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!
The joint distribution

$$p(f, \mathbf{y}) = p(f)\, p(\mathbf{y}|f) = p(\mathbf{y}) p(f|\mathbf{y})$$
$$\implies \mathcal{N}(f|m,\ k)\, \mathcal{N}(\mathbf{y}|\mathbf{f}) = Z_{|\mathbf{y}} \mathcal{N}(f|m_{|\mathbf{y}}, k_{|\mathbf{y}}).$$

Gaussian process prior with zero mean and covariance function k

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

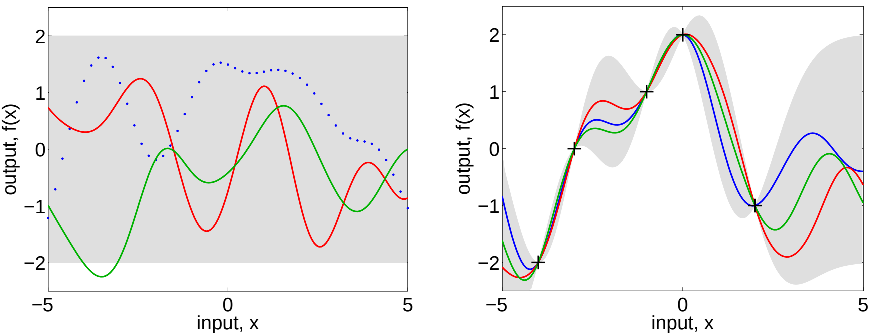
Gaussian likelihood, with noise variance σ^2_{noise}

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

leads to a Gaussian process posterior

$$p(f|\mathbf{y}, \mathcal{M}_i) \sim \mathcal{N}(f|m_{|\mathbf{y}},\ k_{|\mathbf{y}}),$$
$$\text{where} \begin{cases} m_{|\mathbf{y}}(x) = k(x, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1} y, \\ k_{|\mathbf{y}}(x, x') = k(x, x') - k(x, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1} k(\mathbf{x}, x'). \end{cases}$$

Prior and Posterior



Predictive distribution:

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

Some interpretation

Recall our main result:

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

The mean is linear in two ways:

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

The last form is most commonly encountered in the kernel literature.
The variance is the difference between two terms:

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

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 y.