = \frac{1}{m} \text{Var}[P(y|\theta)^{-1}].$$

**We need to compute**

$$\begin{aligned} V \equiv \text{Var}[P(y|\theta)^{-1}] &= \mathbb{E}[P(y|\theta)^{-2}] - \mathbb{E}[P(y|\theta)^{-1}]^2 \\ &= \int \frac{P(y|\theta)P(\theta)}{P(y|\theta)^2 Z} d\theta - Z^{-2} \\ &= Z^{-1} \int \frac{P(\theta)}{P(y|\theta)} d\theta - Z^{-2} \\ &= Z^{-1} \int \frac{N(\theta|0, \tau^2)}{N(y|\theta, \sigma^2)} d\theta - Z^{-2} \\ &= Z^{-1} \frac{\sigma}{\tau} R - Z^{-2}. \end{aligned}$$

**The integral of the ratio of the prior to the likelihood is:**

$$R = \int \exp\left(-\frac{1}{2}\theta^2/\tau^2\right) \exp\left(-\frac{1}{2}(y-\theta)^2/\sigma^2\right) d\theta.$$

**By completing the square in  $\theta$  inside the exponent, we have**

$$R = \exp\left(\frac{1}{2}y^2\sigma^{-2}(1 + \sigma^{-2}/a)\right) \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}a(\theta - h)^2\right) d\theta$$

where  $a \equiv (\tau^{-2} - \sigma^{-2})$  and  $h = y\sigma^{-2}/a$ . Note that the integral diverges if  $a < 0$ , i.e. if  $\tau^2 > \sigma^2$ . Otherwise,

$$R = \exp\left(\frac{1}{2}y^2\sigma^{-2}\left[1 + \frac{\sigma^{-2}}{\tau^{-2} - \sigma^{-2}}\right]\right) \frac{\sigma\sqrt{2\pi}}{\sqrt{1 - \tau^2/\sigma^2}},$$

Therefore as  $\tau \rightarrow \sigma$  from below, this integral diverges. For  $\tau^2 > \sigma^2$ , the variance of the estimator is infinite.

## 4 Bayesian Model Comparison

1. Data points  $\{x_i\}$  come independently from a probability distribution  $P(x)$ . According to model  $H_0$ ,  $P(x)$  is a uniform distribution  $P(x|H_0) = \frac{1}{2}$  for  $x \in (-1, 1)$ . According to model  $H_1$ ,  $P(x)$  is a nonuniform distribution with an unknown parameter  $m \in (-1, 1)$ :

$$P(x|m, H_1) = \frac{1}{2}(1 + mx), \quad (5)$$

for  $x \in (-1, 1)$ . Given the data  $\mathcal{D} = \{0.3, 0.5, 0.7, 0.8, 0.9\}$ , what is the evidence for  $H_0$  and  $H_1$ ?

**Solution:** We note that all the observed data points are within the range of the prior. Under model  $H_0$ , we have

$$P(\mathbf{x}|H_0) = \prod_{i=1}^N P(x_i|H_0) = \left(\frac{1}{2}\right)^N$$

Under model  $H_1$ ,

$$\begin{aligned} P(\mathbf{x}|H_1) &= \int dm P(\mathbf{x}|m, H_1) P(m|H_1) \\ &= \int \left[ \prod_{i=1}^N P(x_i|m, H_1) P(m|H_1) \right] dm \\ &= \left(\frac{1}{2}\right)^N \int_{-1}^1 \prod_{i=1}^N (1 + mx_i) dm \\ &= \left(\frac{1}{2}\right)^4 \int_{-1}^1 (1 + mx_1)(1 + mx_2)(1 + mx_3)(1 + mx_4) dm \\ &= \left(\frac{1}{2}\right)^4 \int_{-1}^1 (1 + S_1m + S_2m^2 + S_3m^3 + Pm^4) dm \end{aligned}$$

where  $S_1, S_2, S_3, P$  are functions of  $\mathbf{x}$ . We find:

$$P(\mathbf{x}|H_1) = \frac{1}{8} [1 + S_2/3 + P/5]$$

where  $S_2 \equiv x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4 = 1.91$  and  $P \equiv x_1x_2x_3x_4 = 0.0756$ . Thus  $P(\mathbf{x}|H_1) = 0.2065$  and  $P(\mathbf{x}|H_0) = 0.0625$ , so the Bayes Factor  $B_{10} = P(\mathbf{x}|H_1)/P(\mathbf{x}|H_0) = 3.3$ . According to the Jeffrey's scale this is "significant" evidence for model  $H_1$ .



2. Datapoints  $\{(x_i, t_i)\}$  are believed to come from a straight line. The experimenter chooses  $x_i$ , and  $t_i$  is Gaussian-distributed about  $y_i = w_0 + w_1 x_i$  with variance  $\sigma^2$ . According to model  $H_1$ , the straight line is horizontal, so  $w_1 = 0$ . According to model  $H_2$ ,  $w_1$  is a parameter with prior distribution  $\text{Normal}(0, 1)$ . Both models assign a prior distribution  $\text{Normal}(0, 1)$  to  $w_0$ . Given the data set  $D = \{(-8, 8), (-2, 10), (6, 11)\}$ , and assuming the noise level is  $\sigma = 1$ , what is the evidence for each model?

## 5 Gaussian Processes as Infinite Basis Expansions

Functions drawn from a Gaussian process prior often have an equivalent description as arising from a linear combination of an infinite set of basis functions. Consider a finite set of  $J > 2$  basis functions with a Gaussian shape centred at values  $c_i$ ,

$$\phi_i(x) = \exp \left[ -\frac{(x - c_i)^2}{l^2} \right] \quad (6)$$

defined on the real line  $x \in \mathbb{R}$ . The centres span a distance  $c_J - c_1 = h$ , and the centres are spaced so that  $\Delta c = c_{i+1} - c_i = h/(J - 1)$ . Suppose a function is formed as a linear combination of these functions:

$$f(x) = \sum_{i=1}^J w_i \phi_i(x). \quad (7)$$

Suppose we put a Gaussian prior on the coefficients,  $w_i \sim N(0, \sigma^2 h/J)$ .

1. What is the mean  $\mathbb{E}[f(x)]$  and the covariance function  $k(x, x') = \text{Cov}[f(x), f(x')]$  ?

**Solution: The expectation is**

$$\mathbb{E}[f(x)] = \sum_{i=1}^J \phi_i(x) \mathbb{E}(w_i) = 0 \quad (8)$$

**The kernel is**

$$\begin{aligned} k(x, x') &= \text{Cov}[f(x), f(x')] = \text{Cov} \left[ \sum_{i=1}^J w_i \phi_i(x), \sum_{j=1}^J w_j \phi_j(x') \right] \\ &= \sum_{i=1}^J \sum_{j=1}^J \phi_i(x) \phi_j(x') \text{Cov}[w_i, w_j] \\ &= \sum_{i=1}^J \sum_{j=1}^J \phi_i(x) \phi_j(x') \delta_{ij} \sigma^2 h/J \\ &= \sum_{i=1}^J \phi_i(x) \phi_i(x') \sigma^2 h/J \\ &= \sigma^2 \sum_{i=1}^J \phi_i(x) \phi_i(x') \frac{J-1}{J} \Delta c \end{aligned} \quad (9)$$

where  $\delta_{ij}$  is a Kronecker delta function.

2. Derive the kernel function  $k(x, x')$  in the limit of an infinite number of basis functions spanning the real line:  $J \rightarrow \infty$  and  $c_1 \rightarrow -\infty$ ,  $h \rightarrow \infty$ .

**Solution:** In the limit of  $J \rightarrow \infty$ , this Riemann sum becomes the integral

$$\begin{aligned} k(x, x') &= \sigma^2 \int_{c_1}^{c_J=c_1+h} \phi_i(x) \phi_i(x') dc \\ &= \sigma^2 \int_{c_1}^{c_1+h} e^{-(x-c)^2/l^2} e^{-(x'-c)^2/l^2} dc \end{aligned} \quad (10)$$

Now letting the basis span the real line,  $c_1, h \rightarrow \infty$ , we have

$$k(x, x') = \sigma^2 \int_{-\infty}^{+\infty} e^{-(x-c)^2/l^2} e^{-(x'-c)^2/l^2} dc \quad (11)$$

Noting that

$$e^{-(x-c)^2/l^2} = \frac{l}{\sqrt{2}} \sqrt{2\pi} N(x|c, l^2/2) = \frac{l}{\sqrt{2}} \sqrt{2\pi} N(c|x, l^2/2), \quad (12)$$

we find

$$\begin{aligned} k(x, x') &= \sigma^2 \left( \frac{l}{\sqrt{2}} \sqrt{2\pi} \right)^2 \int_{-\infty}^{+\infty} N(x|c, l^2/2) N(c|x', l^2/2) dc \\ &= \sigma^2 \left( \frac{l}{\sqrt{2}} \sqrt{2\pi} \right)^2 N(x|x', l^2) \end{aligned} \quad (13)$$

We recognised the integral from previous Gaussian marginalisation examples. Finally,

$$k(x, x') = \frac{l\sigma^2}{2} \sqrt{2\pi} e^{-(x-x')^2/2l^2} \quad (14)$$

Therefore, the squared exponential kernel generates functions that are linear combinations of Gaussian functions of width  $l$ , distributed densely along the real line.

3. What is the variance of the resulting Gaussian process at any  $x$ ?

**Solution:**  $\text{Var}(f(x)) = k(x, x) = \sqrt{\frac{\pi}{2}} l \sigma^2$ .