# 732A96/TDDE15 Advanced Machine Learning
## Gaussian Process Regression and Classification

Jose M. Peña
IDA, Linköping University, Sweden

Lectures 10: Gaussian Process Regression

# Contents

- Linear Regression
- Bayesian Linear Regression
- Gaussian Process Regression
- Squared Exponential Covariance Function
- Gaussian Process Regression: Canadian Wages

# 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

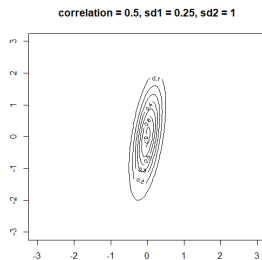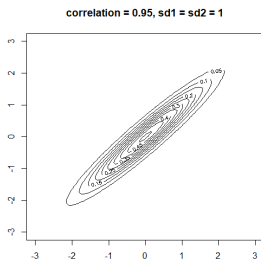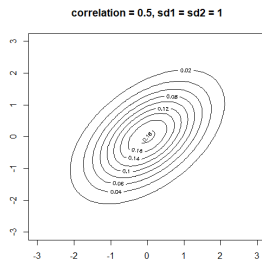▸ Density function of the Gaussian (a.k.a normal) distribution for a $D$-dimensional random variable $\boldsymbol{X}$:
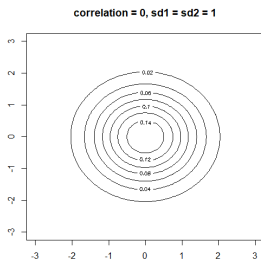
$$\mathcal{N}(\boldsymbol{x}; \mu, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2}(\boldsymbol{x} - \mu)^T \Sigma^{-1}(\boldsymbol{x} - \mu) \right\}$$

▸ Recall that $E[\boldsymbol{X}] = \mu$ and $cov(\boldsymbol{X}) = \Sigma$.
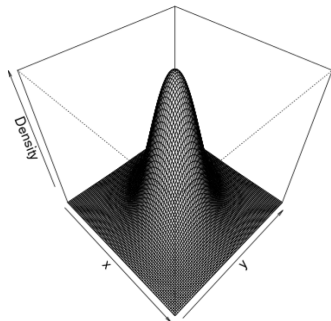
# Gaussian Distribution

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

# Gaussian Distribution

▸ Recall that if

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

then

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

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

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

then

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

# Linear Regression

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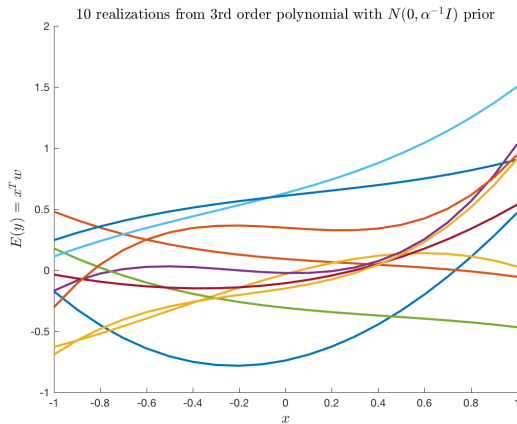- ▶ Posterior distribution:

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

- ▶ 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:

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

# Bayesian Linear Regression

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



10 realizations from 3rd order polynomial with $N(0, \alpha^{-1}I)$ prior

# 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
  - $f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$ where
  - $m(\mathbf{x}) = E[f(\mathbf{x})]$ is the mean function (assumed to be zero hereinafter), and
  - $k(\mathbf{x}, \mathbf{x}') = E[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))]$ is the covariance function, e.g. squared exponential:

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

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

**Correlation functions**
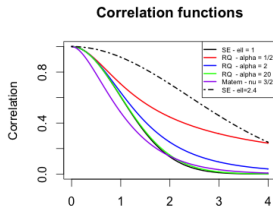
# Gaussian Processes Regression

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

- Note 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 any **finite** number of input points.
- Note that the covariance between the **function values** is written as a function of the **inputs points**. Note that the covariances are non-negative.
- Note that the zero mean assumption affects the location but not the smoothness of the prior. Note also that the posterior mean is not assumed to be zero. However, it may get close to zero in regions with few input points when $\ell$ is small, because the posterior is then similar to the prior. Of course, one can always center or standarize the data.
- 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. $\boldsymbol{f}_* | X_* \sim \mathcal{N}(0, K(X_*, X_*))$.
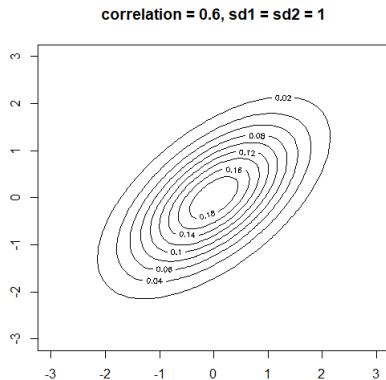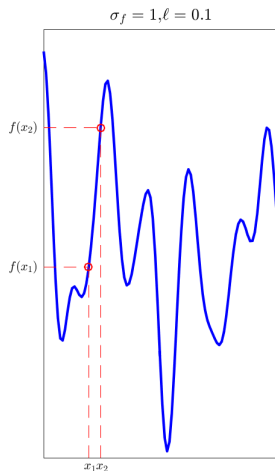- Demo of `GaussianProcesses.R`.

# Squared Exponential Covariance: Smooth Function, Close Points



$\sigma_f = 1, \ell = 1$

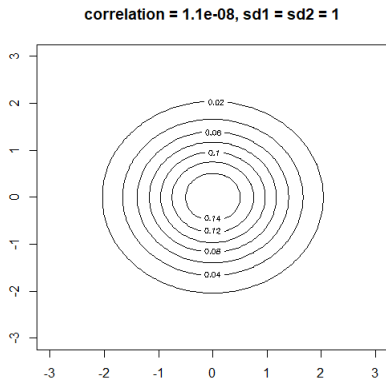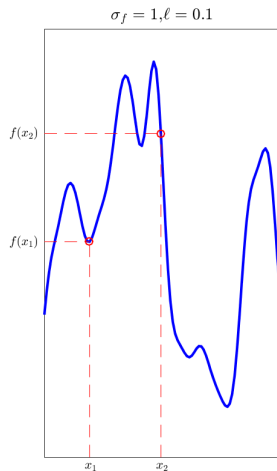correlation = 0.99, sd1 = sd2 = 1
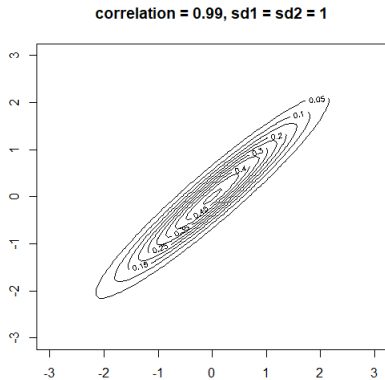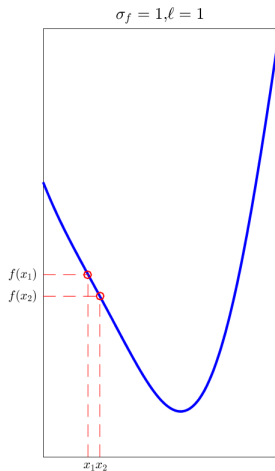
# Squared Exponential Covariance: Smooth Function, Distant Points
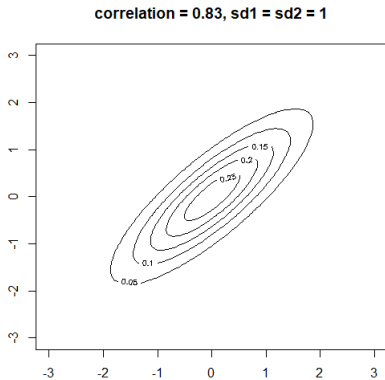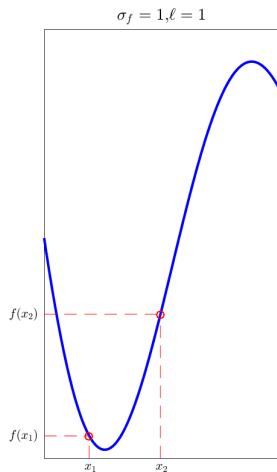
# Squared Exponential Covariance: Jagged Function, Close Points

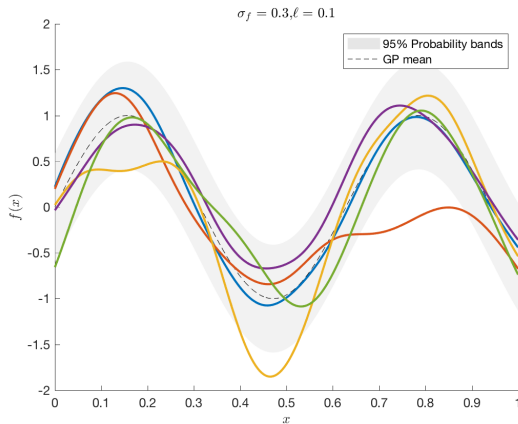# Squared Exponential Covariance: Jagged Function, Distant Points



$\sigma_f = 1, \ell = 0.1$

correlation = 1.1e-08, sd1 = sd2 = 1

# Gaussian Process Sampling: Multivariate Draw

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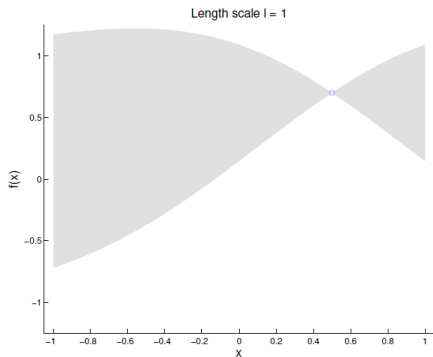  Gaussian distribution $\mathcal{N}(0, K(X_*, X_*))$.

# 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
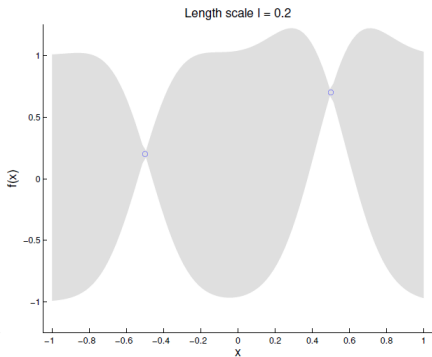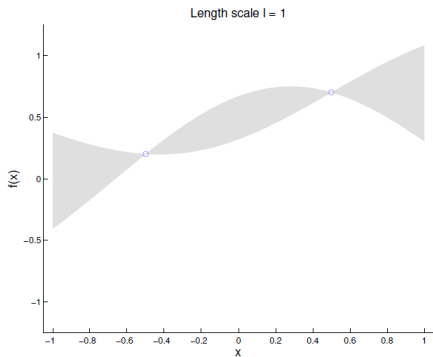
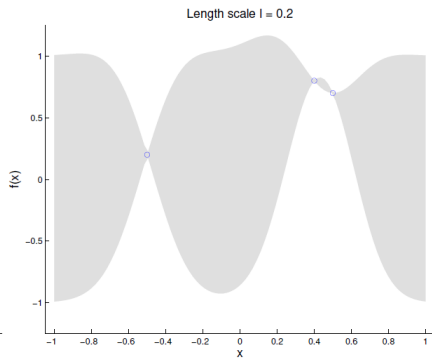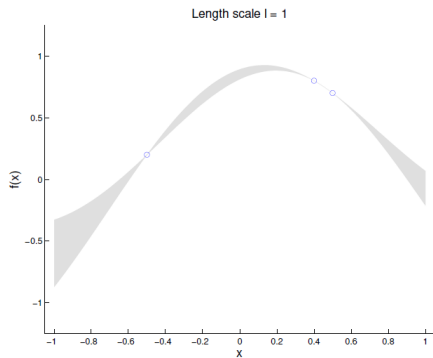$$p(f(x_1), \ldots, f(x_n)) = \prod_{i=1}^{n} p(f(x_i)|f(x_1), \ldots, f(x_{i-1})).$$
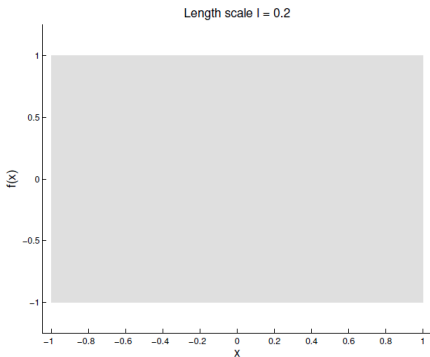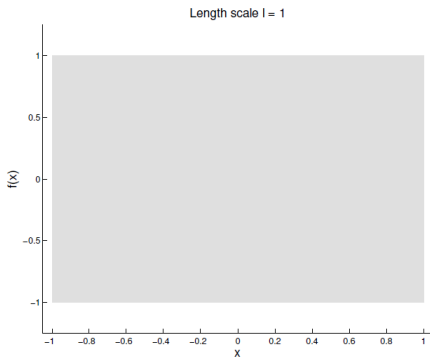
# Gaussian Process Sampling: Before the Second Univariate Draw
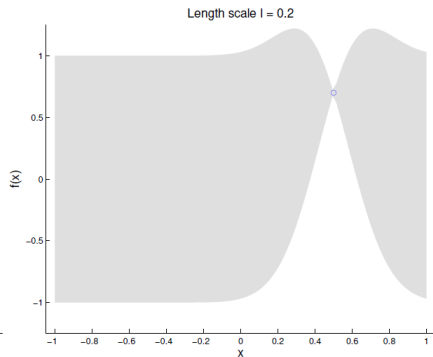
# Gaussian Process Sampling: Before the Third Univariate Draw

# Gaussian Process Sampling: Before the Fourth Univariate Draw

# Gaussian Processes Regression

- With no training data, sample from $\boldsymbol{f}_* | X_* \sim \mathcal{N}(0, K(X_*, X_*))$.
- With **noise-free** training data $\mathcal{D} = \{(\boldsymbol{x}_i, f_i) | i = 1, \dots, n\} = (X, \boldsymbol{f})$, 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 $\mathcal{D} = \{(\boldsymbol{x}_i, y_i) | i = 1, \dots, n\} = (X, \boldsymbol{y})$, build[1]
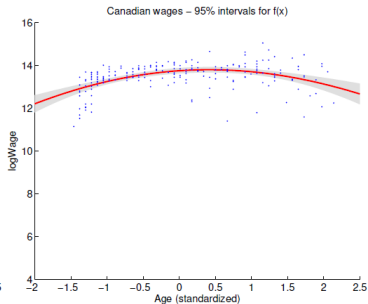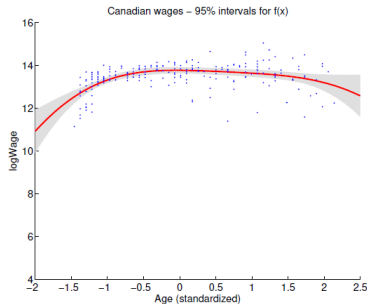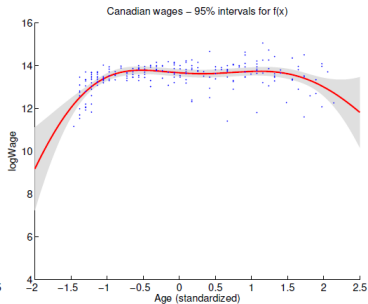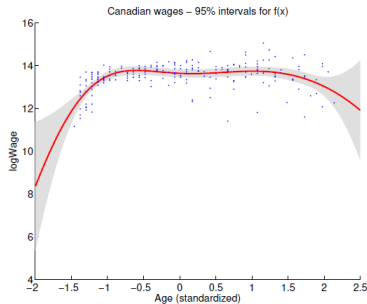
$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} K(X, X) + \sigma_n^2 I & K(X, X_*) \\ K(X_*, X) & K(X_*, X_*) \end{bmatrix}\right)$$

  and sample from $\boldsymbol{f}_* | X_*, X, \boldsymbol{y} \sim \mathcal{N}(K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1}\boldsymbol{y}, K(X_*, X_*) - K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1}K(X, X_*))$.
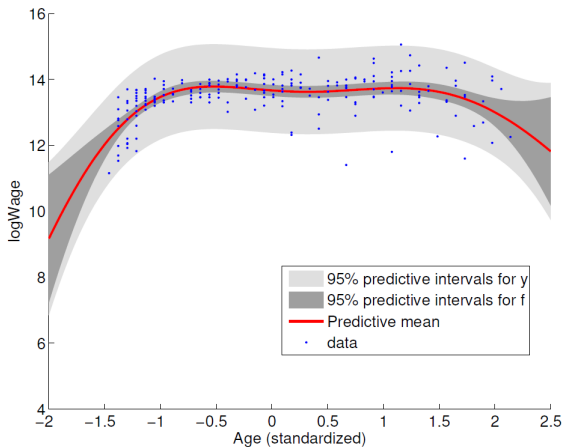
- Demo of `KernLabDemo.R`.

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[1] $cov(y, y') = cov(f(x) + \epsilon, f(x') + \epsilon') =$
$cov(f(x), f(x')) + cov(f(x), \epsilon') + cov(\epsilon, f(x')) + cov(\epsilon, \epsilon') = cov(f(x), f(x')) + \sigma_n^2 \delta_{xx'}$.

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

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Thank you