Nonparametric Bayesian Methods

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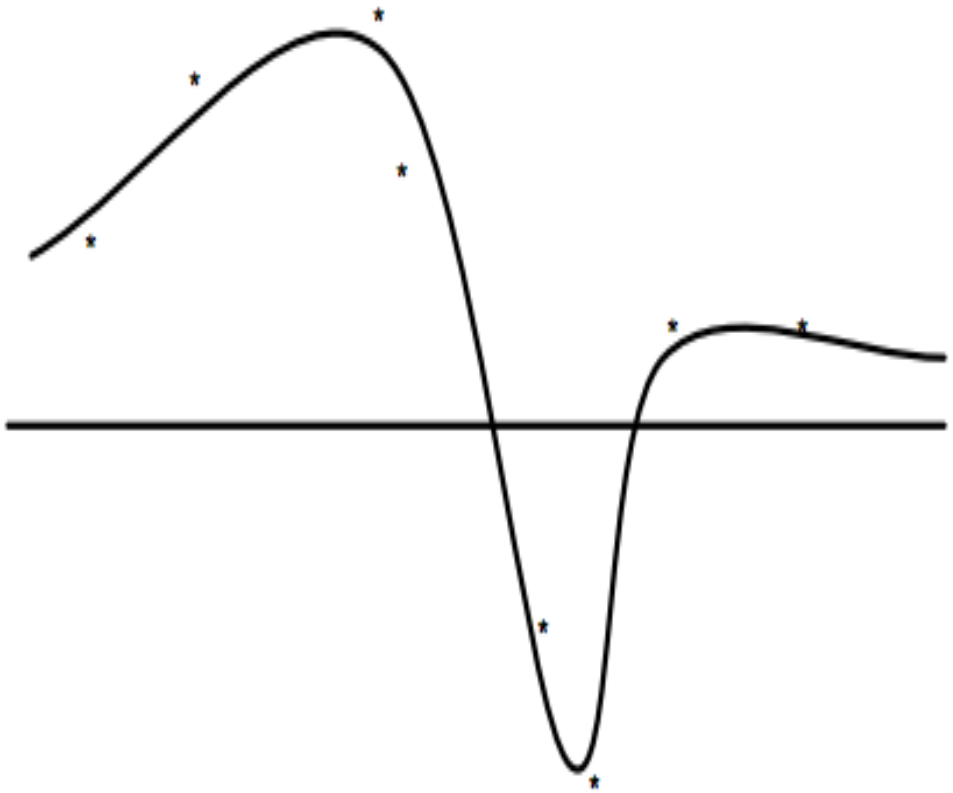
Example 1: Regression

- learning function $f_0 : \mathbb{X} \to \mathbb{Y}$ from training data $\{x_i, y_i\}$.



Regression with Basis Functions

- Assume a set of basis functions $\phi_1, \ldots, \phi_K$ and parameterize a function

$$f(x, \mathbf{w}) = \sum_{k=1}^{K} w_k \phi_k(x)$$

  Parameters $\mathbf{w} = \{w_1, \ldots, w_K\}$.
- Find optimal parameters

$$\text{argmin}_{\mathbf{w}} \sum_{i=1}^{n} \left| y_i - \sum_{k=1}^{K} w_k \phi_k(x_i) \right|^2$$

- As a Bayesian,

$$\begin{aligned} y_i \mid x_i, \mathbf{w} &= f(x_i, \mathbf{w}) + \epsilon_i, \quad \epsilon_i \sim \mathrm{N}(0, \sigma^2) \\ w_k &\sim \mathrm{N}(0, \tau^2) \end{aligned}$$

- Compute posterior $p(\mathbf{w} \mid \{x_i, y_i\})$

Regression with Basis Functions

- What basis functions to use?
- How many basis functions to use?
- Do we really believe that the true $f_0(x)$ can be expressed as $f_0(x) = f(x; \mathbf{w_0})$ for some $\mathbf{w_0}$
- Also $\epsilon_i \sim \mathrm{N}(0, \sigma^2)$. Do we really believe that the noise process is Gaussian?

Gaussian process: a prior for function spaces

- A GP defines a distribution over functions, f, where f is a function mapping some input space $\mathbb{X}$ to $\mathbb{R}$, $f : \mathbb{X} \to \mathbb{R}$. Let's call it $P(f)$.
- Mean and cov function: $m : \mathbb{X} \to \mathbb{R}, c : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$. p.d. function
- $P(f)$ is a Gaussian process if for any finite subset $\{x_1, \ldots, x_n\} \subset \mathbb{X}$, the marginal distribution over that finite subset $P(f)$ has a multivariate Gaussian distribution.

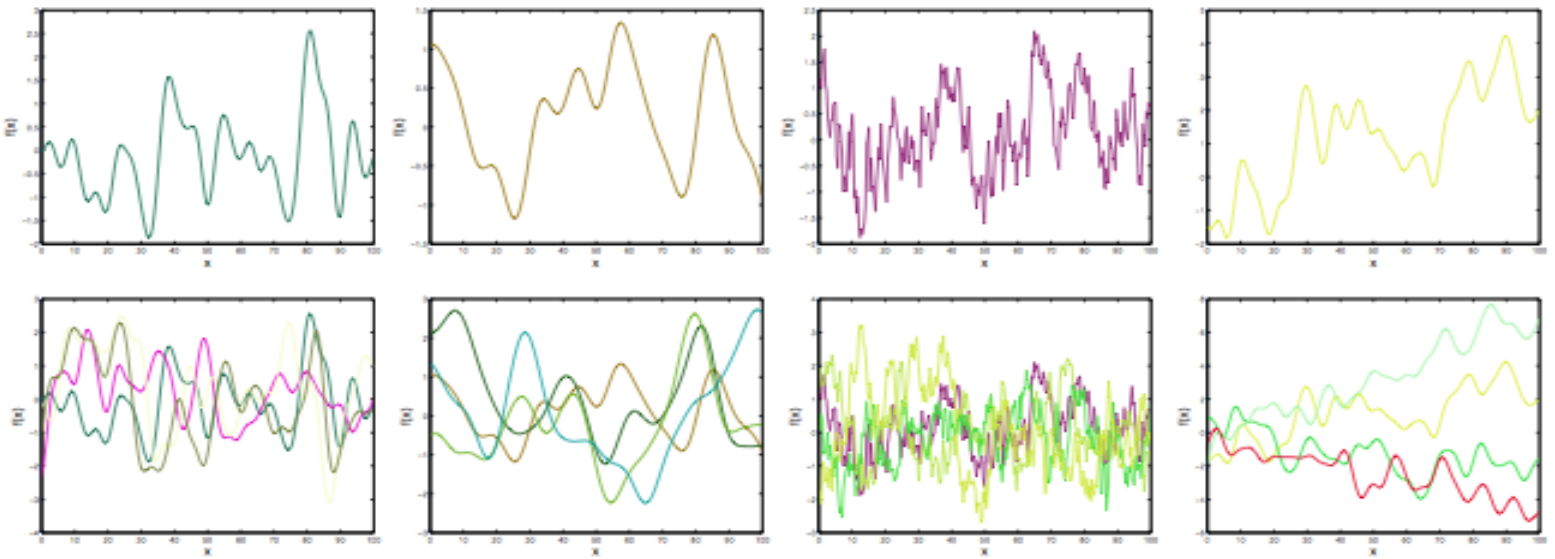
$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix} \sim \mathrm{N}\left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_n) \end{bmatrix}, \begin{bmatrix} c(x_1, x_2) & \cdots & c(x_1, x_n) \\ \vdots & \ddots & \vdots \\ c(x_n, x_1) & \cdots & c(x_n, x_n) \end{bmatrix} \right)$$

- A random function f is a stochastic process. It is a collection of random variables $\{f(x) : x \in \mathbb{X}\}$ one for each possible input value x (Kolmogorov Extension Theorem).

Gaussian process: a prior for function spaces

- E.g. $c(x_i, x_j) = v_0 \exp\{-\kappa|x_i - x_j|^\alpha/\lambda\}$, Gaussian kernel for $\alpha = 2$

Figure: Sample paths of a GP



Gaussian process: why flexible

- Realizations of a GP

$$\{g : g(x) = \sum_{k=1}^{K} w_k C(x, x_k), (x_1, \ldots, x_k) \subset \mathbb{X}, k \in \mathbb{N}, w_k \in \mathbb{R}\}$$

- Heuristics: We want to approximate an arbitrary function $f_0 : \mathbb{X} \to \mathbb{R}$. Setting $c(x, x') = \phi_\sigma(x - x')$, $w_k = f_0(x_k)$

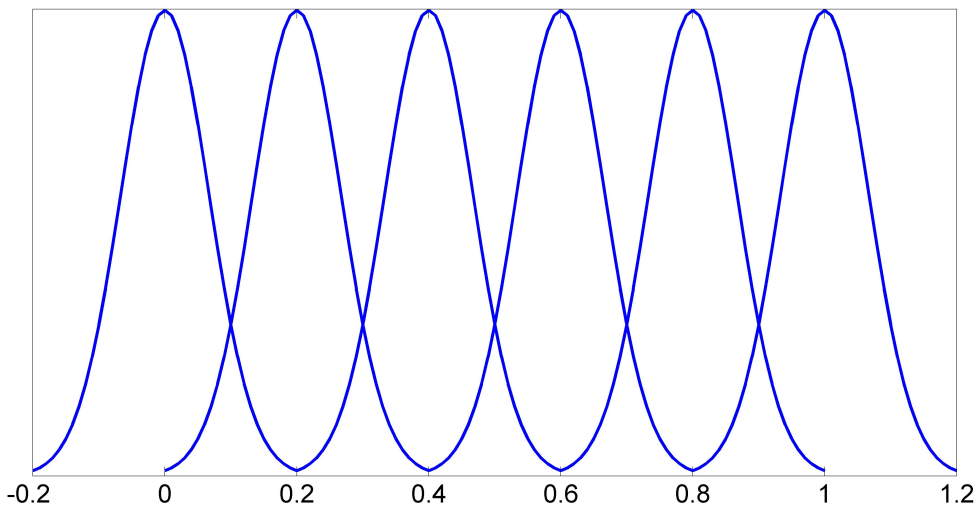
$$\sum_{k=1}^{K} w_k \phi_\sigma(x - x_k) = \sum_{k=1}^{K} f_0(x_k)\phi_\sigma(x - x_k) \approx \phi_\sigma \star f_0 \to f_0 \, as \, \sigma \to 0.$$

RKHS of Gaussian processes

- The RKHS $\mathbb{H}$ is the completion of the linear space

$$f(t) = \sum_{h=1}^{m} a_h C(s_h, t),\ s_h \in [0,1],\ a_h \in \mathbb{R}$$

- Illustration with the squared exponential kernel $C(s,t) = \exp(-\kappa|s-t|^2)$



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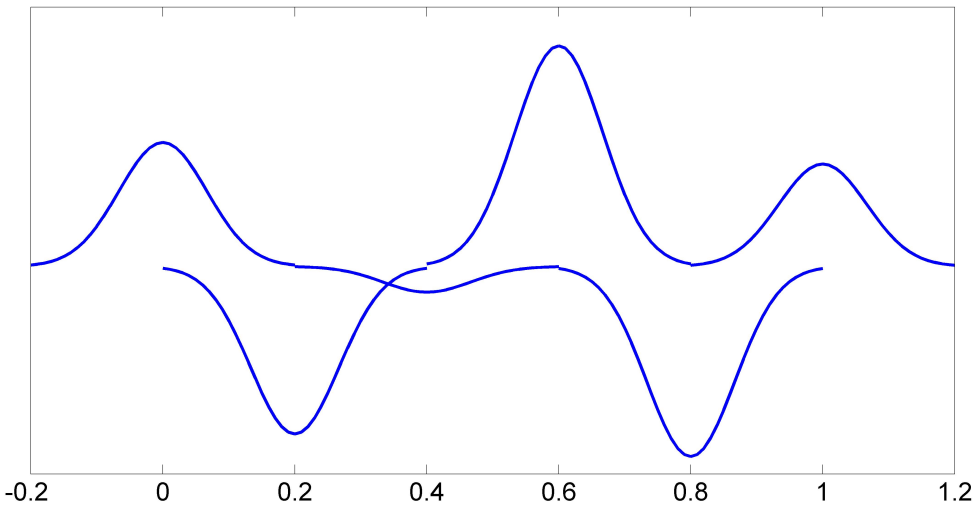
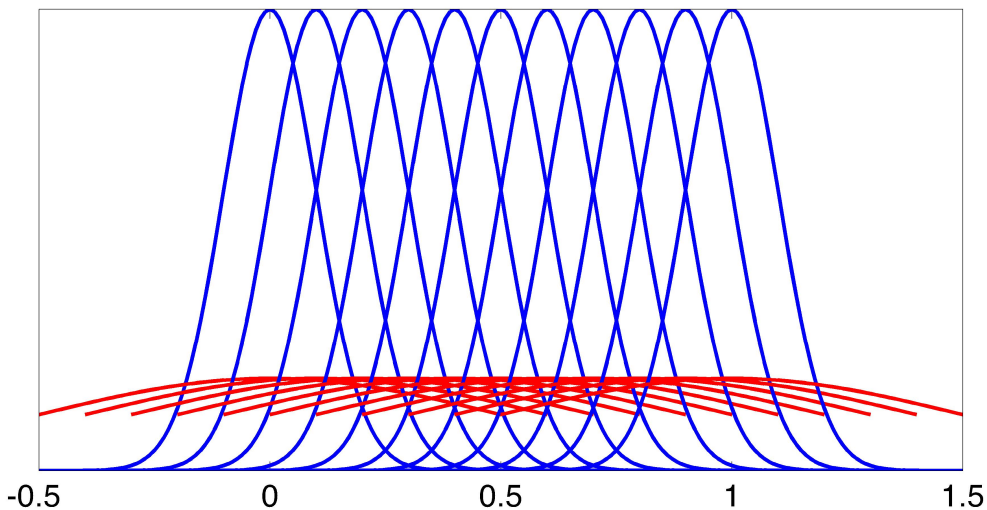


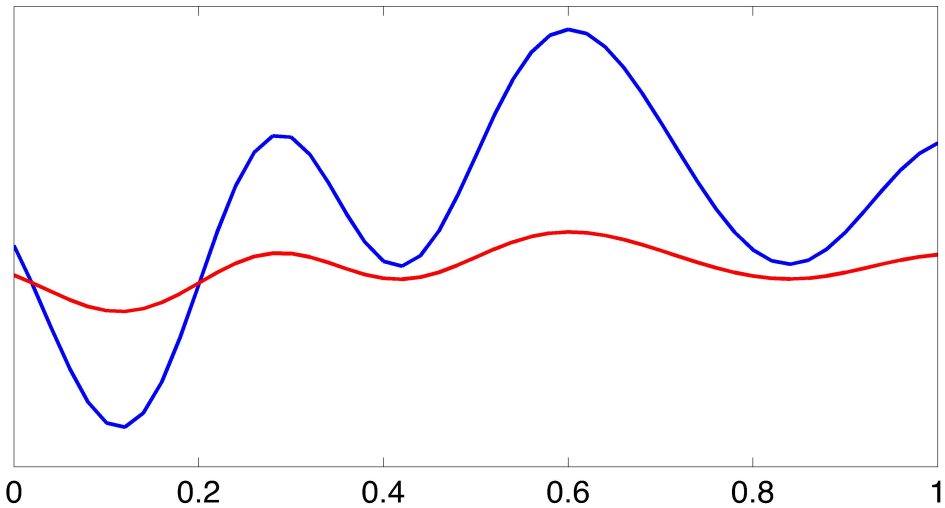
Why scaling works

- A or κ plays the role of an inverse-bandwidth
- Large A implies more peaked kernels
- Stretching the sample paths



Why scaling works

- A or κ plays the role of an inverse-bandwidth
- Large A enables approximation of rougher functions from the RKHS



- van der Vaart & van Zanten (2008): If $A^D \sim \text{gamma}(a, b)$, optimal rate of convergence adaptively over $C^\alpha[0,1]^D$ for any $\alpha > 0$

Gaussian process: posterior and posterior predictive

- How do we compute the posterior and predictive distributions?
- Training set $(x_1, y_1), (x_2, y_2), \ldots, (x_n; y_n)$ and test input x_{n+1}.
- Out of the uncountably many random variables $\{f(x) : x \in \mathbb{X}\}$ making up the GP only $n+1$ has to do with the data: $f(x_1), f(x_2), \ldots, f(x_{n+1})$
- Training data gives observations $f(x_1) = y1, \ldots, f(x_n) = y_n$. The predictive distribution of $f(x_{n+1})$ is simply

$$p(f(x_{n+1}) \mid f(x_1) = y_1, \ldots, f(x_n) = y_n)$$

which is easy to compute since $f(x_1), f(x_2), \ldots, f(x_{n+1})$ is multivariate Gaussian.

Posterior and posterior predictive for noise free observations

- Suppose we know $\{(x_i, f_i), i = 1, \ldots, n\}$
- The joinprior distribution of the training outputs, f, and the test outputs f_* according to the prior is

$$\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathrm{N}\left(\mathbf{0}, \begin{bmatrix} C(X, X) & C(X, X_*) \\ C(X_*, X) & C(X_*, X_*) \end{bmatrix}\right)$$

- If there are n training points and n_* test points then $C(X, X_*)$ denotes the $n \times n_*$ matrix of the covariances evaluated at all pairs of training and test points, and similarly for the other entries $C(X, X)$, $C(X_*, X_*)$ and $C(X_*, X)$.

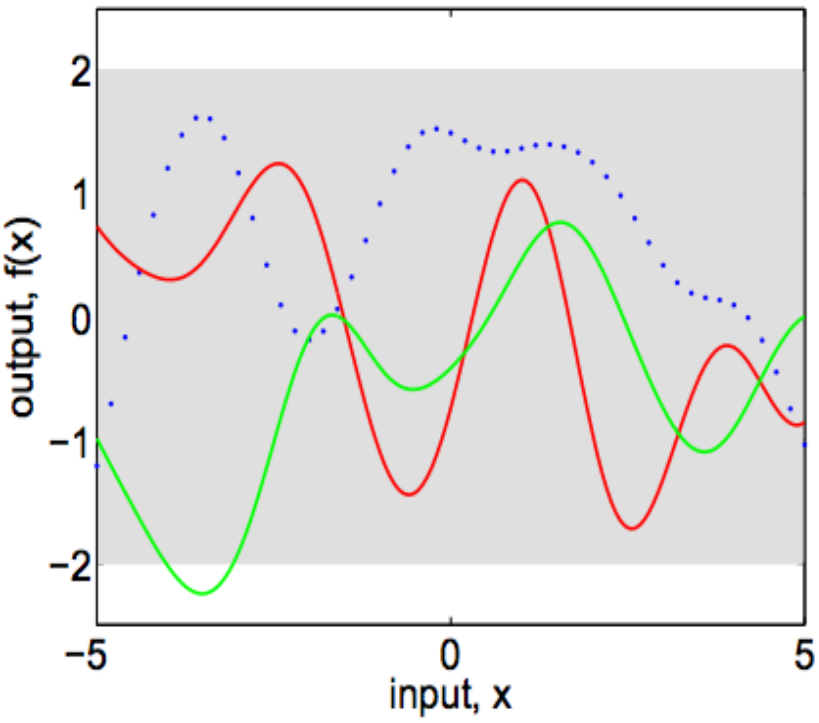
Posterior predictive for noise free observations

- Graphically you may think of generating functions from the prior, and rejecting the ones that disagree with the observations, although this strategy would not be computationally very efficient.
- Fortunately, in probabilistic terms this operation is extremely simple, corresponding to conditioning the joint Gaussian prior distribution on the observations to give

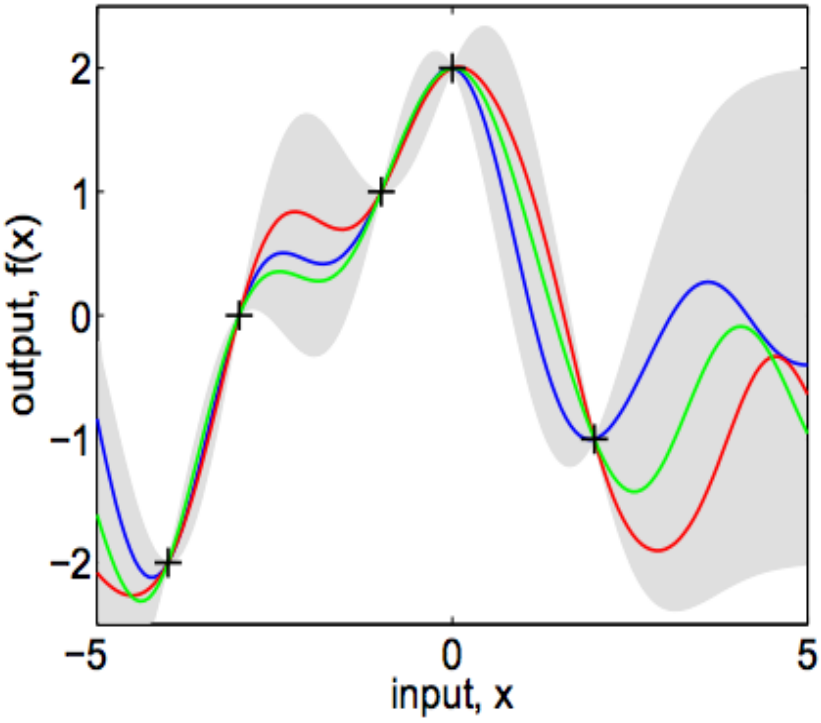
$$f_* \mid X_*, X, f \sim \mathrm{N}(C(X_*, X)C(X, X)^{-1}f,$$
$$C(X_*, X_*) - C(X_*, X)C(X, X)^{-1}C(X, X_*)).$$

- Function values f_* (corresponding to test inputs X_*) can be sampled from the joint posterior distribution by evaluating the mean and covariance matrix

Posterior predictive for noise free observations

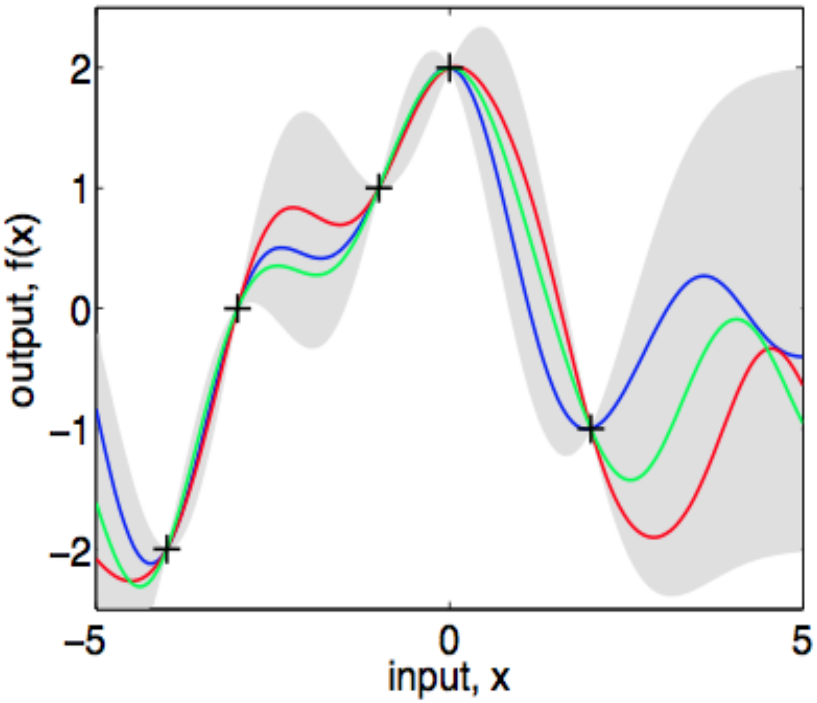


(a), prior

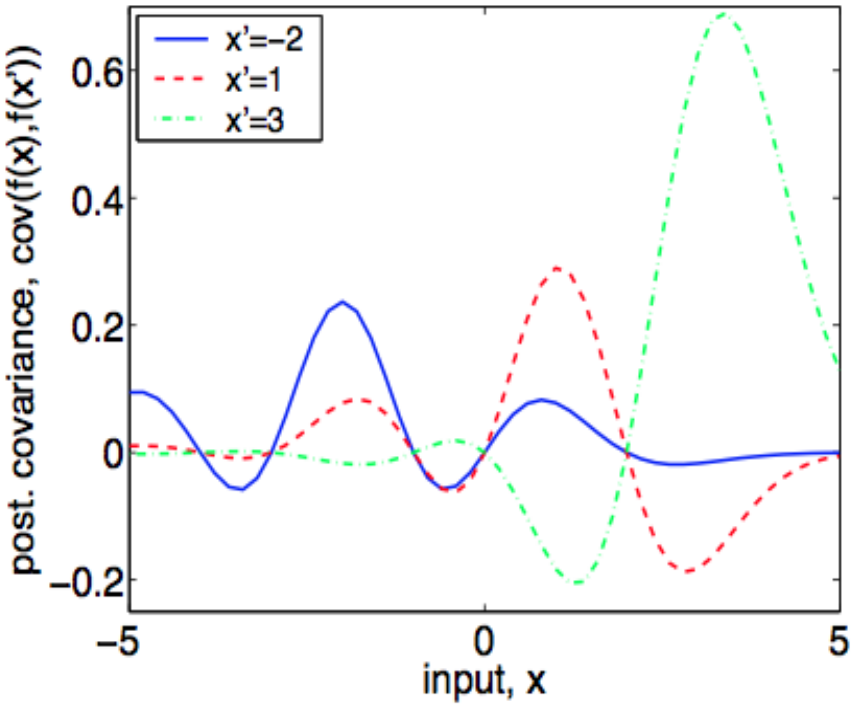


(b), posterior

Posterior covariance



(a), posterior



(b), posterior covariance

Prediction using noisy observations

- It is typical for more realistic modelling situations that we do not have access to function values themselves, but only noisy versions there of $y_i = f(x_i) + \epsilon_i, i = 1, \ldots, n$.
- Assuming additive independent identically distributed Gaussian noise with variance σ^2 , the prior on the noisy observations becomes

$$cov(y_p, y_q) = C(x_p, x_q) + \sigma^2 I_{p=q} \implies cov(y) = C(X, X) + \sigma^2 I,$$

- The joint distribution of the observed target values and the function values at the test locations under the prior as

$$\begin{bmatrix} y \\ f_* \end{bmatrix} \sim \mathrm{N}\left(\mathbf{0}, \begin{bmatrix} C(X, X) + \sigma^2 I & C(X, X_*) \\ C(X_*, X) & C(X_*, X_*) \end{bmatrix}\right)$$

Prediction using noisy observations

- The predictive distribution is

$$f_* \mid X_*, X, y \sim \mathrm{N}(\bar{f}_*, cov(f_*)).$$

where $\bar{f}_* = E[f_* \mid X, y, X_*] = C(X_*, X)[C(X, X) + \sigma^2]^{-1} y$, and

$cov(f_*) = C(X_*, X_*) - C(X_*, X)[C(X, X) + \sigma^2]^{-1} C(X, X_*)$.

- Note first that the mean prediction is a linear combination of observations y; this is sometimes referred to as a linear predictor.
- Another way to look at this equation is to see it as a linear combination of n kernel functions, each one centered on a training point, by writing correspondence with weight-space view compact notation predictive distribution linear predictor representer theorem

$$\bar{f}(x_*) = \sum_{i=1}^{n} \alpha_i C(x_i, x_*), \quad \alpha = (C(X, X) + \sigma^2 I)^{-1} y.$$

Gaussian process predictions using squared exponential cov kernel

Figure: Prediction and predictive intervals