

Note that even if k happens to be a smooth function (this turns out to be a reasonable assumption), the actual realizations $t(x)$, as drawn from the Gaussian process, need not be smooth at all. In fact, they may be even pointwise discontinuous.

Let us have a closer look at the prior distribution resulting from these assumptions. The standard setting is $\mu = 0$, which implies that we have no prior knowledge about the particular value of the estimate, but assume that small values are preferred. Then, for a given set of $(t(x_1), \dots, t(x_m)) =: \mathbf{t}$, the prior density function $p(\mathbf{t})$ is given by

$$p(\mathbf{t}) = (2\pi)^{-\frac{m}{2}} (\det K)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} \mathbf{t}^\top K^{-1} \mathbf{t} \right). \quad (16.38)$$

In most cases, we try to avoid inverting K . By a simple substitution,

$$\mathbf{t} = K\alpha, \quad (16.39)$$

we have $\alpha \sim \mathcal{N}(0, K^{-1})$, and consequently

$$p(\alpha) = (2\pi)^{-\frac{m}{2}} (\det K)^{+\frac{1}{2}} \exp \left(-\frac{1}{2} \alpha^\top K \alpha \right). \quad (16.40)$$

Taking logs, we see that this term is identical to $\Omega[f]$ from the regularization framework (4.80). This result thus connects Gaussian process priors and estimators using the Reproducing Kernel Hilbert Space framework: Kernels favoring smooth functions, as described in Chapters 2, 4, 11, and 13, translate immediately into covariance kernels with similar properties in a Bayesian context.

16.3.3 Simple Hypotheses

Let us analyze in more detail which functions are considered simple by a Gaussian process prior. As we know, hypotheses of low complexity correspond to vectors $\mathbf{y}$ for which $\mathbf{y}^\top K^{-1} \mathbf{y}$ is small. This is in particular the case for the (normalized) eigenvectors $\mathbf{v}_i$ of K with large eigenvalues λ_i , since

$$K\mathbf{v}_i = \lambda_i \mathbf{v}_i \text{ yields } \mathbf{v}_i^\top K^{-1} \mathbf{v}_i = \lambda_i^{-1}. \quad (16.41)$$

In other words, the estimator is biased towards solutions with small λ_i^{-1} . This means that the spectrum and eigensystem of K represent a practical means of actually *viewing* the effect a certain prior has on the degree of smoothness of the estimates.

Let us consider a practical example: For a Gaussian covariance kernel (see also (2.68)),

$$k(x, x') = \exp \left(-\frac{\|x - x'\|^2}{2\omega^2} \right), \quad (16.42)$$

where $\omega = 1$, and under the assumption of a uniform distribution on $[-5, 5]$, we obtain the functions depicted in Figure 16.4 as simple base hypotheses for our estimator. Note the similarity to a Fourier decomposition: This means that the kernel has a strong preference for slowly oscillating functions.

RKHS
Regularization