Gaussian Processes for Machine Learning

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Outline

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Section 1

Gaussian Process

Gaussian Process

Definition

A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.

$$f \sim \mathcal{GP}(m(\cdot), k(\cdot,\cdot)) \Leftrightarrow f(t_1, \ldots, t_n) \sim \mathcal{N}(\mu, K),$$

where $\mu = (m(t_1), \ldots, m(t_n))^T$, $K \in \mathbb{R}^{n \times n}$, $K_{ij} = k(t_i, t_j)$.
$m : \mathbb{R} \to \mathbb{R}$ is called the mean function of the gaussian process f.
$k : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+$ is the covariance function of f.

Mean and covariance functions completely determine a gaussian process.

Example

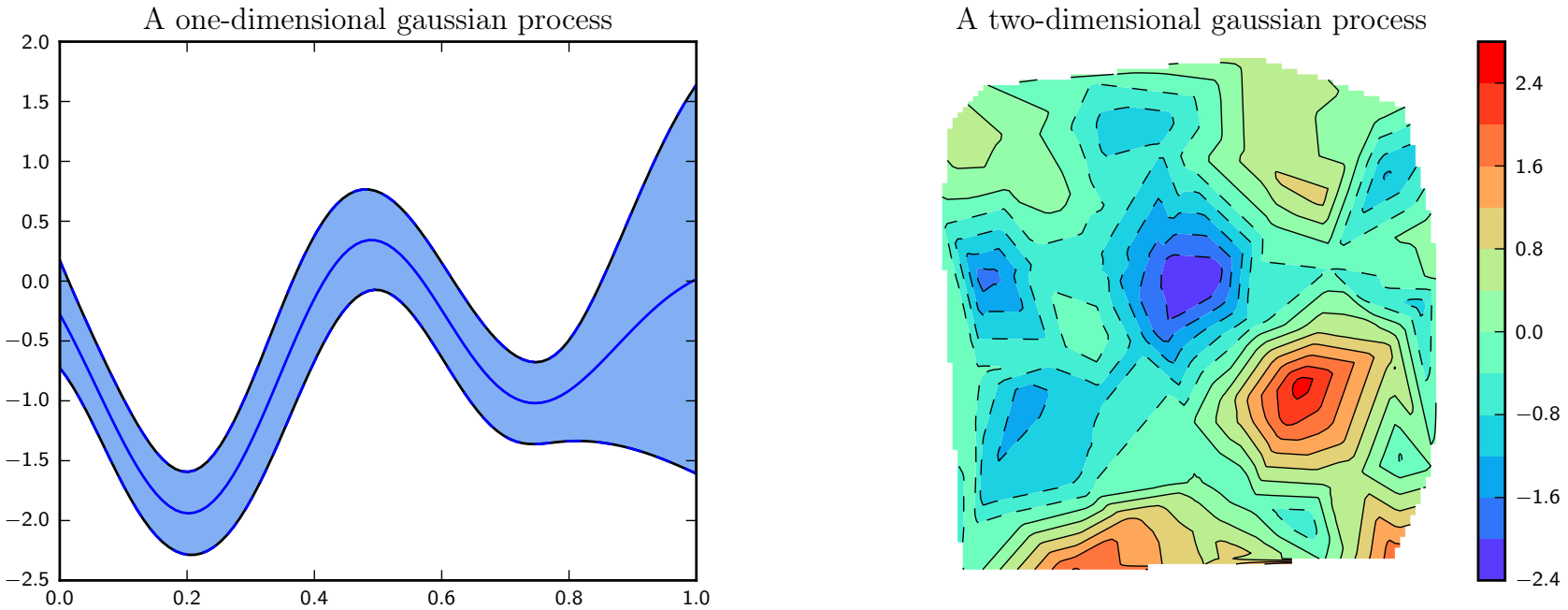


Figure: Examples of gaussian processes

Covariance functions

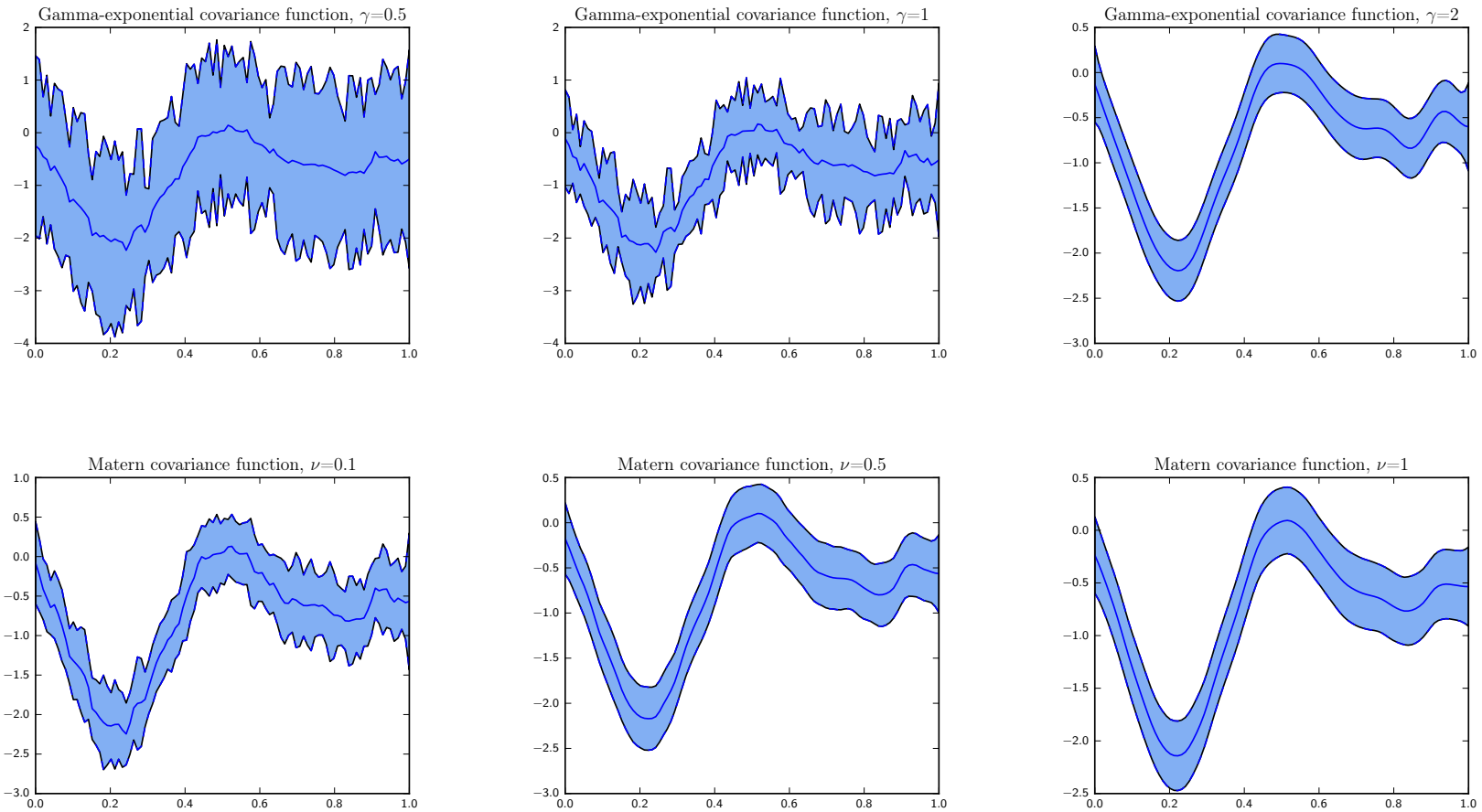


Figure: Gamma-exponential and Matern covariance functions

Section 2

Gaussian Process Regression

Problem statement and notation

- $\{(x_i, f_i)|i = 1, \ldots, n\}$ — dataset, considered to be generated from a Gaussian process $f \sim \mathcal{GP}(m(\cdot), k(\cdot, \cdot))$, let $x \in \mathbb{R}^d$.
- $X \in \mathbb{R}^{n \times d}$ — the matrix, comprised of data points $x_1, \ldots, x_n$.
- $f \in \mathbb{R}^n$ — the vector of target values $f_1, \ldots, f_n$.
- $y \in \mathbb{R}^n$ — the noisy version of f: $y \sim \mathcal{N}(y|f, \sigma_n^2 I)$
- $X_* \in \mathbb{R}^{k \times d}$ — new (test) data points.
- $f_* \in \mathbb{R}^k$ — the desired vector of process values at new data points X_*.
- $K(X, X) \in \mathbb{R}^{n \times n}$ — the matrix, comprised of pairvise values of the covariance function $k(\cdot, \cdot)$ of the underlying process:

$$K(X, X)_{ij} = k(x_i, x_j).$$

- $K(X, X_*) \in \mathbb{R}^{n \times k}$ — the matrix, defined similarly to the $K(X, X)$.
- $K(X_*, X) = K(X, X_*)$.

We want to obtain the predictive distribution

$$p(f_*|X_*, X, y).$$

Noise-free case

Let us consider the noise-free case first:

$$y = f.$$

We put the following prior on our model: the data is generated from a zero-mean gaussian process with covariance function $k(\cdot, \cdot)$:

$$f \sim \mathcal{GP}(0, k(\cdot, \cdot)).$$

This prior is not limiting, because zero-mean prior does not imply a zero-mean predictive distribution.

Noise-free case

As f and f_* are assumed to be generated from the same gaussian proces, we have the following joint distribution

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

Marginalizing this distribution, we obtain the predictive

$$f_*|X_*, X, f \sim \mathcal{N}(\hat{m}, \hat{K}),$$

where

$$\mathbb{E}[f_*|f] = \hat{m} = K(X_*,X)K(X,X)^{-1}f,$$

$$\text{cov}(f_*|f) = \hat{K} = K(X_*,X_*) - K(X_*,X)K(X,X)^{-1}K(X,X_*).$$

Noisy case

In the noisy case, we have a slightly different model:

$$y = f + \varepsilon,$$

where $\varepsilon \sim \mathcal{N}(0, \sigma_n^2 I)$.
We can then rewrite the joint distribution as

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

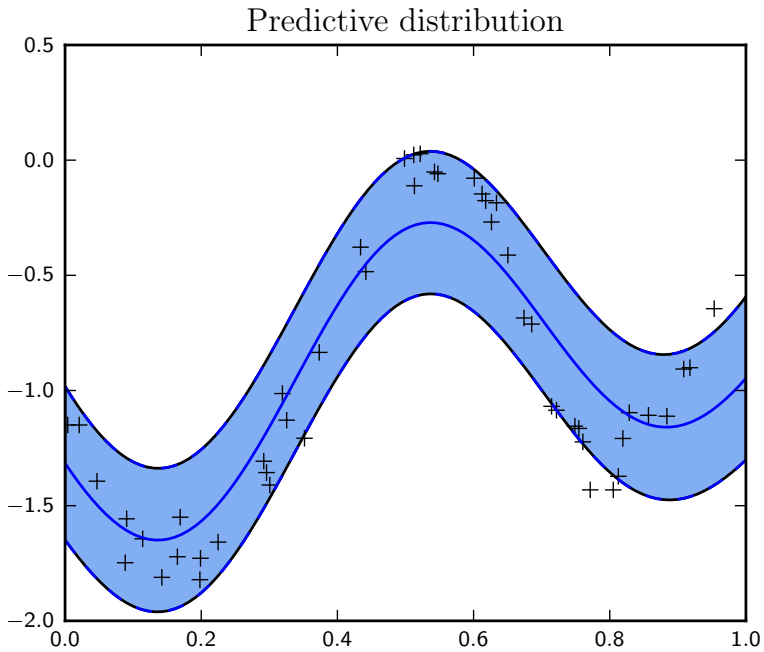
Marginalizing it once again we obtain the predictive

$$f_*|y \sim \mathcal{N}(\hat{m}, \hat{K}),$$

$$\mathbb{E}[f_*|y] = \hat{m} = K(X_*,X)(K(X,X) + \sigma_n^2 I)^{-1} y,$$

$$\operatorname{cov}(f_*|y) = \hat{K} = K(X_*,X_*) - K(X_*,X)(K(X,X) + \sigma_n^2 I)^{-1} K(X,X_*).$$

Example



As we can see, the method struggles to explain the data. In order to deal with this problem, we can tweak the covariance function. The covariance functions usualy have a set of parameters, which we will refer to as covariance (or kernel) hyper-parameters. Varying these parameters, we can find a better model for the data.

Marginal likelihood

In order to find the best set of kernel hyper-parameters, we maximize the marginal likelihood with respect to them. In the case of gaussian process regression, this likelihood is given by

$$p(y) = \mathcal{N}(y|0, K(X,X) + \sigma_n^2 I) =$$

$$= -\frac{1}{2} y^T (K(X,X) + \sigma_n^2 I)^{-1} y - \frac{1}{2} \log |K(X,X) + \sigma_n^2 I| - \frac{n}{2} \log 2\pi.$$

If $k(\cdot, \cdot)$ is a differentiable function of it's hyper-parameters (which is usually true), $p(y)$ also is, and can be maximized with gradient-based optimization methods.

Example

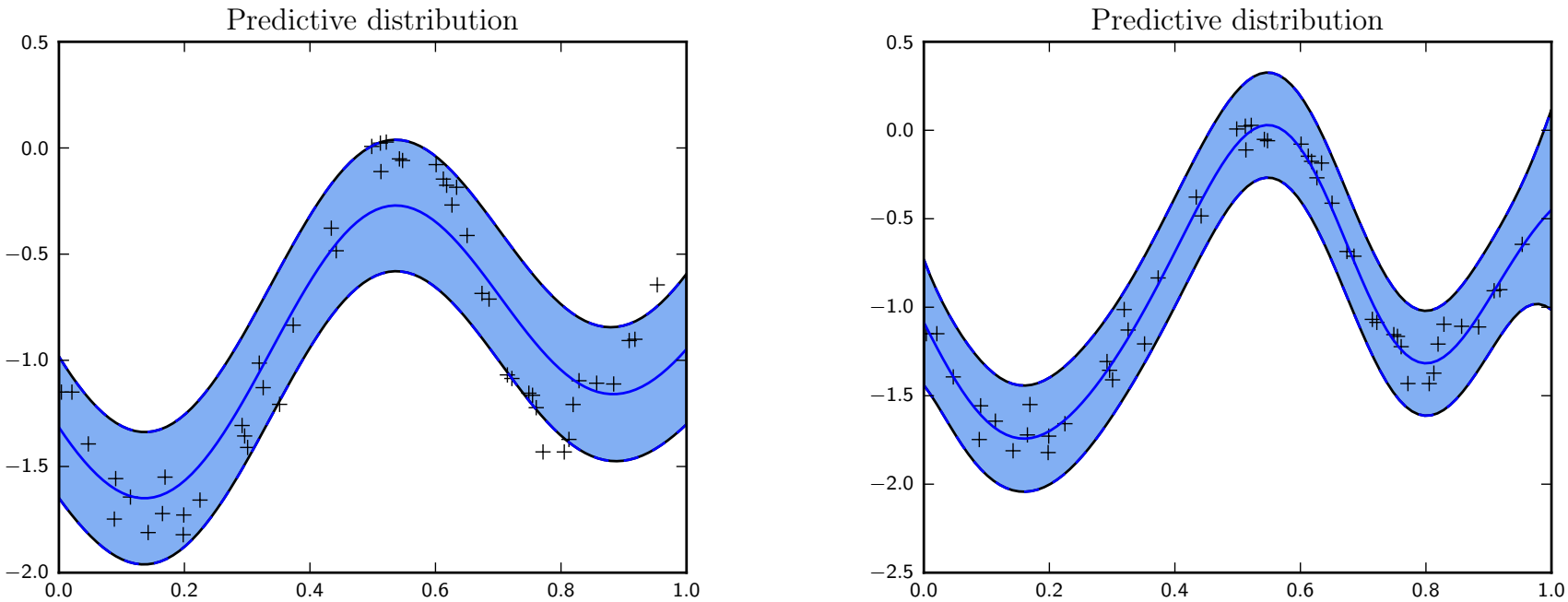


Figure: Predictive distribution before and after hyper-parameter adaptation

As we can see, after adaptation of kernel hyper-parameters, the method does a better job, explaining the data.

Computational Complexity

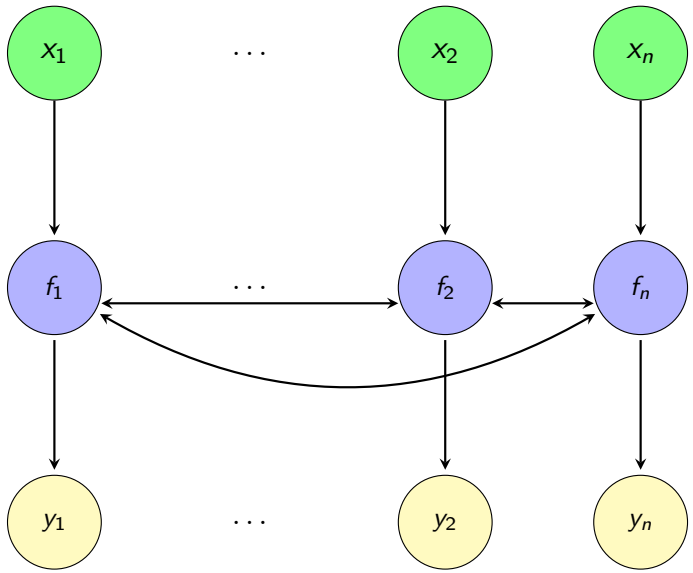
The computational complexity of the gaussian process regression is determined by the complexity of inversing the $K(X, X)$ matrix, and thus scales as $O(n^3)$. This complexity makes the method unaplicable to big problems and thus approximate aproaches are needed.

Section 3

Inducing Inputs

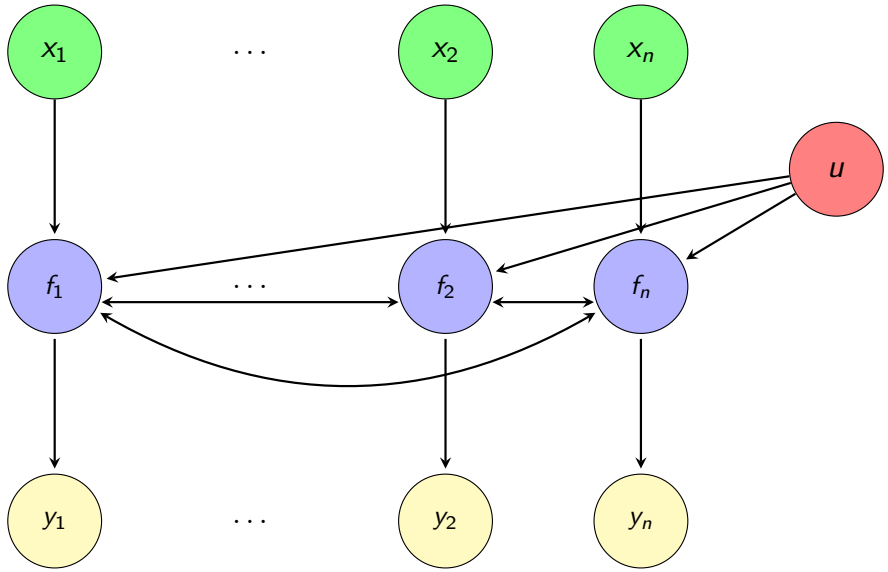
Inducing Inputs

The graphical model for the gaussian process regression looks like this.



Inducing Inputs

Now we slightly change the model, adding a set of latent variables u.



The joint probability of latent and observable variables now is given by

$$p(y, f, u) = p(y|f)p(f|u)p(u).$$

Inducing Inputs

The latent variables u are referred to as inducing inputs. The intuition behind them is that they are considered as the values of the process at new data points $z_1, \ldots, z_m$. We will have to introduce some more notation now.

- $Z_m \in \mathbb{R}^{m \times d}$ — the matrix, comprised of the coordinates of the inducing inputs inputs $z_1, \ldots, z_m$.
- $K_{nn} = K(X, X)$
- $K_{mm} = K(Z_m, Z_m)$
- $K_{mn} = K(Z_m, X)$
- $K_{nm} = L(X, Z_m) = K_{mn}^T$

As u_i are considered to be generated from the same gaussian process, as f_i, we have the following formulas.

$$p(u) = \mathcal{N}(u|0, K_{mm}),$$

$$p(f|u) = \mathcal{N}(f|K_{nm}K_{mm}^{-1}u, \tilde{K}),$$

where $\tilde{K} = K_{nn} - K_{nm}K_{mm}^{-1}K_{mn}$.

Evidence Lower Bound

The standard variational lower bound for the marginal likelihood $p(y)$ for our augmented model is

$$p(y) \geq \mathbb{E}_{q(u,f)} \log \frac{p(y,u,f)}{q(u,f)} = \mathbb{E}_{q(u,f)} p(y|f) - \mathrm{KL}\left(q(u,f) \,||\, p(u,f)\right).$$

Our model implies $\mathbb{E}_{q(u,f)} p(y|f) = \mathbb{E}_{q(f)} p(y|f)$, where $q(f)$ is the marginal of $q(u,f)$.
We will consider the variational distributions of the following form:

$$q(u,f) = p(f|u)q(u),$$

where $q(u) \sim \mathcal{N}(u|\mu, \Sigma)$. This implies $q(f)$

$$q(f) = \int p(u|f)q(u)du =$$

$$\mathcal{N}(f|K_{nm}K_{mm}^{-1}\mu, K_{nn} + K_{nm}K_{mm}^{-1}(\Sigma - K_{mm})K_{mm}^{-1}K_{mn}).$$

Evidence Lower Bound

Now, consider the KL-divergence in the lower bound we've devised.

$$\mathrm{KL}\left(q(u,f) \mid\mid p(u,f)\right) = \mathrm{KL}\left(q(u)p(f|u) \mid\mid p(u)p(f|u)\right) = \mathrm{KL}\left(q(u) \mid\mid p(u)\right).$$

Finally, the lower bound is

$$p(y) \geq \mathbb{E}_{q(f)} p(y|f) + \mathrm{KL}\left(q(u) \mid\mid p(u)\right).$$

Note, that although, we've devised this bound for the regression problem, we never used the fact, that we are actually performing regression. This bound holds for binary classification problem as well.
However, in the case of GP-regression, the right-hand side of the bound can be computed analytically in a closed form.

SVI method

Substituting the normal distributions $q(u)$, $p(u)$, $q(f)$ and $p(y|f)$ back into the lower bound, we obtain the following inequality.

$$p(y) \geq \sum_{i=1}^{n} \left(\log \mathcal{N}(y_i | k_i^T K_{mm}^{-1} \mu, \sigma_n^2) - \frac{1}{2\sigma_n^2} \tilde{K}_{ii} - \frac{1}{2} \mathrm{tr}(\Sigma \Lambda_i) \right) -$$

$$- \frac{1}{2} \left(\log \frac{|K_{mm}|}{|\Sigma|} - m + \mathrm{tr}(K_{mm}^{-1} \Sigma) + \mu^T K_{mm}^{-1} \mu \right),$$

where $\Lambda_i = \frac{1}{\sigma_n^2} K_{mm}^{-1} k_i k_i^T K_{mm}^{-1}$, and k_i is the i-th column of the matrix K_{mn}. This lower can be maximized with respect to kernel hyper-parameters and variational parameters μ, Σ using the stochastic optimization techniques. The authors of the method sudgest using the stochastic gradient descent with natural gradients for variational parameters. The complexity of computing a stochastic update for one object is $O(m^3)$.

Titsias's method

The lower bound we devised can also be maximized with respect to variational parameters analytically. The optimal distribution $q^*(u) \sim \mathcal{N}(u|\hat{u}, \Lambda^{-1})$, where

$$\Lambda = \frac{1}{\sigma_n} K_{mm}^{-1} K_{mn} K_{nm} K_{mm}^{-1} + K_{mm}^{-1},$$

$$\hat{u} = \frac{1}{\sigma_n} \Lambda^{-1} K_{mm}^{-1} K_{mn} y.$$

Substituting this distribution back to the ELBO, we obtain

$$p(y) \geq -\frac{1}{2} \left(n \log 2\pi + \log |B| + y^T B^{-1} y + \frac{1}{\sigma_n^2} \text{tr}(\tilde{K}) \right),$$

where $B = \sigma_n^2 I + K_{nm} K_{mm}^{-1} K_{mn}$. The complexity of computing the optimal distribution parameters, the lower bound and it's gradients is $O(nm^2)$. However, we can not apply stochastic optimization in this case.

Example

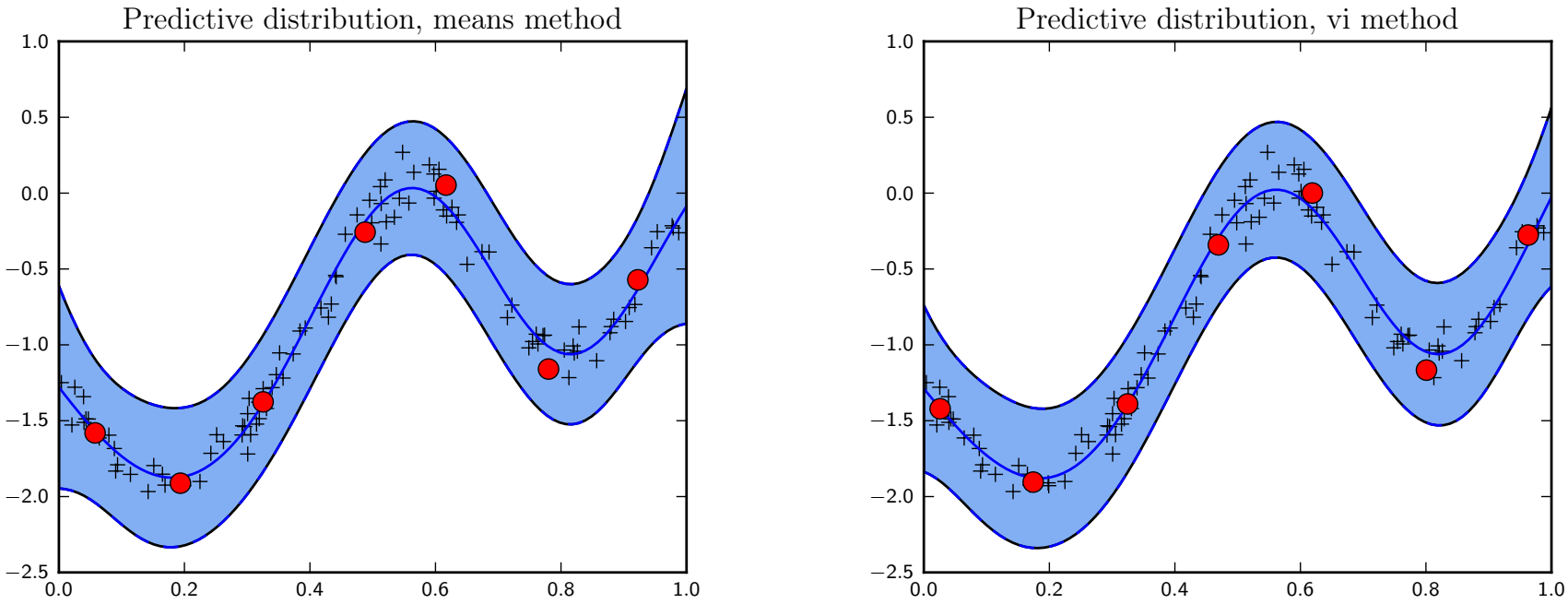


Figure: Example of two implementations of the Titsias's method. The vi method maximizes the lower bound with respect to the positions of inducing inputs, while the means method just uses the K-means cluster centers as inducing point positions.