732A96/TDDE15 Advanced Machine Learning

Gaussian Process Regression and Classification

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Lectures 10: Gaussian Process Regression

Contents

Literature

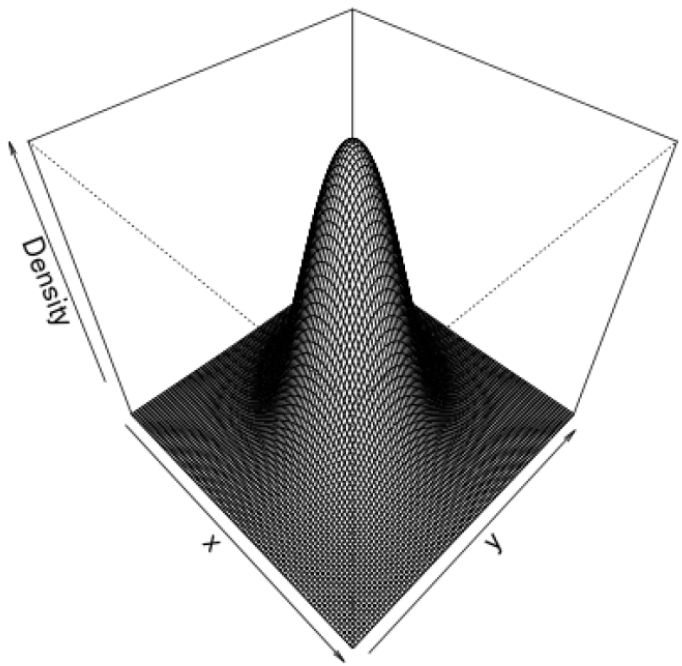
- Main source
  - Rasmussen, C. E. and Williams, K. I. *Gaussian Processes for Machine Learning*. MIT Press, 2006. Chapters 2.1-2.5.
- Additional source
  - Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Chapters 6.4.1-6.4.2.

Gaussian Distribution

- Density function of the Gaussian (a.k.a normal) distribution for a D-dimensional random variable $\boldsymbol{x}$:

$$\mathcal{N}(\boldsymbol{x}|\mu,\Sigma) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\Sigma|^{1/2}}\exp\left\{-\frac{1}{2}(\boldsymbol{x}-\mu)^T\Sigma^{-1}(\boldsymbol{x}-\mu)\right\}$$

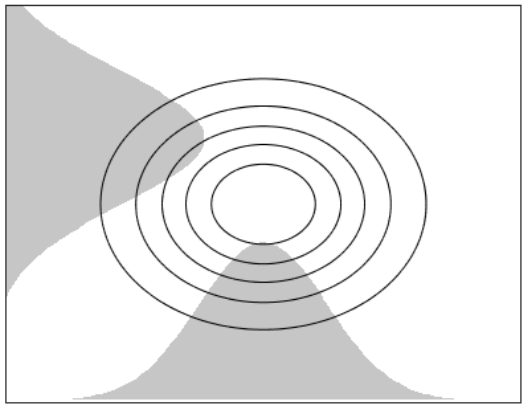
- Recall that $E[\boldsymbol{x}] = \mu$ and $var(\boldsymbol{x}) = \Sigma$.



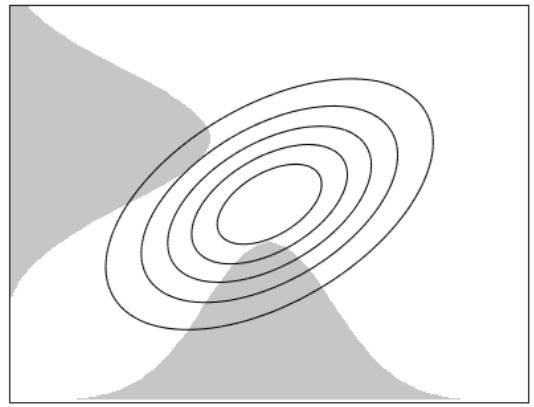
Gaussian Distribution

- Example: $\mathcal{N}(x_1, x_2|\mu, \Sigma)$ with $\Sigma = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$.

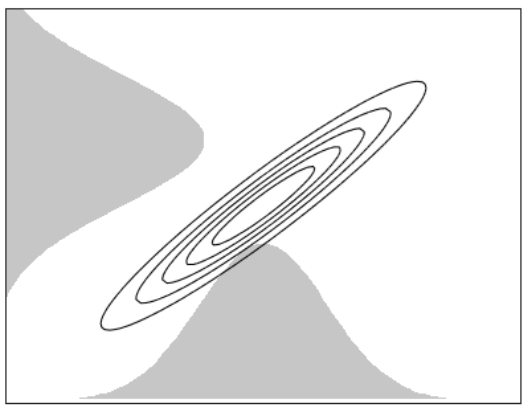
$\rho = 0, \sigma_1 = 1, \sigma_2 = 1$



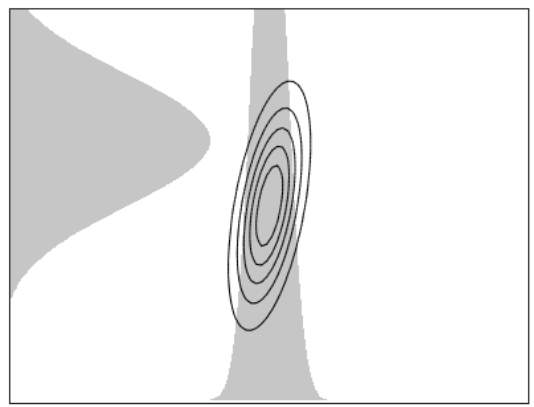
$\rho = 0.5, \sigma_1 = 1, \sigma_2 = 1$



$\rho = 0.95, \sigma_1 = 1, \sigma_2 = 1$



$\rho = 0.5, \sigma_1 = 1/4, \sigma_2 = 1$



Gaussian Distribution

- Recall that if

$$p(x) = \mathcal{N}(x|\mu, \Lambda^{-1})$$
$$p(y|x) = \mathcal{N}(y|Ax + B, L^{-1})$$

then

$$p(x, y) = \mathcal{N}(x, y|A\mu + B, R^{-1})$$

where

$$R^{-1} = \begin{pmatrix} \Lambda^{-1} & \Lambda^{-1}A^T \\ A\Lambda^{-1} & L^{-1} + A\Lambda^{-1}A^T \end{pmatrix}.$$

- Recall also that if $p(x) = \mathcal{N}(x|\mu, \Sigma)$ and $\Lambda = \Sigma^{-1}$ and

$$x = (x_a, x_b)^T \qquad \mu = (\mu_a, \mu_b)^T$$
$$\Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix} \qquad \Lambda = \begin{pmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{pmatrix}$$

then

$$p(x_a) = \mathcal{N}(x_a|\mu_a, \Sigma_{aa})$$
$$p(x_a|x_b) = \mathcal{N}(x_a|\mu_{a|b}, \Lambda_{aa}^{-1}) \quad \text{where } \mu_{a|b} = \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(x_b - \mu_b) \text{ or}$$
$$p(x_a|x_b) = \mathcal{N}(x_a|\mu_{a|b}, \Sigma_{a|b}) \quad \text{where } \mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b)$$
$$\text{and } \Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}.$$

Linear Regression

- Training data: $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)|i = 1, \ldots, n\} = (X, \boldsymbol{y})$.
- Deterministic function: $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{w}$.
- Additive noisy observations: $y = f(\boldsymbol{x}) + \epsilon$.
- Gaussian noise: $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$.
- Likelihood function: $p(\boldsymbol{y}|X, \boldsymbol{w}) = \mathcal{N}(X^T \boldsymbol{w}, \sigma_n^2 I) \propto \exp\left\{\frac{1}{2\sigma_n^2}||\boldsymbol{y} - X^T \boldsymbol{w}||^2\right\}$.
- To obtain $\boldsymbol{w}^{ML}$,
  - take the derivative of the log lik function wrt $\boldsymbol{w}$, and
  - set it to zero, and
  - solve to obtain $\boldsymbol{w}^{ML} = (XX^T)^{-1}X\boldsymbol{y}$.
- Minimizing the least squared error (i.e., $\frac{1}{2}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T \boldsymbol{w})^2$) gives the same result. This justifies the use of LSE.

Bayesian Linear Regression

- Prior distribution: $\boldsymbol{w} \sim \mathcal{N}(0, \Sigma_p)$, e.g. ridge regression $\Sigma_p = \alpha^{-1} I$.
- Posterior distribution:

$$\log p(\boldsymbol{w}|X, \boldsymbol{y}) \propto \log p(\boldsymbol{y}|X, \boldsymbol{w}) + \log p(\boldsymbol{w}) \propto \frac{1}{2\sigma_n^2} \|\boldsymbol{y} - X^T \boldsymbol{w}\|^2 - \frac{1}{2} \boldsymbol{w}^T \Sigma_p^{-1} \boldsymbol{w}.$$

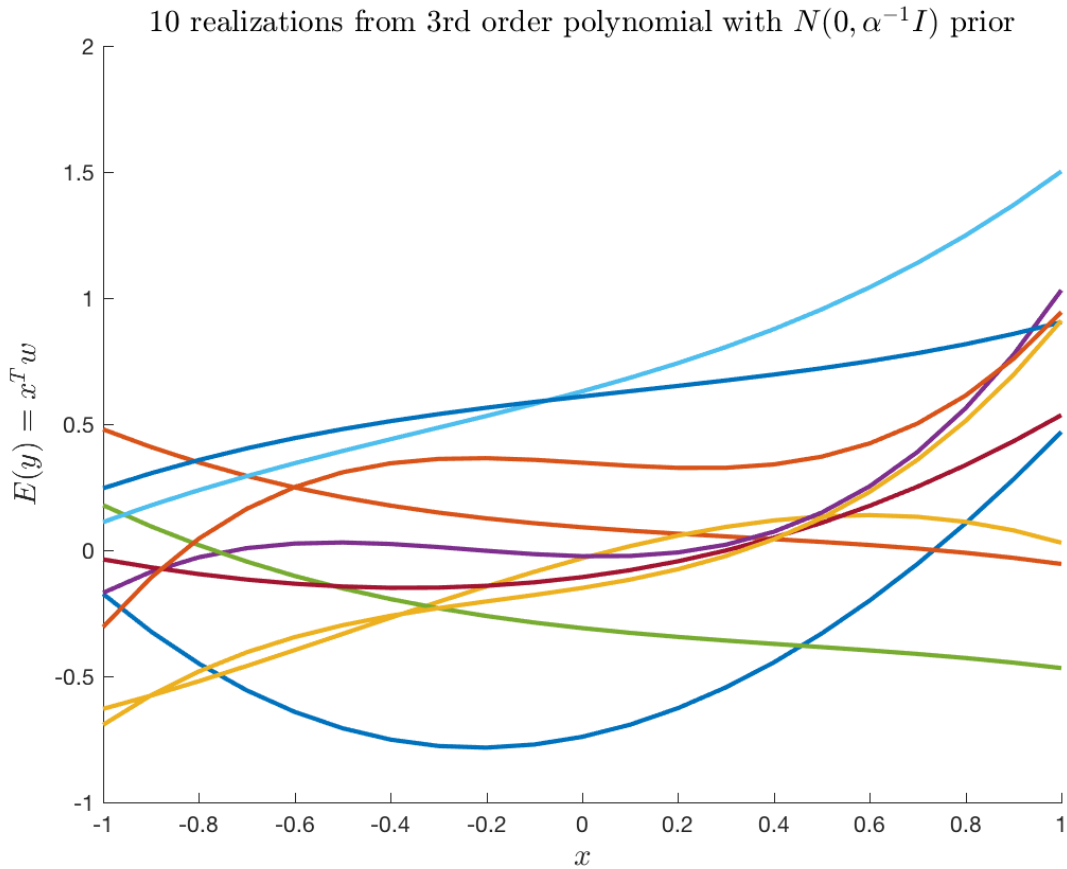
- So, $\boldsymbol{w}^{MAP}$ can be seen as a penalized/regularized ML estimate.
- Specifically, $p(\boldsymbol{w}|X, \boldsymbol{y}) = \mathcal{N}(\bar{\boldsymbol{w}} = \frac{1}{\sigma_n^2} A^{-1} X \boldsymbol{y}, A^{-1})$ where $A = \sigma_n^{-2} X X^T + \Sigma_p^{-1}$, and thus $\boldsymbol{w}^{MAP} = \bar{\boldsymbol{w}}$.
- A full Bayesian approach does not use $\boldsymbol{w}^{MAP}$ but the predictive distribution:

$$p(f_*|\boldsymbol{x}_*, X, \boldsymbol{y}) = \int p(f_*|\boldsymbol{x}_*, \boldsymbol{w}) p(\boldsymbol{w}|X, \boldsymbol{y}) d\boldsymbol{w} = \mathcal{N}(\frac{1}{\sigma_n^2} \boldsymbol{x}_* A^{-1} X \boldsymbol{y}, \boldsymbol{x}_*^T A^{-1} \boldsymbol{x}_*).$$

- The above carries over to the feature space $\phi(\boldsymbol{x})$. The kernel trick applies. See p. 12 of Rasmussen and Williams.

Bayesian Linear Regression

- A prior on $\boldsymbol{w}$ is a prior on f.

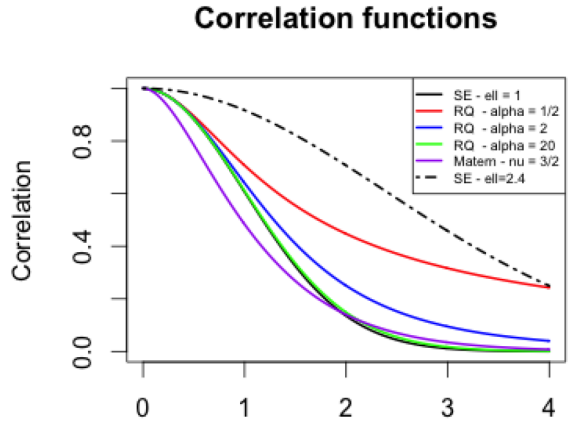


Gaussian Processes Regression

- A GP defines a prior distribution over functions directly, instead of indirectly through weights as before. Therefore, a GP operates on the space of functions rather than on the space of weights. Operating in either space is equivalent. A GP defines a prior over functions by defining a prior over a finite number of input points.
- Formally, a GP is a collection of random variables, any finite number of which have a joint Gaussian distribution. Hence, a GP is defined as
  - $f(\boldsymbol{x}) \sim \mathcal{GP}(m(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}'))$ where
  - $m(\boldsymbol{x}) = E[f(\boldsymbol{x})]$ is the mean function (assumed to be zero hereinafter), and
  - $k(\boldsymbol{x}, \boldsymbol{x}') = E[(f(\boldsymbol{x}) - m(\boldsymbol{x}))(f(\boldsymbol{x}') - m(\boldsymbol{x}'))]$ is the covariance function, e.g. squared exponential:

$$k(\boldsymbol{x}, \boldsymbol{x}') = cov(f(\boldsymbol{x}), f(\boldsymbol{x}')) = \sigma_f^2 \exp\left\{ - \frac{||\boldsymbol{x} - \boldsymbol{x}'||^2}{2\ell^2} \right\}$$

i.e. highly correlated function values for close input points. Intuitively, σ_f^2 is the overall variance of the function, and ℓ is the distance we have to move in the input space for the function to vary significantly.



Gaussian Processes Regression

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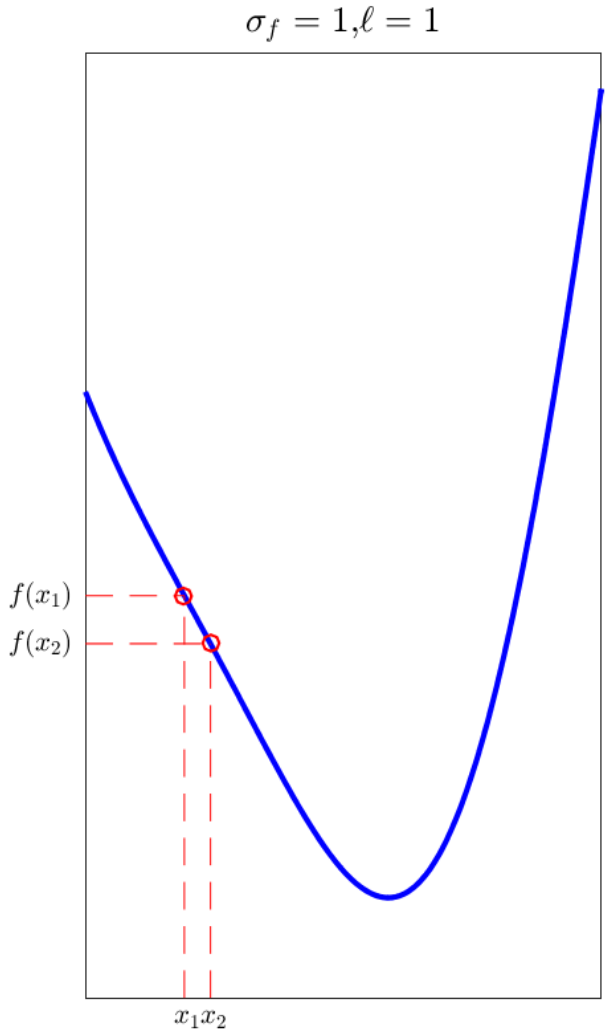
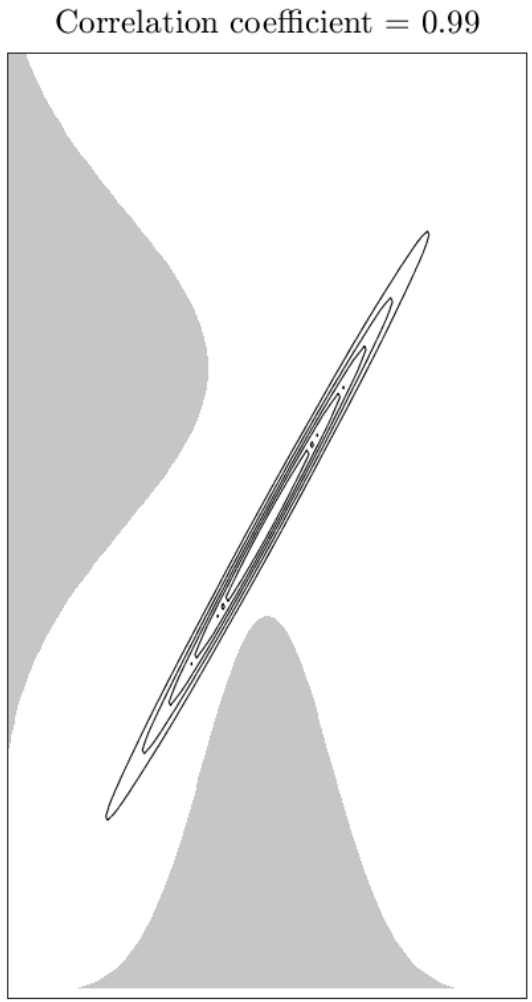
  i.e. highly correlated function values for close input points. Intuitively, σ_f^2 is the overall variance of the function, and ℓ is the distance we have to move in the input space for the function to vary significantly.

- Note that the covariance between the function values is written as a function of the inputs points.
- Note also that each random variable or dimension in a GP is a function value at an input point. Hence, a GP specifies a probability distribution over functions at a finite number of input points.
- We can sample the function space by sampling the GP at any number of chosen input points X_*. To do so, we sample a multivariate Gaussian distribution with the corresponding covariance matrix, i.e. $\boldsymbol{f}_* | X_* \sim \mathcal{N}(0, K(X_*, X_*))$.
- Demo of `GaussianProcesses.R`.

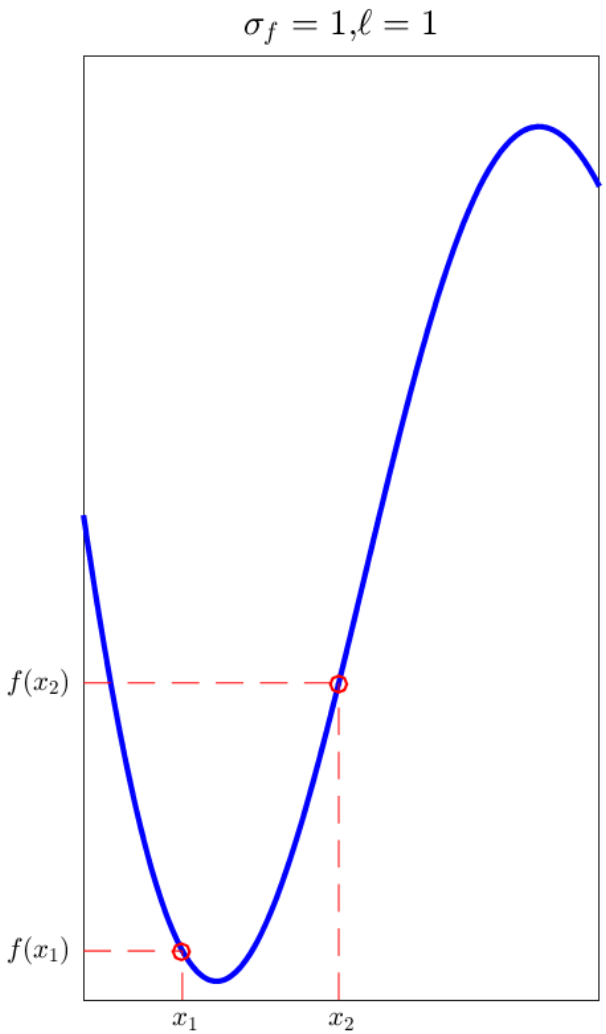
Squared Exponential Covariance: Smooth Function, Close Points

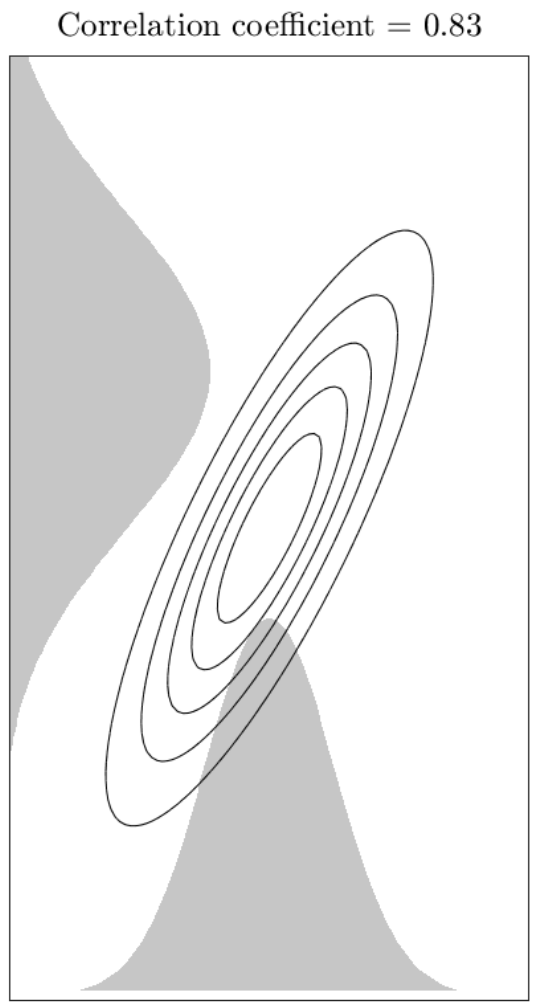
- If $\sigma_f = 1$, then $k(x, x) = 1$, $0 \leq k(x, x') \leq 1$, and $k(x, x') = \rho(f(x), f(x'))$.



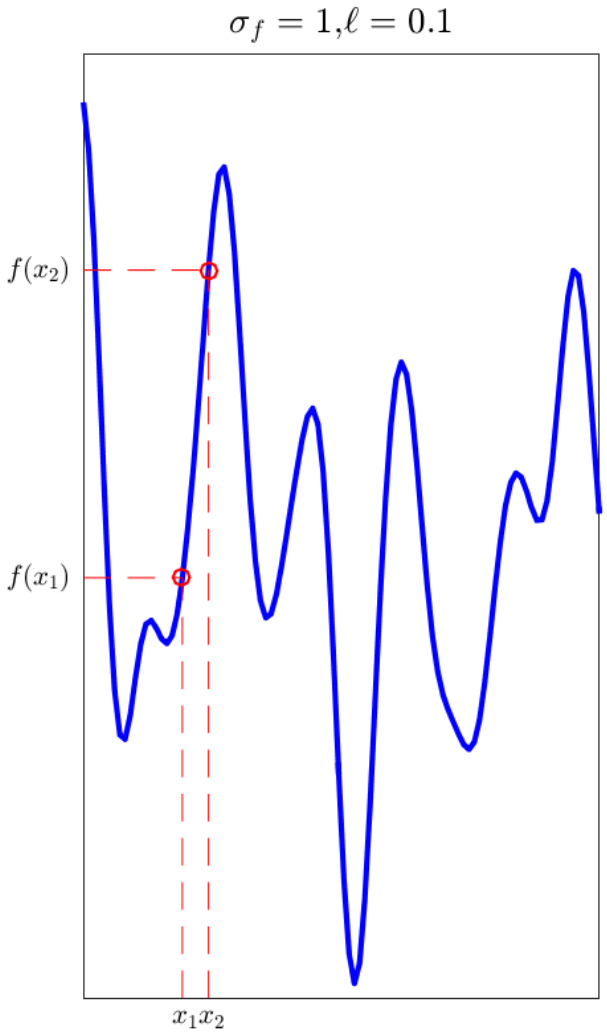


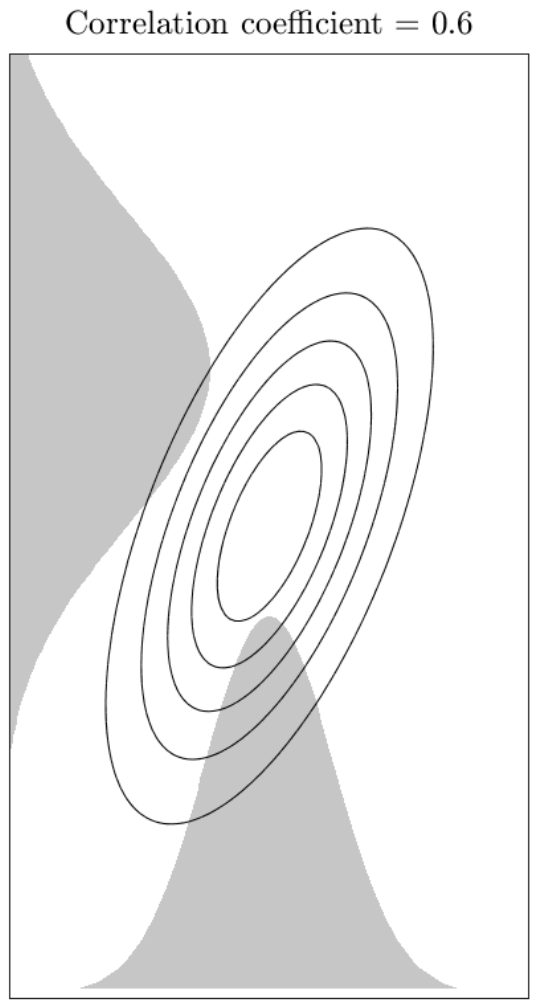
Squared Exponential Covariance: Smooth Function, Distant Points



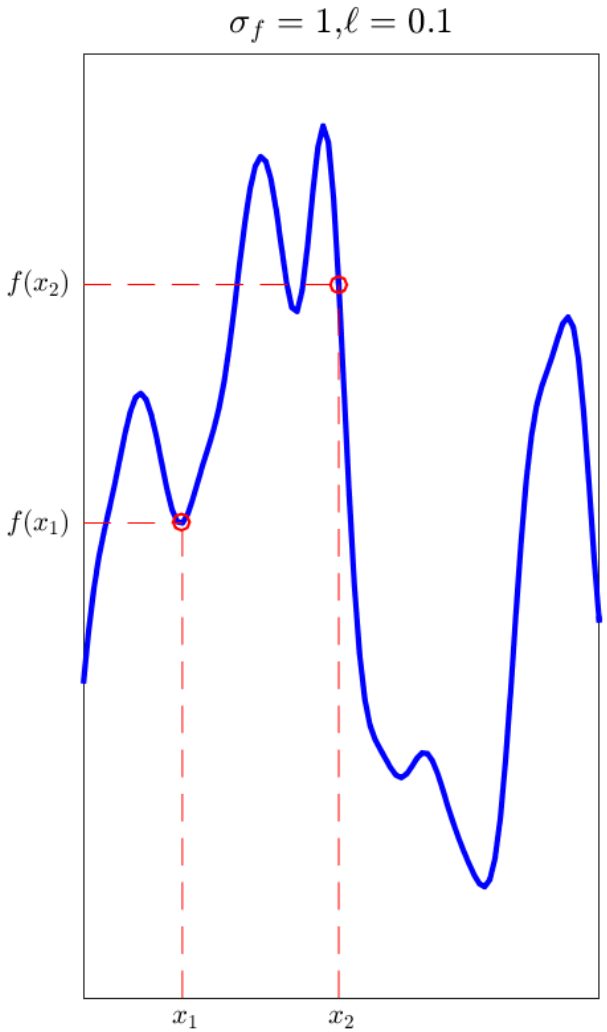


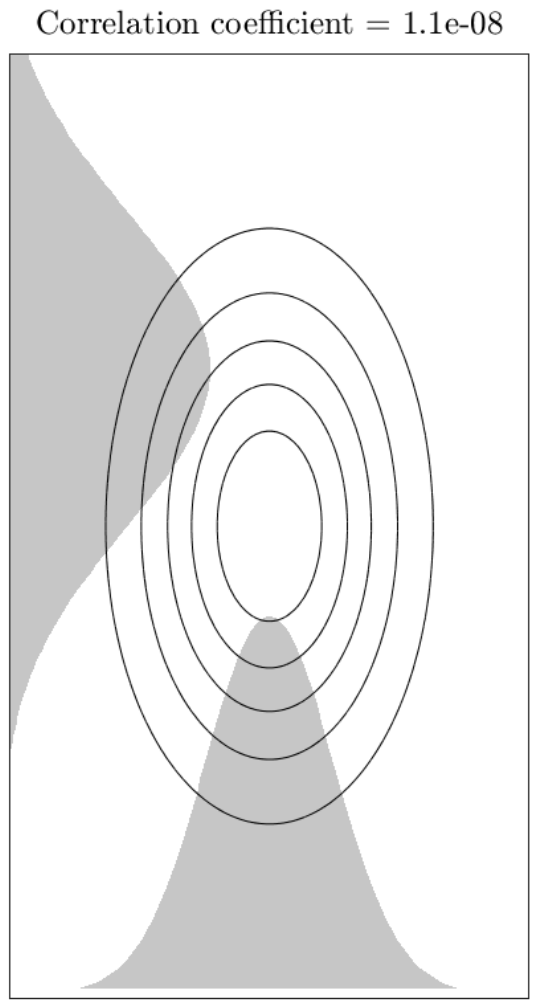
Squared Exponential Covariance: Jagged Function, Close Points





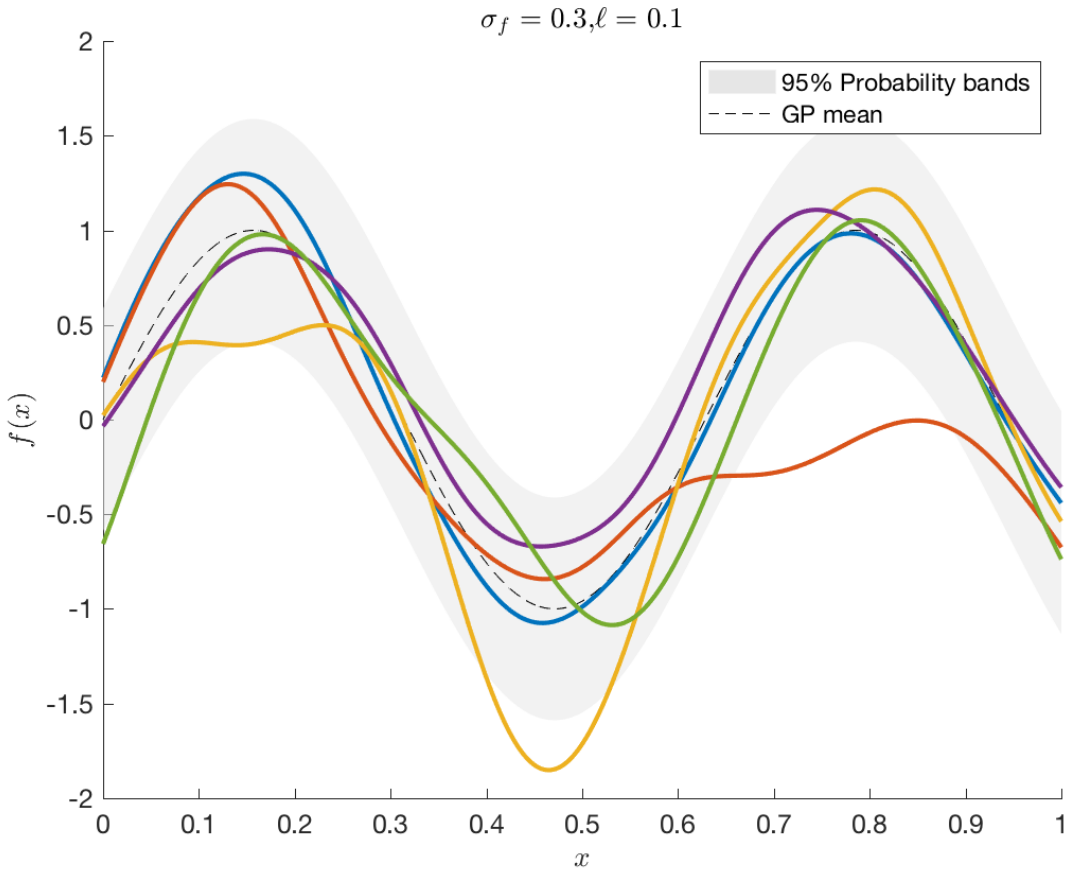
Squared Exponential Covariance: Jagged Function, Distant Points





Gaussian Process Sampling: Multivariate Draw

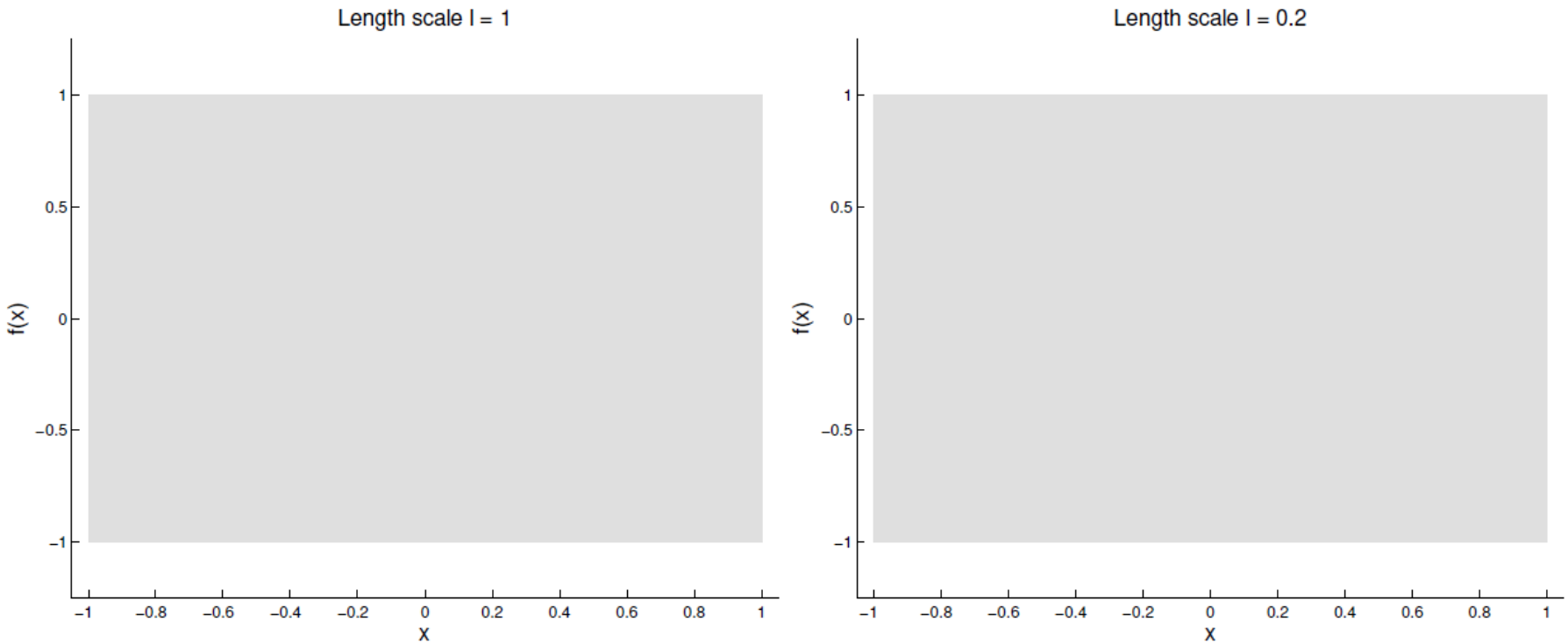
- To sample a GP at points $X_* = \{x_1, \ldots, x_n\}$, we sample a multivariate Gaussian distribution $\mathcal{N}(0, K(X_*, X_*))$.



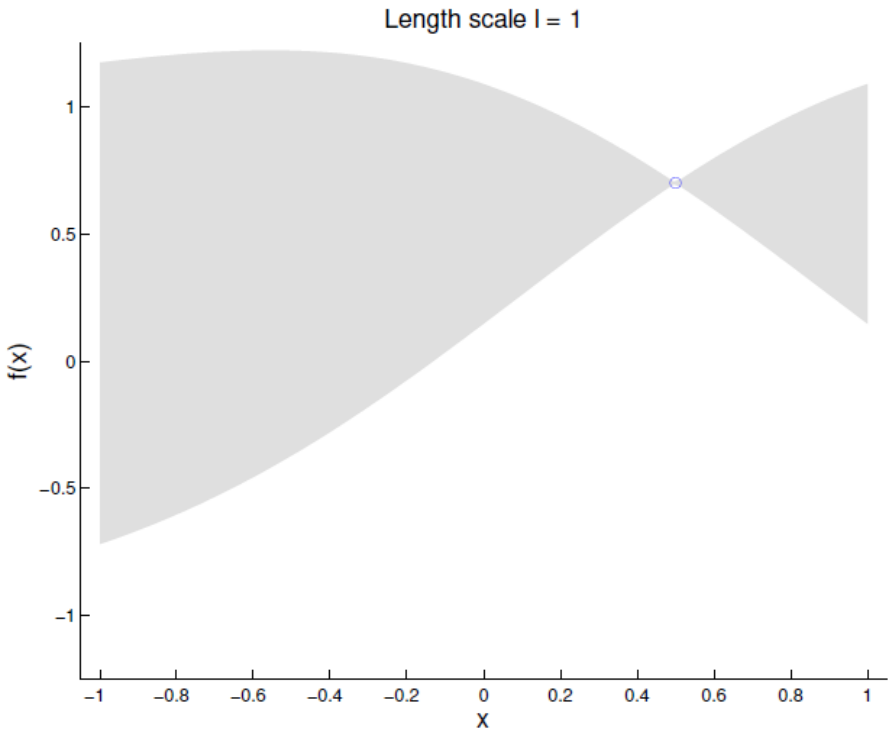
Gaussian Process Sampling: Before the First Univariate Draw

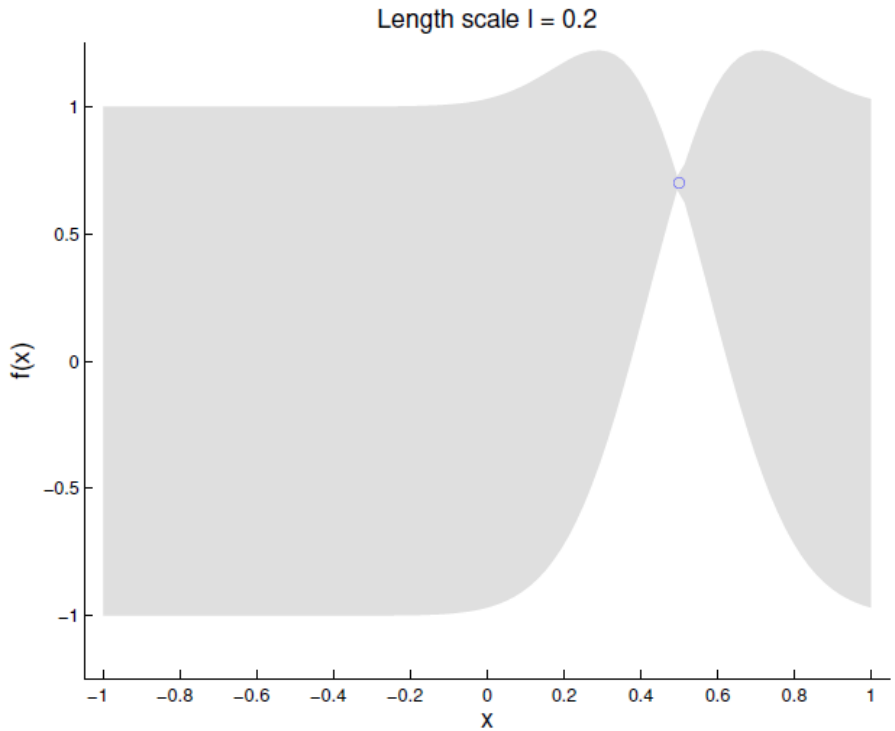
- To sample a GP at points $X_* = \{x_1, \ldots, x_n\}$, we can alternatively sample univariate Gaussian distributions, since

$$p(f(x_1), \ldots, f(x_n)) = \prod_{i=1}^{n} p(f(x_i)|f(x_1), \ldots, f(x_{i-1})).$$

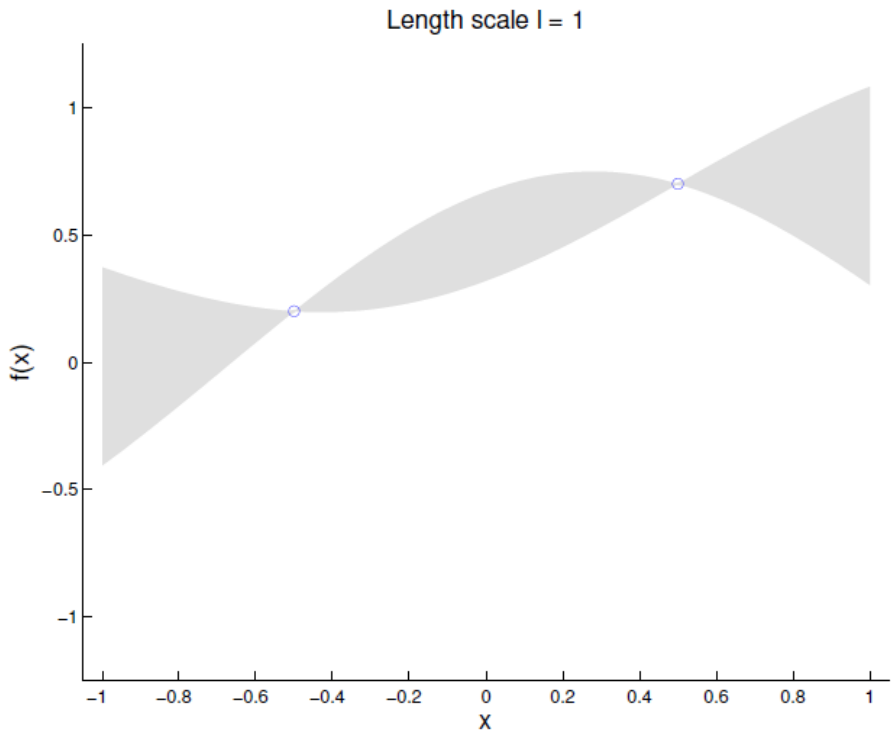


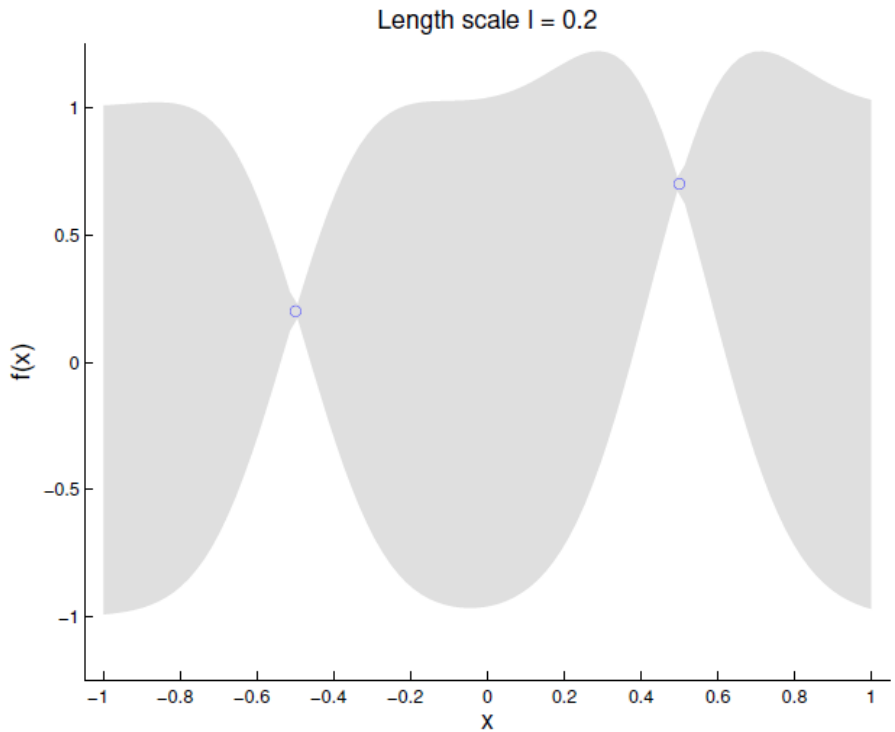
Gaussian Process Sampling: Before the Second Univariate Draw



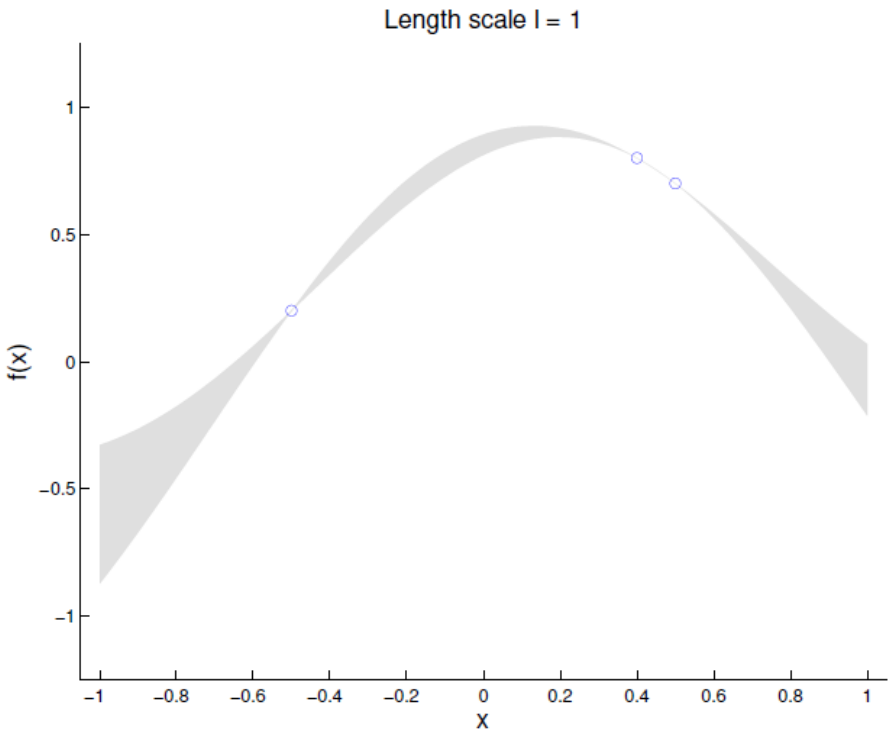


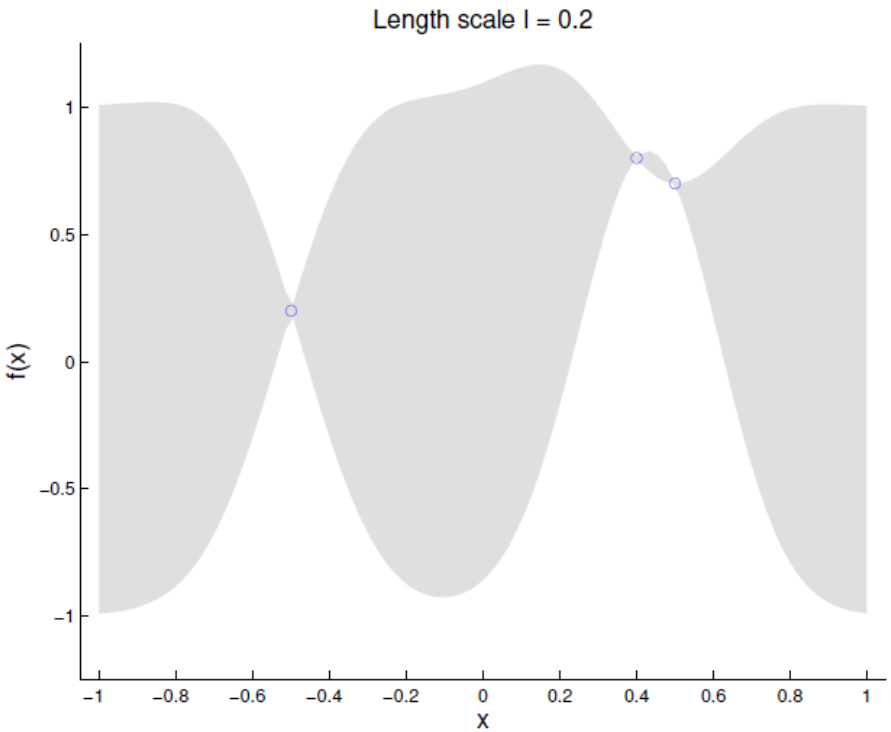
Gaussian Process Sampling: Before the Third Univariate Draw





Gaussian Process Sampling: Before the Fourth Univariate Draw





Gaussian Processes Regression

- With no data, sample from $\boldsymbol{f}_*|X_* \sim \mathcal{N}(0, K(X_*, X_*))$.
- With noise-free training data $\mathcal{D} = \{(\boldsymbol{x}_i, f_i)|i = 1, \ldots, n\} = (X, \boldsymbol{f})$, build

$$\begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} K(X, X) & K(X, X_*) \\ K(X_*, X) & K(X_*, X_*) \end{bmatrix}\right)$$

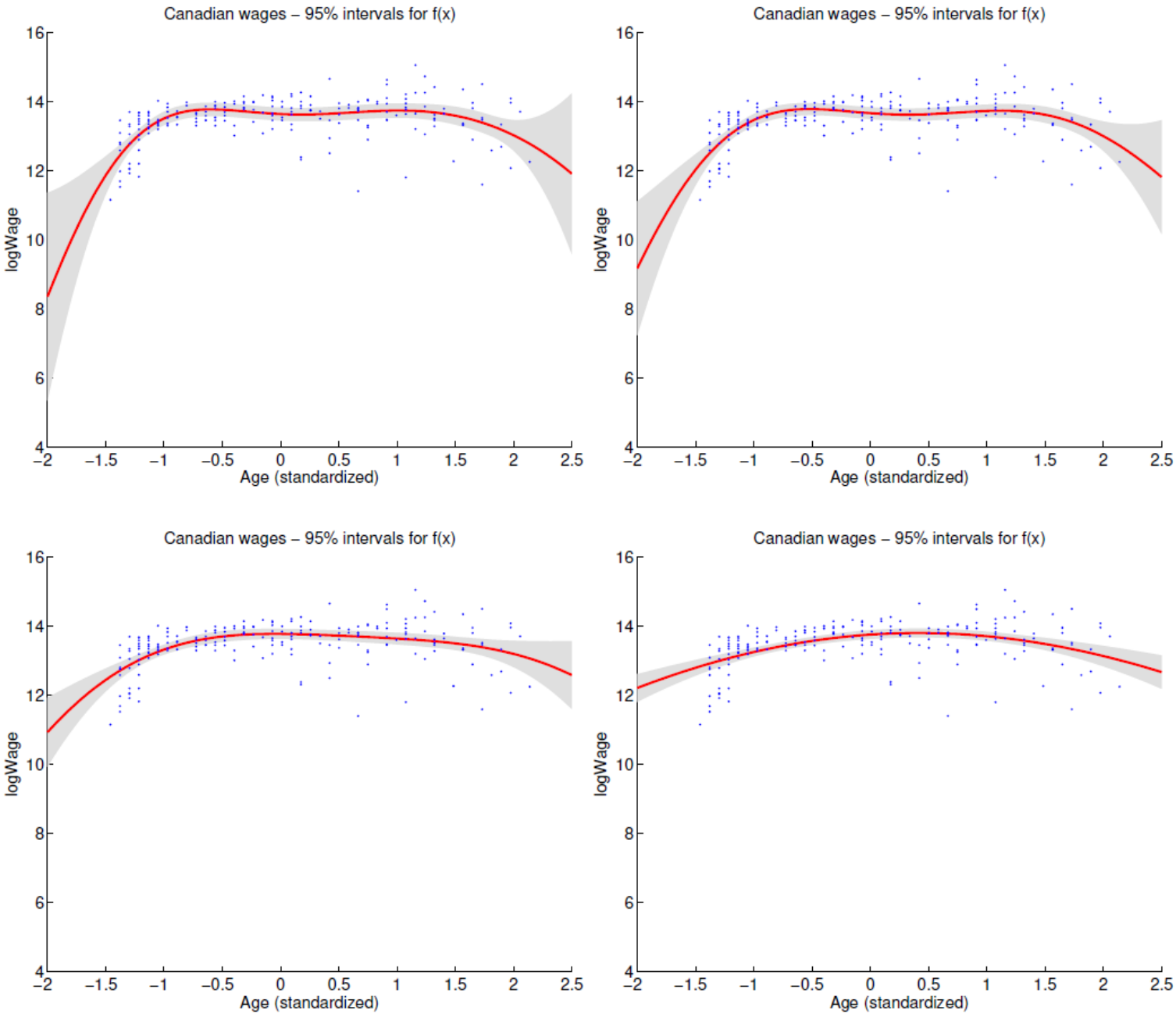
  and sample from $\boldsymbol{f}_*|X_*, X, \boldsymbol{f} \sim \mathcal{N}(K(X_*, X)K(X, X)^{-1}\boldsymbol{f}, K(X_*, X_*) - K(X_*, X)K(X, X)^{-1}K(X, X_*))$.
- With noisy training data $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)|i = 1, \ldots, n\} = (X, \boldsymbol{y})$, build[1]

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} K(X, X) + \sigma_n^2 I & K(X, X_*) \\ K(X_*, X) & K(X_*, X_*) \end{bmatrix}\right)$$

  and sample from $\boldsymbol{f}_*|X_*, X, \boldsymbol{y} \sim \mathcal{N}(K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1}\boldsymbol{y}, K(X_*, X_*) - K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1}K(X, X_*))$.
- See p. 17 of Rasmussen and Williams for the correspondence between the weight and function space views: Every covariance function can be mapped into a set of features, and vice versa.
- Demo of `KernLabDemo.R`.

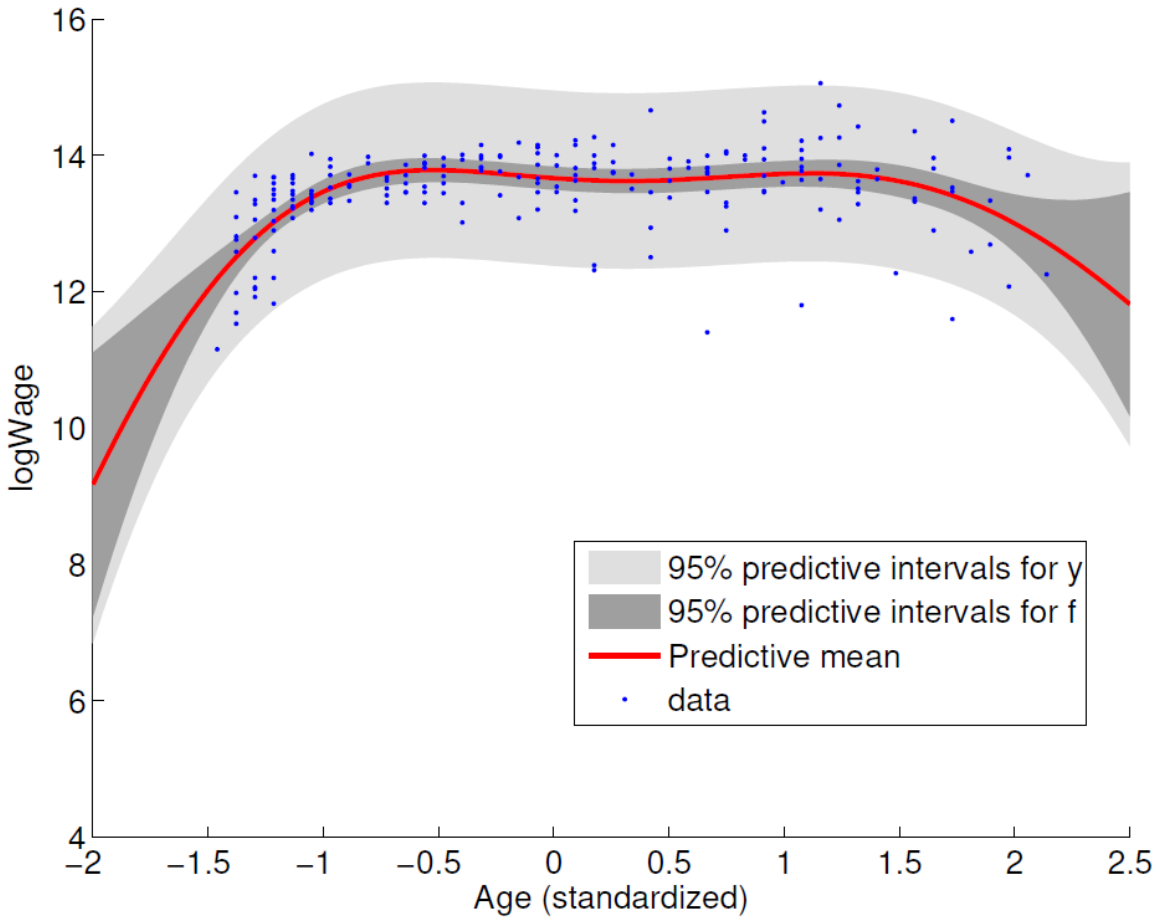
[1] $cov(X + Y, Z + W) = cov(X, Z) + cov(X, W) + cov(Y, Z) + cov(Y, W)$ for independent random variables X, Y, Z and W.

Gaussian Process Regression: Canadian Wages ($\ell = 0.2, 0.5, 1, 2$)



Gaussian Process Regression: Canadian Wages ($\ell = 0.5$)

- Predictive interval for $\boldsymbol{f}_*$: mean($\boldsymbol{f}_*$) $\pm$ 1.96 sqrt(var($\boldsymbol{f}_*$)).
- Predictive interval for $\boldsymbol{y}_*$: mean($\boldsymbol{f}_*$) $\pm$ 1.96 sqrt(var($\boldsymbol{f}_*$) + σ_n^2).



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Thank you