Posterior Gaussian Process

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Key concepts

- we are not interested in random functions
- we want to *condition* on the training data
- when both prior and likelihood are Gaussian, then
  - posterior is a Gaussian process
  - predictive distributions are Gaussian
- pictorial representation of prior and posterior
- interpretation of predictive equations

Gaussian Process Inference

Recall Bayesian inference in a parametric model.

The posterior is proportional to the prior times the likelihood.

The predictive distribution is the predictions marginalized over the parameters.

How does this work in a Gaussian Process model?

Answer: in our non-parametric model, the "parameters" are the function itself!

Non-parametric Gaussian process models

In our non-parametric model, the "parameters" are the function itself!

Gaussian likelihood, with noise variance σ^2_{noise}

$$p(\mathbf{y}|\mathbf{x}, f, \mathcal{M}_i) \sim \mathcal{N}(\mathbf{f},\ \sigma^2_{\text{noise}} I),$$

Model with 1-input-1-output function:
y = f(x) + sigma_noise* N(0,1)

Gaussian process prior with zero mean and covariance function k

$$p(f|\mathcal{M}_i) \sim \mathcal{GP}(m \equiv 0,\ k),$$

Leads to a Gaussian process posterior

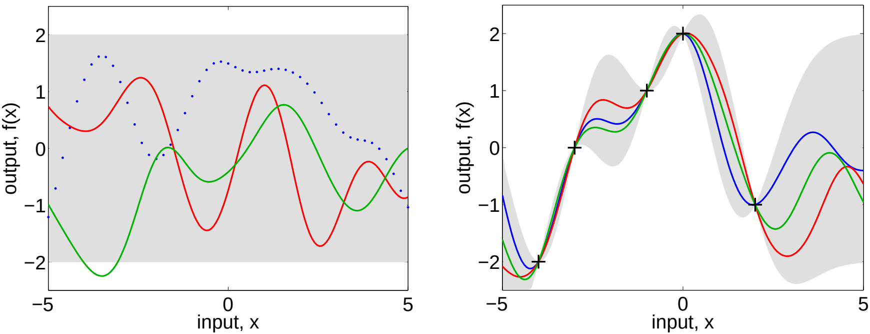
$$p(f|\mathbf{x}, \mathbf{y}, \mathcal{M}_i) \sim \mathcal{GP}(m_{\text{post}},\ k_{\text{post}}),$$

$$\text{where} \begin{cases} m_{\text{post}}(x) = \underline{k}(x, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1}\mathbf{y}, \\ k_{\text{post}}(x, x') = k(x, x') - \underline{k}(x, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1}\underline{k}(\mathbf{x}, x'), \end{cases}$$

And a Gaussian predictive distribution:

$$p(y_*|x_*, \mathbf{x}, \mathbf{y}, \mathcal{M}_i) \sim \mathcal{N}\Big(\underline{\mathbf{k}}(x_*, \mathbf{x})^\top [K + \sigma^2_{\text{noise}} I]^{-1}\mathbf{y},$$
$$k(x_*, x_*) + \sigma^2_{\text{noise}} - \underline{\mathbf{k}}(x_*, \mathbf{x})^\top [K + \sigma^2_{\text{noise}} I]^{-1}\underline{\mathbf{k}}(x_*, \mathbf{x})\Big).$$

Prior and Posterior



Predictive distribution:

$$\begin{aligned} p(y_*|x_*,\mathbf{x},\mathbf{y}) \;\sim\; \mathcal{N}\Big(&\mathbf{k}(x_*,\mathbf{x})^\top[K+\sigma^2_{\text{noise}}I]^{-1}\mathbf{y}, \\ &k(x_*,x_*)+\sigma^2_{\text{noise}}-\mathbf{k}(x_*,\mathbf{x})^\top[K+\sigma^2_{\text{noise}}I]^{-1}\mathbf{k}(x_*,\mathbf{x})\Big) \end{aligned}$$

Some interpretation

Recall our main result:

$$f_*|x_*, \mathbf{x}, \mathbf{y} \;\sim\; \mathcal{N}\big(\cancel{K}(x_*, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1}\mathbf{y},$$
$$\cancel{K}(x_*, x_*) - \cancel{K}(x_*, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1}\cancel{K}(\mathbf{x}, x_*)\big).$$

The mean is linear in two ways:

$$\mu(x_*) \;=\; \mathbf{k}(x_*, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1}\mathbf{y} = \sum_{n=1}^{N} \beta_n y_n \;=\; \sum_{n=1}^{N} \alpha_n k(x_*, x_n).$$

The last form is most commonly encountered in the kernel literature.

The variance is the difference between two terms:

$$V(x_*) \;=\; k(x_*, x_*) - \mathbf{k}(x_*, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1}\mathbf{k}(\mathbf{x}, x_*),$$

the first term is the *prior variance*, from which we subtract a (positive) term, telling how much the data $\mathbf{x}$ has explained.
Note, that the variance is independent of the observed outputs $\mathbf{y}$.