

Chapter 1

Expressing Structure through Kernels

1.1 Derivation of Component Marginal Variance

In this section, we derive the posterior marginal variance and covariance of the additive components of a gp. These formulas let us plot the marginal variance of each component separately. These formulas can also be used to examine the posterior covariance between pairs of components.

Let us assume that our function \mathbf{f} is a sum of two functions, \mathbf{f}_1 and \mathbf{f}_2 , where $\mathbf{f} = \mathbf{f}_1 + \mathbf{f}_2$. If \mathbf{f}_1 and \mathbf{f}_2 are a priori independent, and $\mathbf{f}_1 \sim \text{gp}(\mu_1, k_1)$ and $\mathbf{f}_2 \sim \text{gp}(\mu_2, k_2)$, then

$$\begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_1^* \\ \mathbf{f}_2 \\ \mathbf{f}_2^* \\ \mathbf{f} \\ \mathbf{f}^* \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_1^* \\ \mu_2 \\ \mu_2^* \\ \mu_1 + \mu_2 \\ \mu_1^* + \mu_2^* \end{bmatrix}, \begin{bmatrix} \mathbf{k}_1 & \mathbf{k}_1^* & 0 & 0 & \mathbf{k}_1 & \mathbf{k}_1^* \\ \mathbf{k}_1^* & \mathbf{k}_1^{**} & 0 & 0 & \mathbf{k}_1^* & \mathbf{k}_1^{**} \\ 0 & 0 & \mathbf{k}_2 & \mathbf{k}_2^* & \mathbf{k}_2 & \mathbf{k}_2^* \\ 0 & 0 & \mathbf{k}_2^* & \mathbf{k}_2^{**} & \mathbf{k}_2^* & \mathbf{k}_2^{**} \\ \mathbf{k}_1 & \mathbf{k}_1^* & \mathbf{k}_2 & \mathbf{k}_2^* & \mathbf{k}_1 + \mathbf{k}_2 & \mathbf{k}_1^* + \mathbf{k}_2^* \\ \mathbf{k}_1^* & \mathbf{k}_1^{**} & \mathbf{k}_2^* & \mathbf{k}_2^{**} & \mathbf{k}_1^* + \mathbf{k}_2^* & \mathbf{k}_1^{**} + \mathbf{k}_2^{**} \end{bmatrix} \right) \quad (1.1)$$

where $\mathbf{k}_1 = k_1(\mathbf{X}, \mathbf{X})$ and $\mathbf{k}_1^* = k_1(\mathbf{X}^*, \mathbf{X})$.

By the formula for Gaussian conditionals:

$$\mathbf{x}_A | \mathbf{x}_B \sim \mathcal{N}(\mu_A + \Sigma_{AB} \Sigma_{BB}^{-1} (\mathbf{x}_B - \mu_B), \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA}), \quad (1.2)$$

we get that the conditional variance of a Gaussian conditioned on its sum with another

Gaussian is given by

$$\mathbf{f}_1^* | \mathbf{f} \sim \mathcal{N} \left(\mu_1^* + \mathbf{k}_1^{*\top} (\mathbf{K}_1 + \mathbf{K}_2)^{-1} (\mathbf{f} - \mu_1 - \mu_2), \mathbf{k}_1^{**} - \mathbf{k}_1^{*\top} (\mathbf{K}_1 + \mathbf{K}_2)^{-1} \mathbf{k}_1^* \right). \quad (1.3)$$

The covariance between the two components, conditioned on their sum is given by:

$$\text{cov}(\mathbf{f}_1^*, \mathbf{f}_2^*) | \mathbf{f} = -\mathbf{k}_1^{*\top} (\mathbf{K}_1 + \mathbf{K}_2)^{-1} \mathbf{k}_2^* \quad (1.4)$$

These formulae express the posterior model uncertainty about different components of the signal, integrating over the possible configurations of the other components.