9. Gaussian Processes - Regression

Repetition: Regularized Regression

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\left(\mathbf{w}^T\phi(x) - t_i\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

$$\nabla\tilde{E}(\mathbf{w}) = \sum_{i=1}^{N}\left(\mathbf{w}^T\phi(x) - t_i\right)\phi(x)^T + \lambda\mathbf{w}^T \doteq \mathbf{0}^T$$

$$\mathbf{w} = (\lambda I + \Phi^T\Phi)^{-1}\Phi^T\mathbf{t}$$

Before, we solved for **w** using the pseudoinverse.

But: we can kernelize this problem as well!

First step: Matrix inversion lemma

Kernelized Regression

Thus, we have:

$$\mathbf{w} = (\lambda I_D + \Phi^T\Phi)^{-1}\Phi^T\mathbf{t} = \Phi^T(\lambda I_N + \Phi\Phi^T)^{-1}\mathbf{t}$$

by defining: $K = \Phi\Phi^T$ $\qquad$ $\mathbf{a} = (\lambda I_N + K)^{-1}\mathbf{t}$

we get:

$$y(\mathbf{x}) = \phi(\mathbf{x})^T\mathbf{w} = \phi(\mathbf{x})^T\Phi^T\mathbf{a}$$

$$= \mathbf{k}(\mathbf{x})^T(K + \lambda I_N)^{-1}\mathbf{t}$$

(same result as last lecture)

This means that the predicted output is a **linear combination** of the training outputs, where the coefficients depend on the similarities to the training input.

Motivation

- We have found a way to predict function values of y for new input points $\mathbf{x}$
- As we used regularized regression, we can equivalently find the **predictive distribution** by marginalizing out the parameters $\mathbf{w}$
- Can we find a closed form for that distribution?
- How can we model the uncertainty of our prediction?
- Can we use that for classification?

Gaussian Marginals and Conditionals

Before we start, we need some formulae:

Assume we have two variables $\mathbf{x}_a$ and $\mathbf{x}_b$ that are jointly Gaussian distributed, i.e. $\mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \Sigma)$

with

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \qquad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix}$$

Then the cond. distribution $p(\mathbf{x}_a \mid \mathbf{x}_b) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_{a|b}, \Sigma_{a|b})$

where $\boldsymbol{\mu}_{a|b} = \boldsymbol{\mu}_a + \Sigma_{ab}\Sigma_{bb}^{-1}(\mathbf{x}_b - \boldsymbol{\mu}_b)$

and $\Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$ "Schur Complement"

The marginal is $p(\mathbf{x}_a) = \mathcal{N}(\mathbf{x}_a \mid \boldsymbol{\mu}_a, \Sigma_{aa})$

Gaussian Marginals and Conditionals

Main idea of the proof for the conditional (using inverse of block matrices):

$$\begin{pmatrix}\Sigma_{aa} & \Sigma_{ab}\\ \Sigma_{ba} & \Sigma_{bb}\end{pmatrix}^{-1} = \begin{pmatrix} I & 0 \\ -\Sigma_{bb}^{-1}\Sigma_{ba} & I\end{pmatrix}\begin{pmatrix}(\Sigma/\Sigma_{bb})^{-1} & 0\\ 0 & \Sigma_{bb}^{-1}\end{pmatrix}\begin{pmatrix} I & -\Sigma_{ab}\Sigma_{bb}^{-1}\\ 0 & I\end{pmatrix}$$

The lower line corresponds to a quadratic form that is only dependent on $p(\mathbf{x}_b)$, i.e. the rest can be identified with the conditional Normal distribution $p(\mathbf{x}_a \mid \mathbf{x}_b)$.

(for details see, e.g. Bishop or Murphy)

Definition

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

The number of random variables can be **infinite**!

This means: a GP is a Gaussian distribution over **functions**!

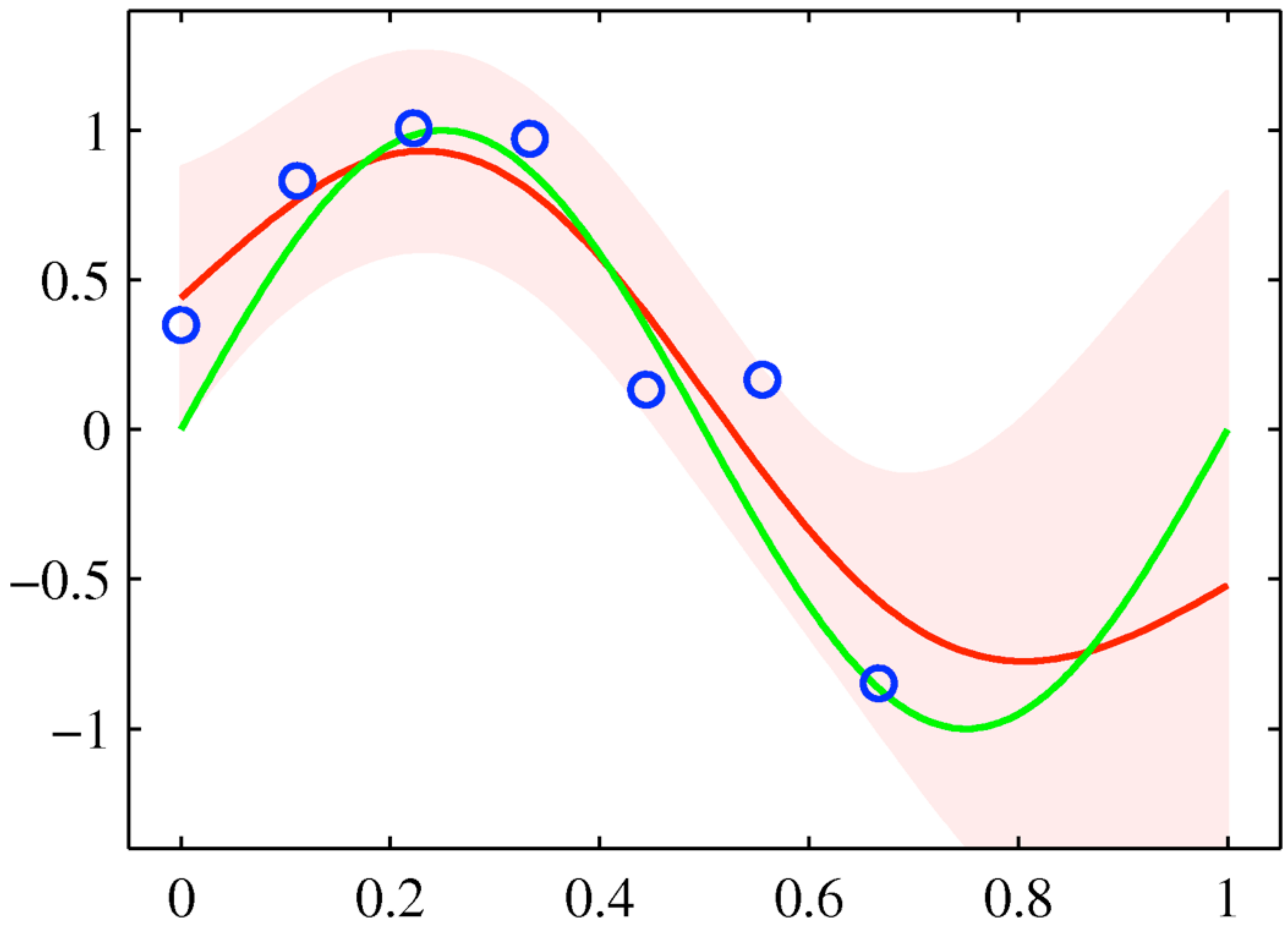
To specify a GP we need:

mean function: $m(\mathbf{x}) = \mathbb{E}[y(\mathbf{x})]$

covariance function:

$$k(\mathbf{x}_1, \mathbf{x}_2) = \mathbb{E}[y(\mathbf{x}_1) - m(\mathbf{x}_1)y(\mathbf{x}_2) - m(\mathbf{x}_2)]$$

Example



- green line: sinusoidal data source
- blue circles: data points with Gaussian noise
- red line: mean function of the Gaussian process

How Can We Handle Infinity?

Idea: split the (infinite) number of random variables into a finite and an infinite subset.

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_f \\ \mathbf{x}_i \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu}_f \\ \boldsymbol{\mu}_i \end{pmatrix}, \begin{pmatrix} \Sigma_f & \Sigma_{fi} \\ \Sigma_{fi}^T & \Sigma_i \end{pmatrix} \right)$$

finite part

infinite part

From the marginalization property we get:

$$p(\mathbf{x}_f) = \int p(\mathbf{x}_f, \mathbf{x}_i) d\mathbf{x}_i = \mathcal{N}(\mathbf{x}_f \mid \boldsymbol{\mu}_f, \Sigma_f)$$

This means we can use finite vectors.

A Simple Example

In Bayesian linear regression, we had $y(\mathbf{x}) = \phi(\mathbf{x})^T \mathbf{w}$ with prior probability $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \Sigma_p)$. This means:

$$\mathbb{E}[y(\mathbf{x})] = \phi(\mathbf{x})^T \mathbb{E}[\mathbf{w}] = \mathbf{0}$$

$$\mathbb{E}[y(\mathbf{x}_1) y(\mathbf{x}_2))] = \phi(\mathbf{x}_1)^T \mathbb{E}[\mathbf{w}\mathbf{w}^T] \phi(\mathbf{x}_2) = \phi(\mathbf{x}_1)^T \Sigma_p \phi(\mathbf{x}_2)$$

Any number of function values $y(\mathbf{x}_1), \dots, y(\mathbf{x}_N)$ is jointly Gaussian with zero mean.

The covariance function of this process is

$$k(\mathbf{x}_1, \mathbf{x}_2) = \phi(\mathbf{x}_1)^T \Sigma_p \phi(\mathbf{x}_2)$$

In general, any valid kernel function can be used.

The Covariance Function

The most used covariance function (kernel) is:

$$k(\mathbf{x}_p, \mathbf{x}_q) = \sigma_f^2 \exp(-\frac{1}{2l^2}(\mathbf{x}_p - \mathbf{x}_q)^2) + \sigma_n^2 \delta_{pq}$$

signal variance

length scale

noise variance

It is known as “squared exponential”, “radial basis function” or “Gaussian kernel”.

Other possibilities exist, e.g. the exponential kernel:

$$k(\mathbf{x}_p, \mathbf{x}_q) = \exp(-\theta |\mathbf{x}_p - \mathbf{x}_q|)$$

This is used in the “Ornstein-Uhlenbeck” process.

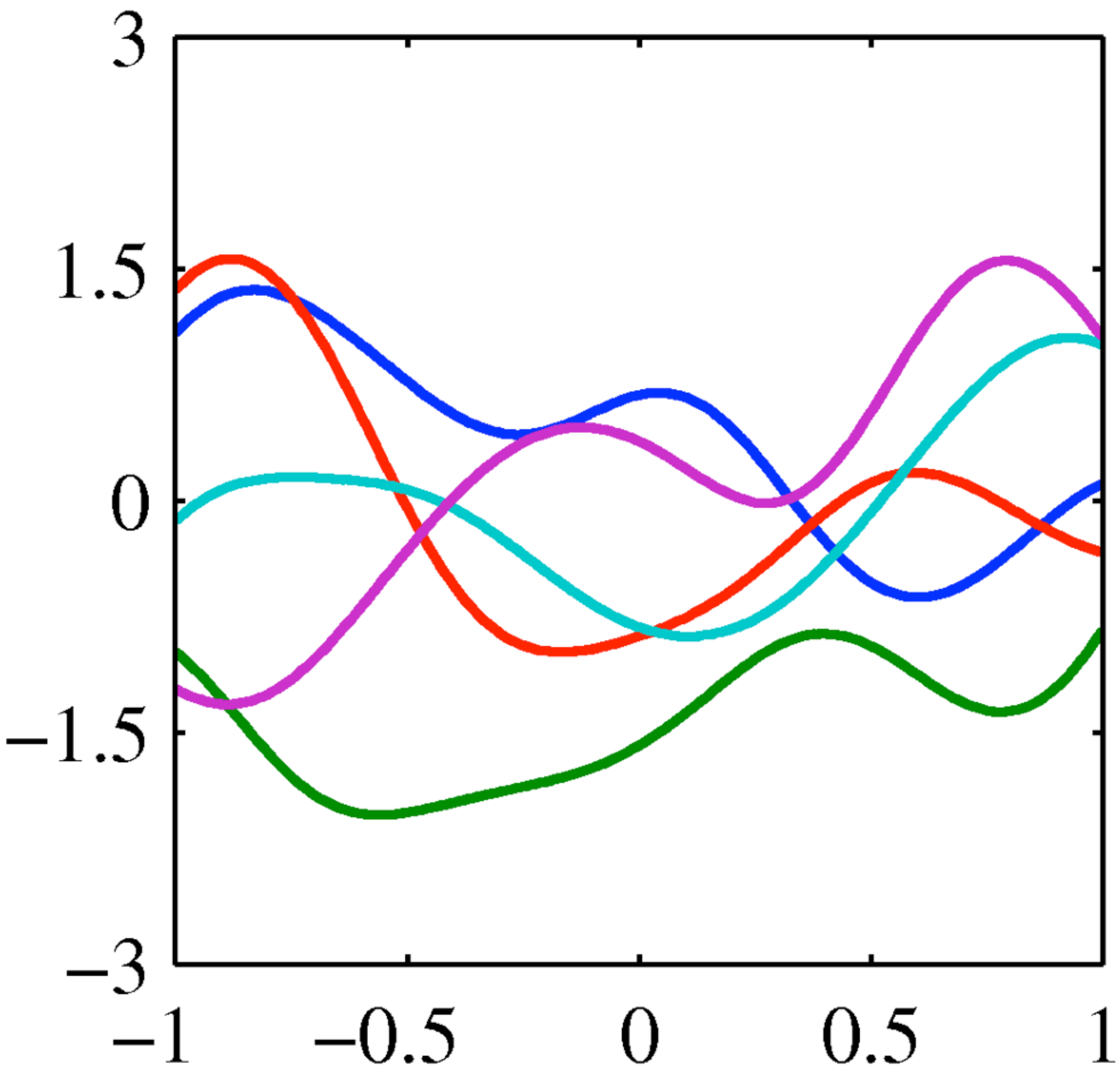
Sampling from a GP

Just as we can sample from a Gaussian distribution, we can also generate samples from a GP. **Every sample will then be a function!**

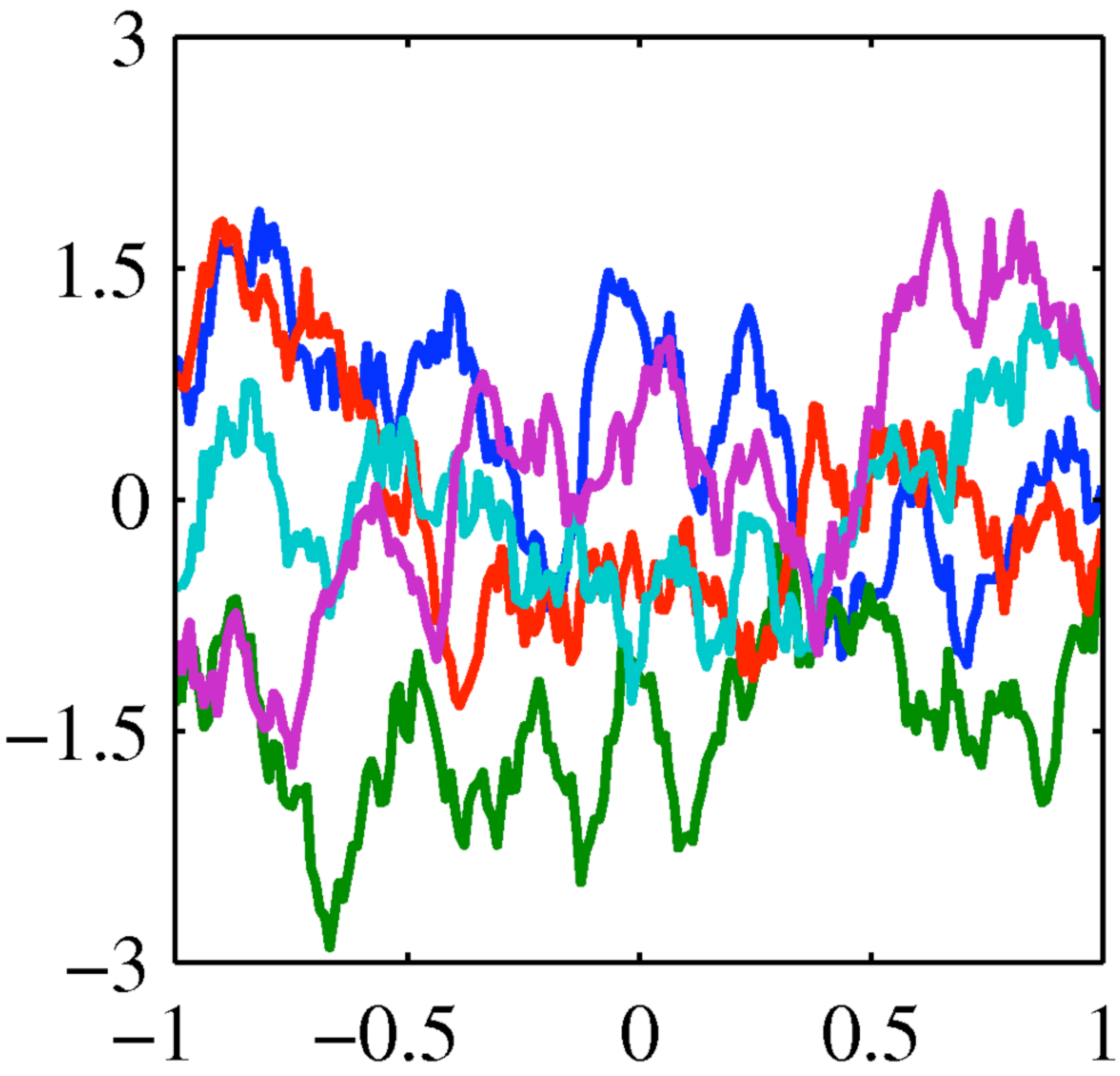
Process:

1. Choose a number of input points $\mathbf{x}_1^*, \ldots, \mathbf{x}_M^*$
2. Compute the covariance matrix K where
$$K_{ij} = k(\mathbf{x}_i^*, \mathbf{x}_j^*)$$
3. Generate a random Gaussian vector from
$$\mathbf{y}_* \sim \mathcal{N}(\mathbf{0}, K)$$
4. Plot the values $\mathbf{x}_1^*, \ldots, \mathbf{x}_M^*$ versus $y_1^*, \ldots, y_M^*$

Sampling from a GP



Squared exponential kernel



Exponential kernel

Prediction with a Gaussian Process

Most often we are more interested in predicting new function values for given input data.

We have:

training data $\mathbf{x}_1, \dots, \mathbf{x}_N \qquad y_1, \dots, y_N$

test input $\mathbf{x}_1^*, \dots, \mathbf{x}_M^*$

And we want test outputs $y_1^*, \dots, y_M^*$

The joint probability is

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{y}_* \end{pmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{pmatrix} K(X,X) & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{pmatrix}\right)$$

and we need to compute $p(\mathbf{y}^* \mid \mathbf{x}^*, X, \mathbf{y})$.

Prediction with a Gaussian Process

In the case of only one test point $\mathbf{x}^*$ we have

$$K(X, \mathbf{x}^*) = \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_*) \\ \vdots \\ k(\mathbf{x}_N, \mathbf{x}_*) \end{pmatrix} = \mathbf{k}_*$$

Now we compute the conditional distribution

$$p(y^* \mid \mathbf{x}^*, X, \mathbf{y}) = \mathcal{N}(y_* \mid \mu_*, \Sigma_*)$$

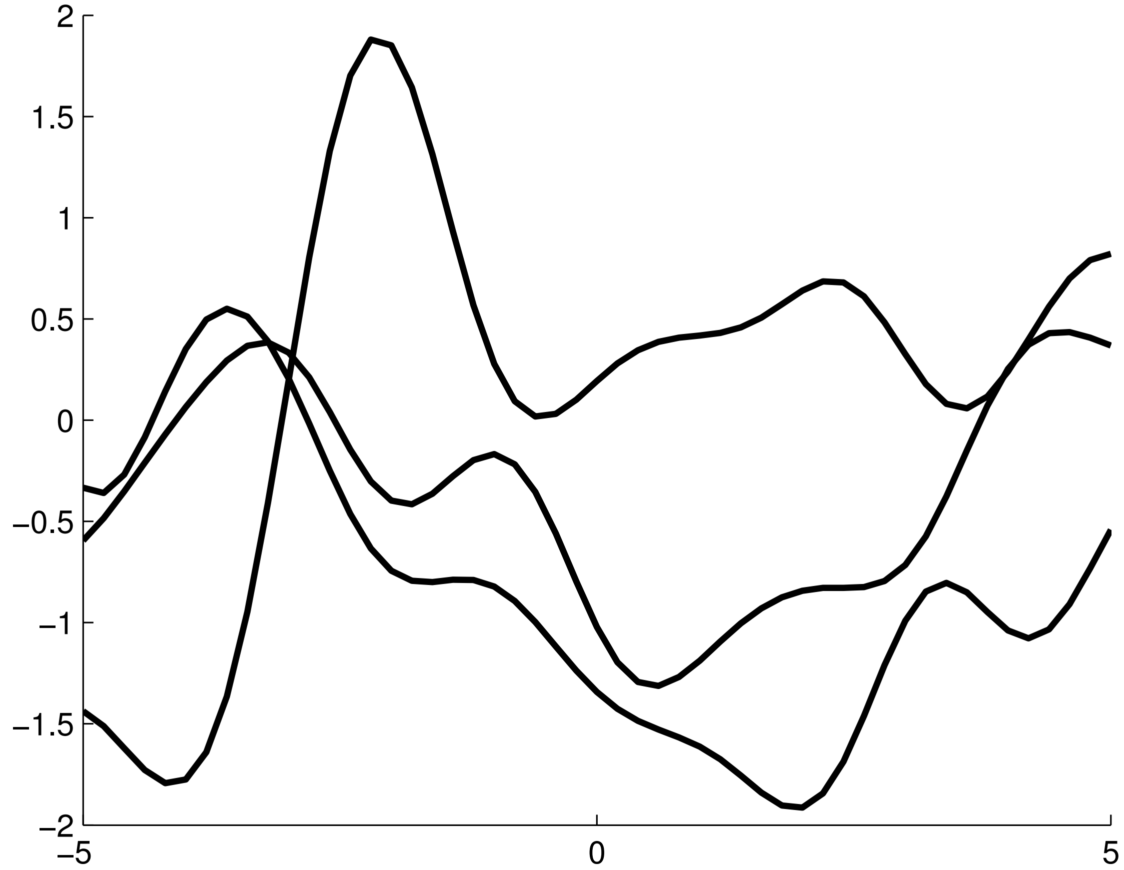
where

$$\mu_* = \mathbf{k}_*^T K^{-1} \mathbf{t}$$

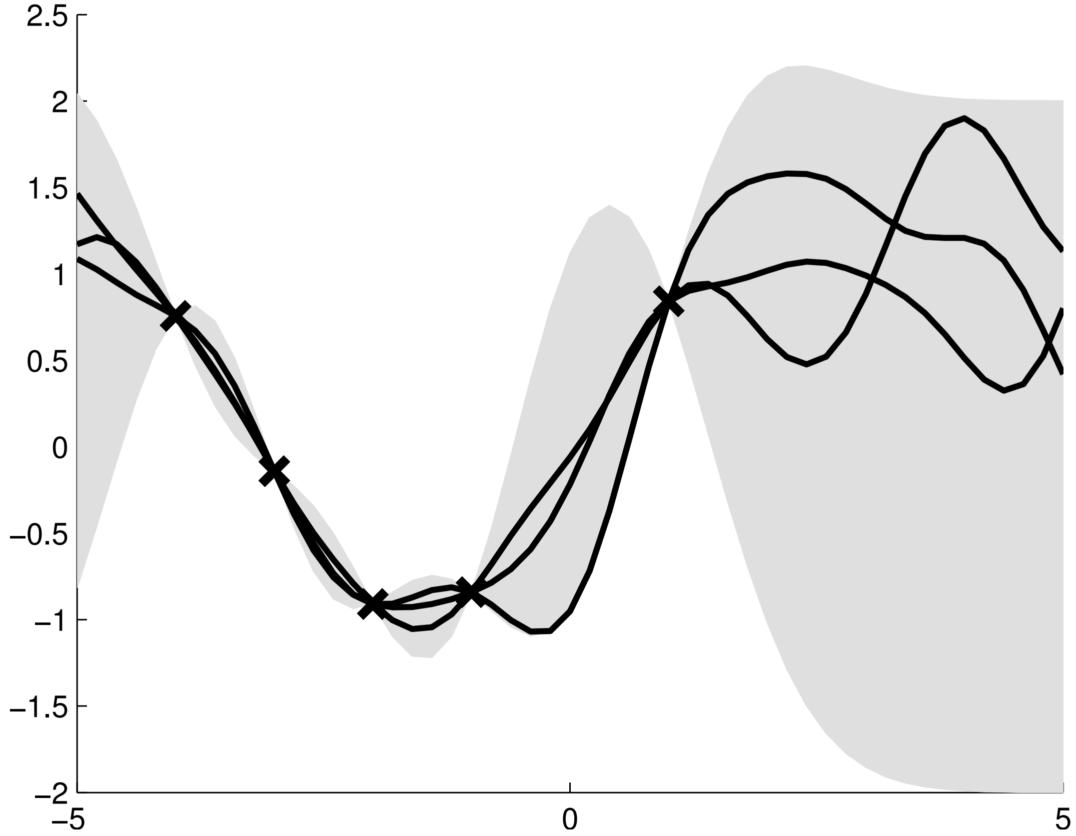
$$\Sigma_* = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^T K^{-1} \mathbf{k}_*$$

This defines the **predictive distribution.**

Example



Functions sampled from
a Gaussian Process prior



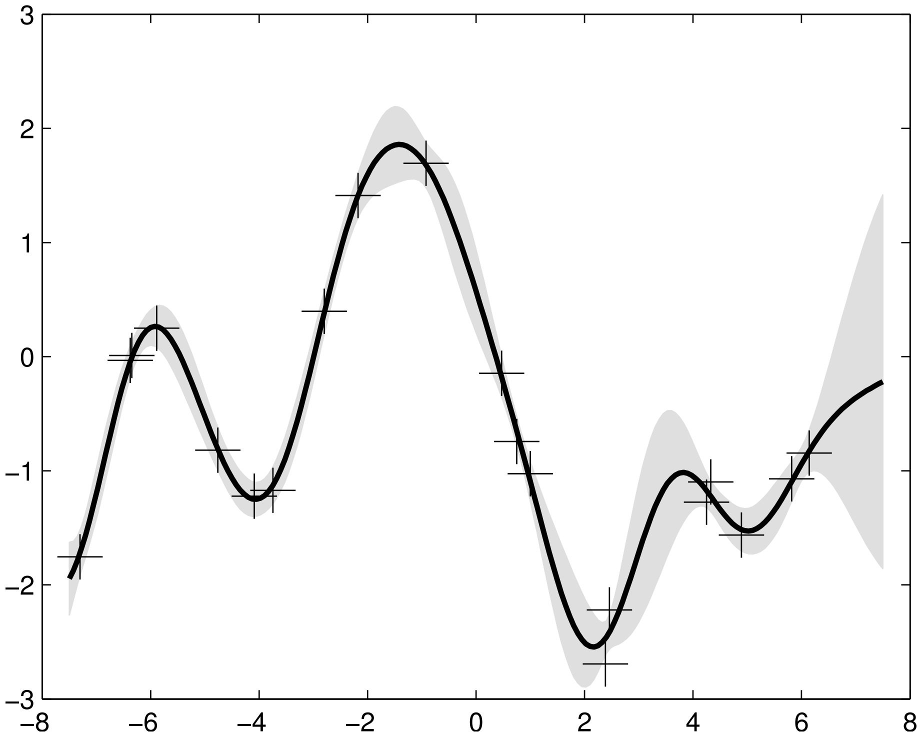
Functions sampled from the
predictive distribution

The predictive distribution is itself a Gaussian process.

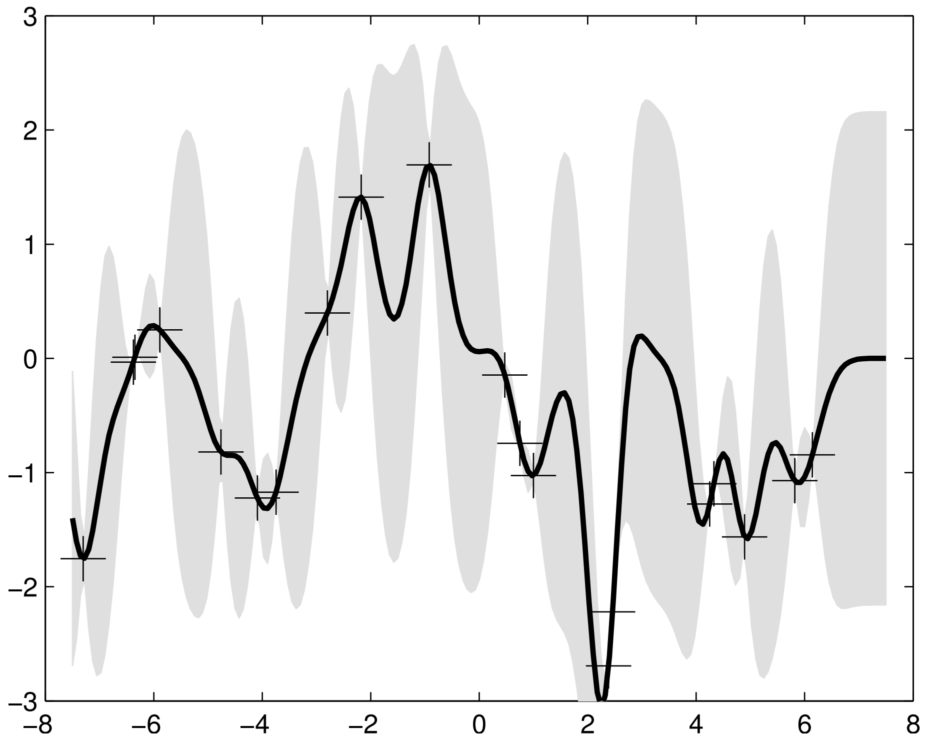
It represents the posterior after observing the data.

The covariance is low in the vicinity of data points.

Varying the Hyperparameters



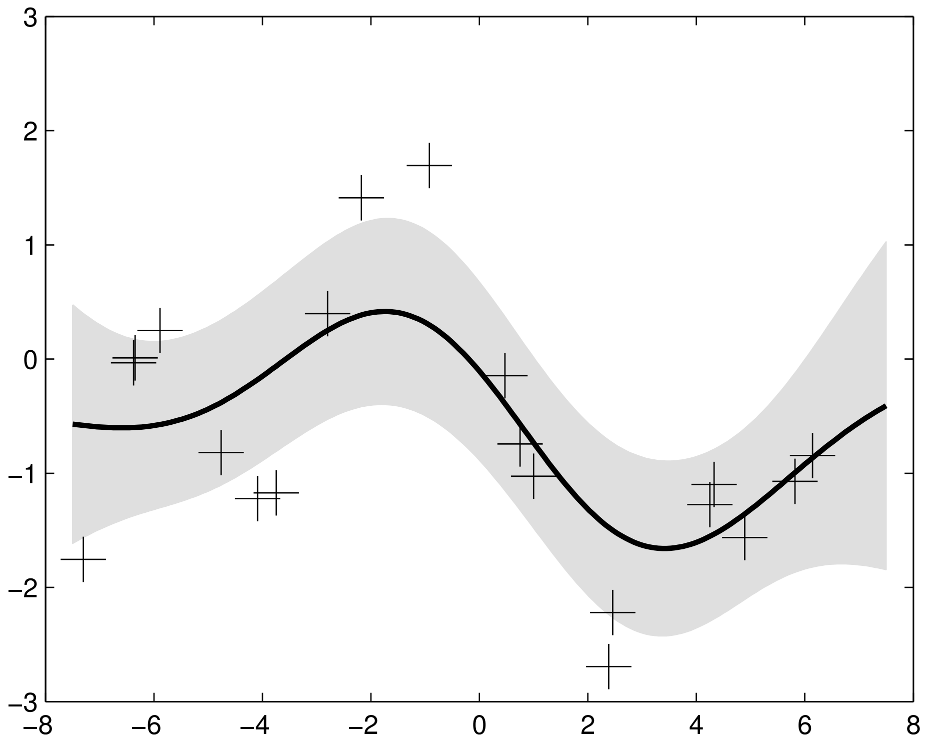
$l = \sigma_f = 1, \quad \sigma_n = 0.1$



$l = 0.3,$

$\sigma_f = 1.08,$

$\sigma_n = 0.0005$



$l = 3$

$\sigma_f = 1.16$

$\sigma_n = 0.89$

- 20 data samples
- GP prediction with different kernel hyper parameters

Varying the Hyperparameters

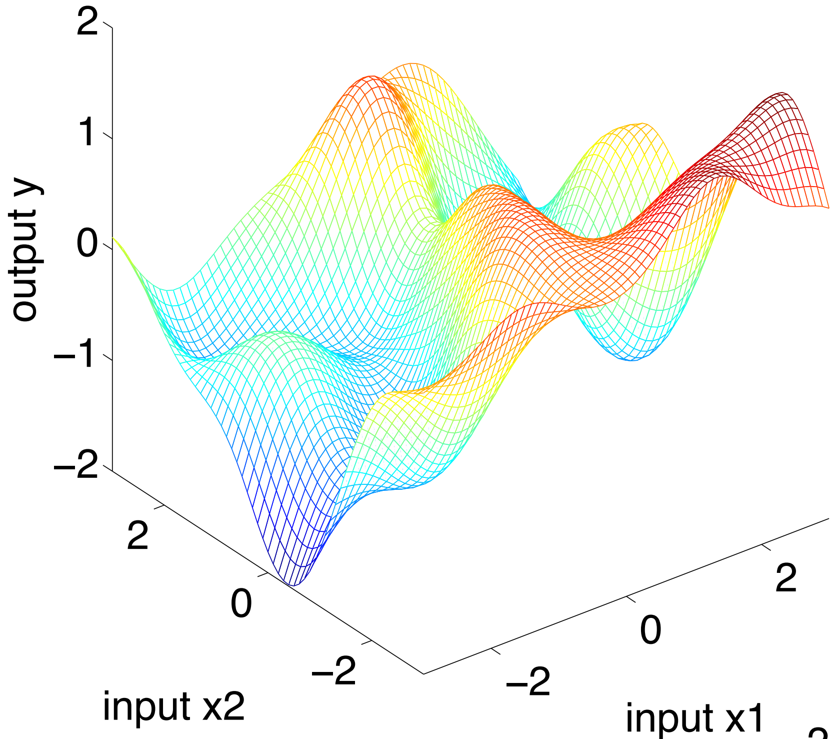
The squared exponential covariance function can be generalized to

$$k(\mathbf{x}_p, \mathbf{x}_q) = \sigma_f^2 \exp(-\frac{1}{2}(\mathbf{x}_p - \mathbf{x}_q)^T M(\mathbf{x}_p - \mathbf{x}_q)) + \sigma_n^2 \delta_{pq}$$

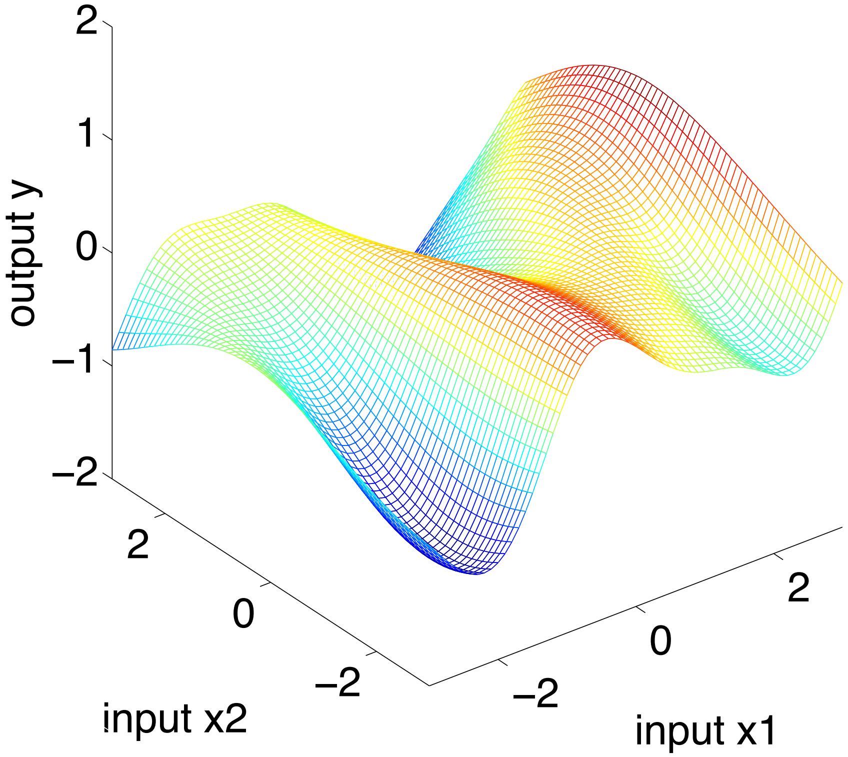
where M can be:

- $M = l^{-2} I$: this is equal to the above case
- $M = \operatorname{diag}(l_1, \ldots, l_D)^{-2}$: every feature dimension has its own length scale parameter
- $M = \Lambda\Lambda^T + \operatorname{diag}(l_1, \ldots, l_D)^{-2}$: here Λ has less than D columns

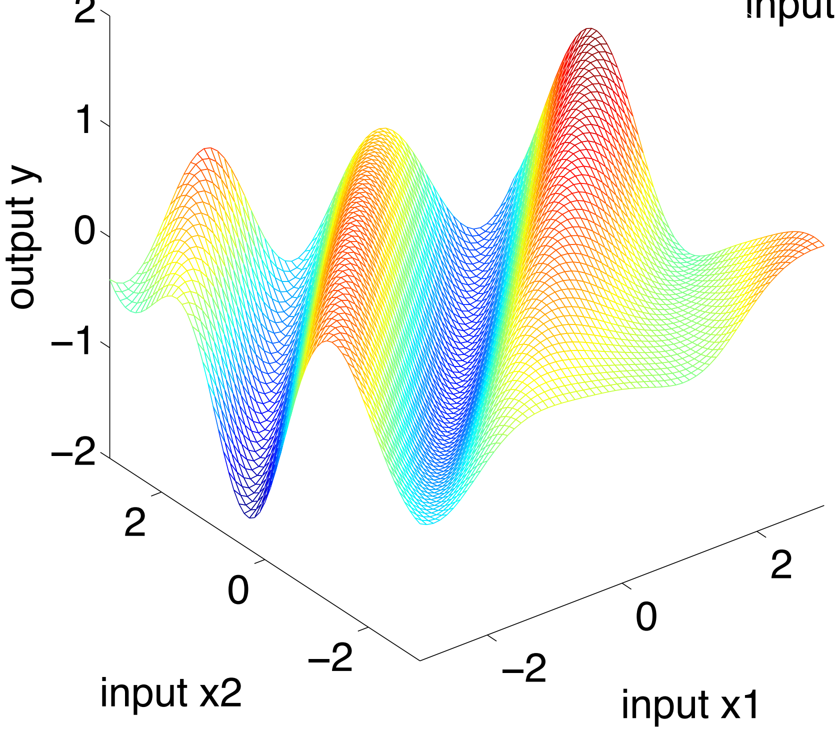
Varying the Hyperparameters



$$M = I$$



$$M = \mathrm{diag}(1, 3)^{-2}$$



$$M = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + \mathrm{diag}(6, 6)^{-2}$$

Implementation

Algorithm 1: GP regression

```
**Data**: training data $(X, \mathbf{y})$, test data $\mathbf{x}_*$
**Input**: Hyper parameters $\sigma_f^2$, $l$, $\sigma_n^2$
$K_{ij} \leftarrow k(\mathbf{x}_i, \mathbf{x}_j)$
$L \leftarrow \texttt{cholesky}(K + \sigma_n^2 I)$
$\boldsymbol{\alpha} \leftarrow L^T \backslash (L \backslash \mathbf{y})$
$\mathbb{E}[f_*] \leftarrow \mathbf{k}_*^T \boldsymbol{\alpha}$
$\mathbf{v} \leftarrow L \backslash \mathbf{k}_*$
$\texttt{var}[f_*] \leftarrow k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^T \mathbf{v}$
$\log p(\mathbf{y} \mid X) \leftarrow -\frac{1}{2}\mathbf{y}^T \boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{N}{2} \log(2\pi)$
```

Training Phase

Test Phase

- Cholesky decomposition is numerically stable
- Can be used to compute inverse efficiently

Estimating the Hyperparameters

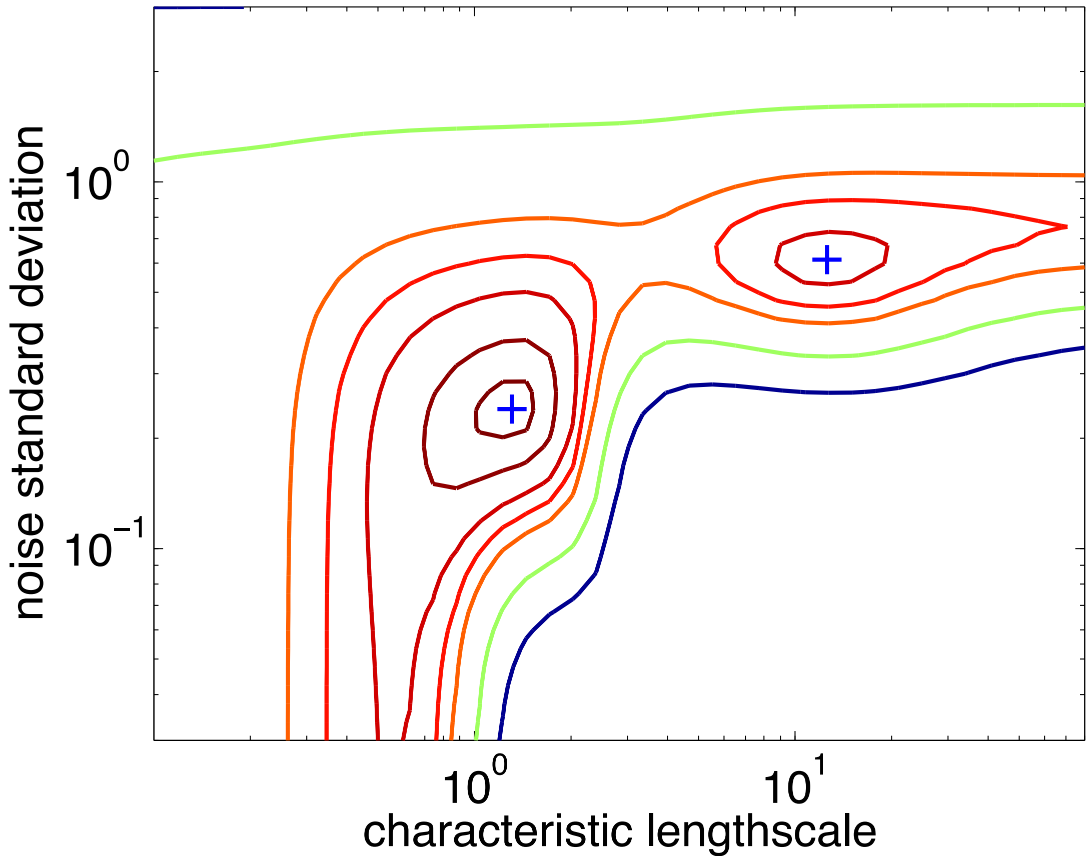
To find optimal hyper parameters we need the **marginal likelihood:**

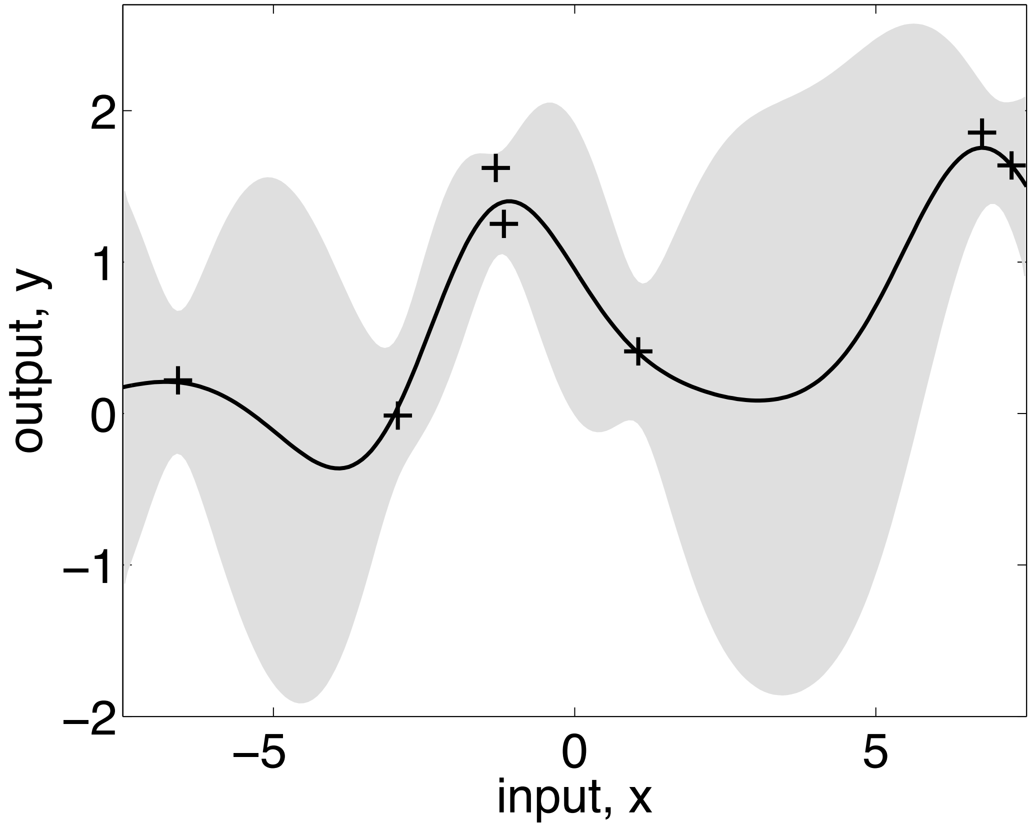
$$p(\mathbf{y} \mid X) = \int p(\mathbf{y} \mid \mathbf{f}, X) p(\mathbf{f} \mid X) d\mathbf{f}$$

This expression implicitly depends on the hyper parameters, but $\mathbf{y}$ and X are given from the training data. It can be computed in closed form, as all terms are Gaussians.

We take the logarithm, compute the derivative and set it to 0. This is the **training** step.

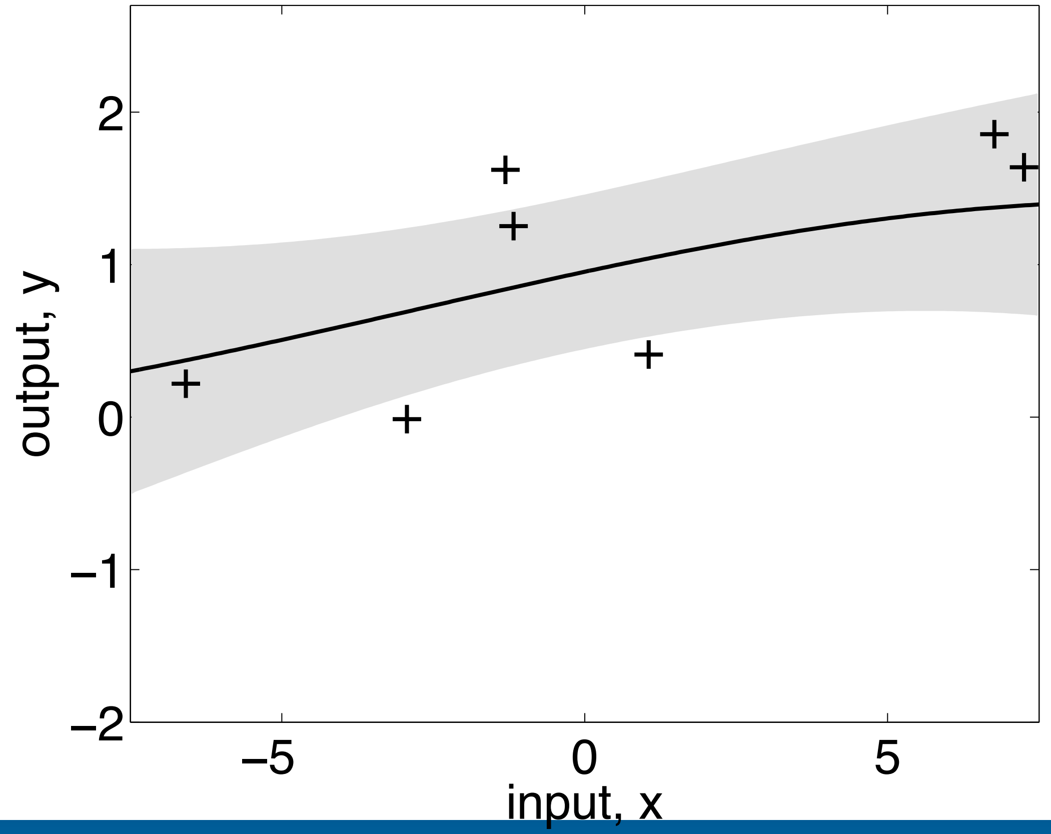
Estimating the Hyperparameters





The log marginal likelihood is not necessarily concave, i.e. it can have local maxima.

The local maxima can correspond to sub-optimal solutions.



Automatic Relevance Determination

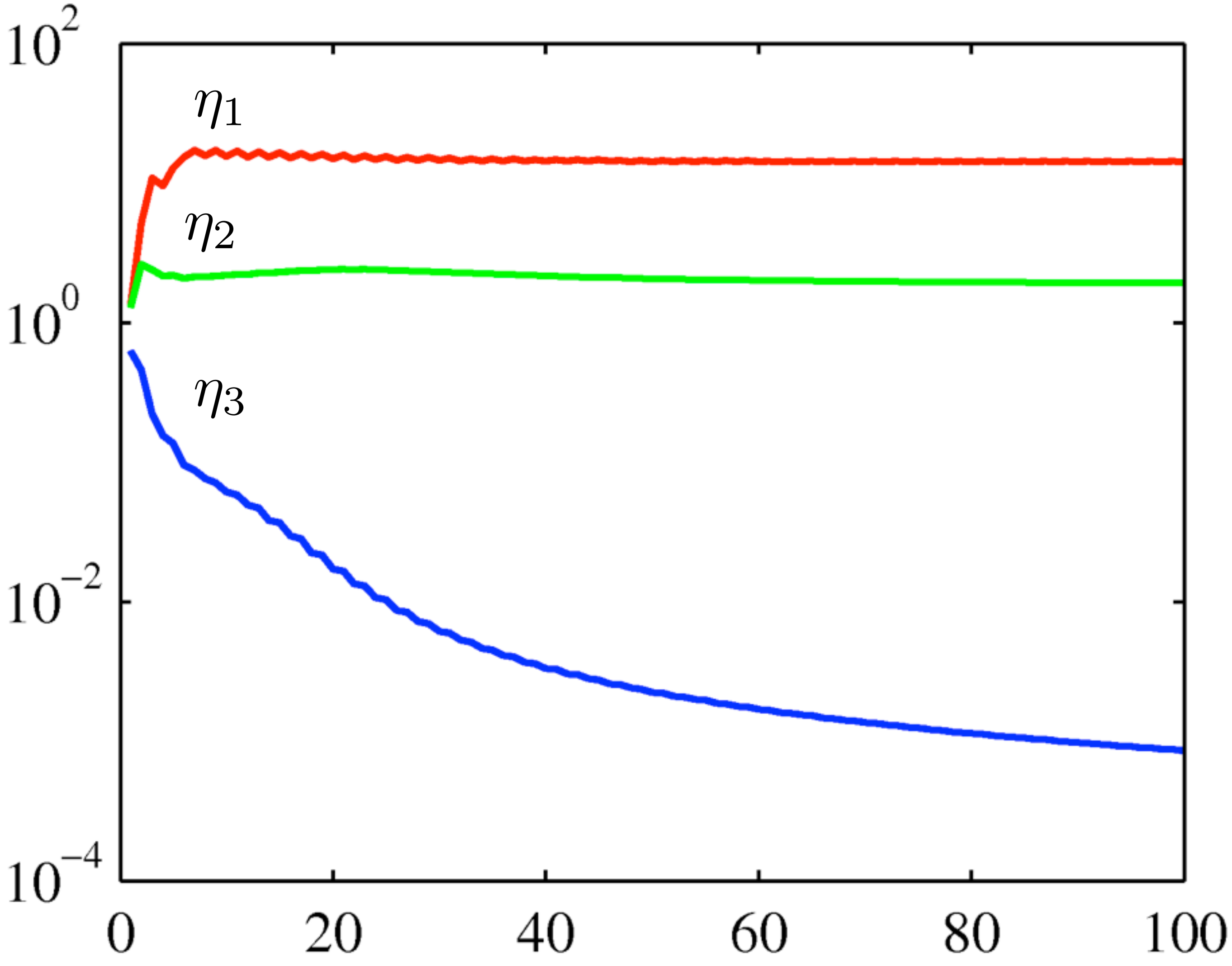
- We have seen how the covariance function can be generalized using a matrix M
- If M is diagonal this results in the kernel function

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f \exp\left(\frac{1}{2}\sum_{i=1}^{D} \eta_i (x_i - x_i')^2\right)$$

- We can interpret the η_i as weights for each feature dimension
- Thus, if the length scale $l_i = 1/\eta_i$ of an input dimension is large, the input is less relevant
- During training this is done automatically

Automatic Relevance Determination

3-dimensional data, parameters η_1 η_2 η_3 as they evolve during training



During the optimization process to learn the hyper-parameters, the reciprocal length scale for one parameter decreases, i.e.:

This hyper parameter is not very relevant!

Gaussian Processes - Classification

Gaussian Processes For Classification

In regression we have $y \in \mathbb{R}$, in binary classification we have $y \in \{-1; 1\}$

To use a GP for classification, we can apply a **sigmoid** function to the posterior obtained from the GP and compute the class probability as:

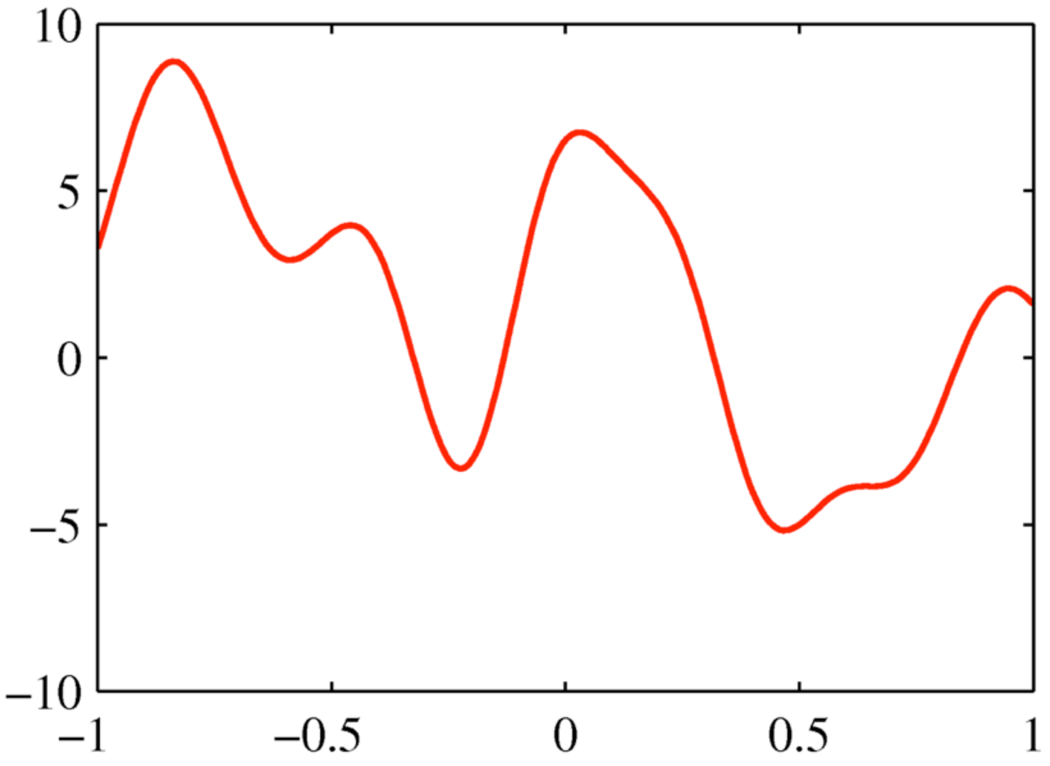
$$p(y = +1 \mid \mathbf{x}) = \sigma(f(\mathbf{x}))$$

If the sigmoid function is symmetric: $\sigma(-z) = 1 - \sigma(z)$ then we have $p(y \mid \mathbf{x}) = \sigma(yf(\mathbf{x}))$.

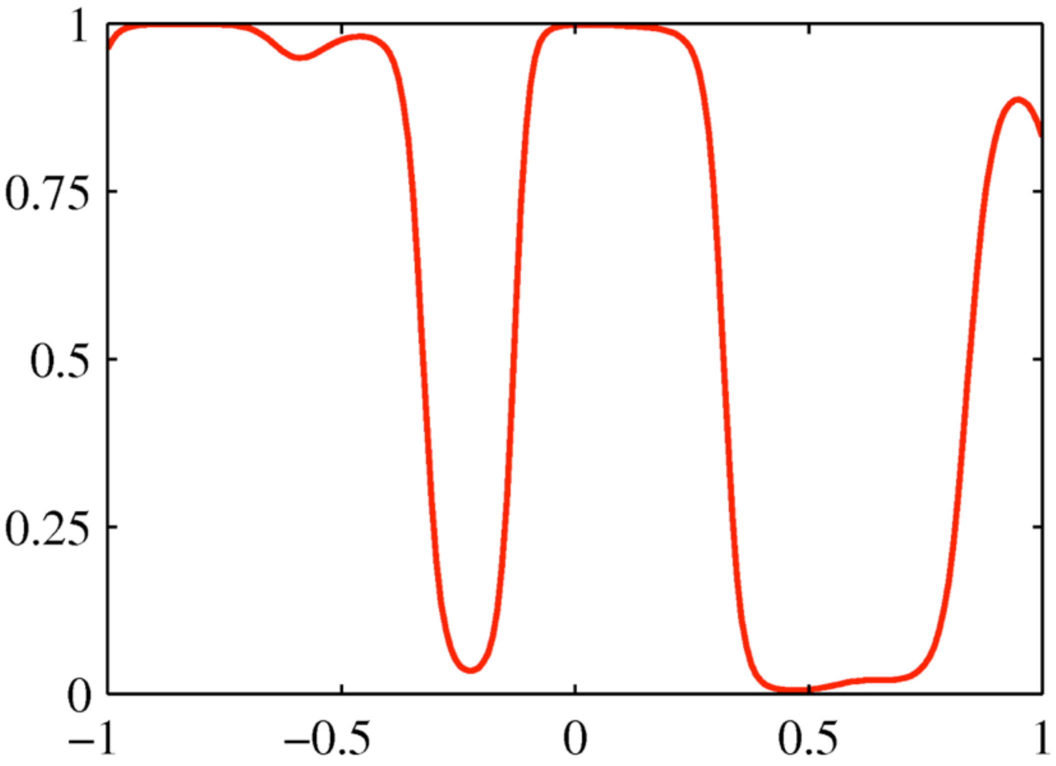
A typical type of sigmoid function is the logistic sigmoid:

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

Application of the Sigmoid Function



Function sampled from a Gaussian Process

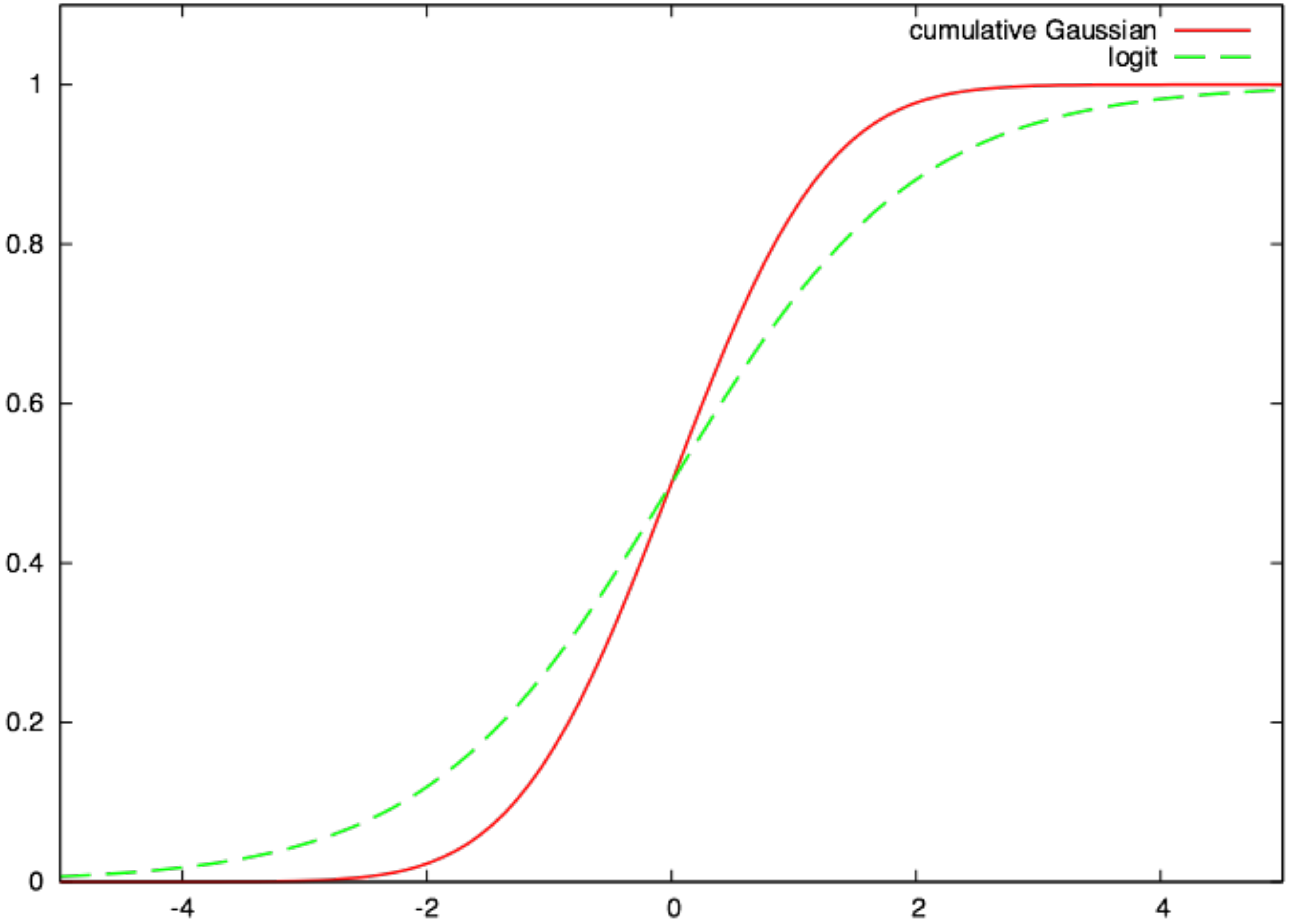


Sigmoid function applied to the GP function

Another symmetric sigmoid function is the **cumulative Gaussian:**

$$\Phi(z) = \int_{-\infty}^{z} \mathcal{N}(x \mid 0, 1) dx$$

Visualization of Sigmoid Functions



The cumulative Gaussian is slightly steeper than the logistic sigmoid

The Latent Variables

In regression, we directly estimated f as

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$

and values of f where observed in the training data. Now only labels +1 or -1 are observed and f is treated as a set of **latent variables.**

A major advantage of the Gaussian process classifier over other methods is that it **marginalizes** over all latent functions rather than maximizing some model parameters.

Class Prediction with a GP

The aim is to compute the predictive distribution

$$p(y_* = +1 \mid X, \mathbf{y}, \mathbf{x}_*) = \int \underbrace{p(y_* \mid f_*)}_{\sigma(f_*)} p(f_* \mid X, \mathbf{y}, \mathbf{x}_*) df_*$$

Class Prediction with a GP

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$$p(y_* = +1 \mid X, \mathbf{y}, \mathbf{x}_*) = \int p(y_* \mid f_*) p(f_* \mid X, \mathbf{y}, \mathbf{x}_*) df_*$$

we marginalize over the latent variables from the training data:

$$p(f_* \mid X, \mathbf{y}, \mathbf{x}_*) = \int p(f_* \mid X, \mathbf{x}_*, \mathbf{f}) p(\mathbf{f} \mid X, \mathbf{y}) d\mathbf{f}$$

predictive distribution of the latent variable (from regression)

Class Prediction with a GP

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$$p(y_* = +1 \mid X, \mathbf{y}, \mathbf{x}_*) = \int p(y_* \mid f_*) p(f_* \mid X, \mathbf{y}, \mathbf{x}_*) df_*$$

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we need the posterior over the latent variables:

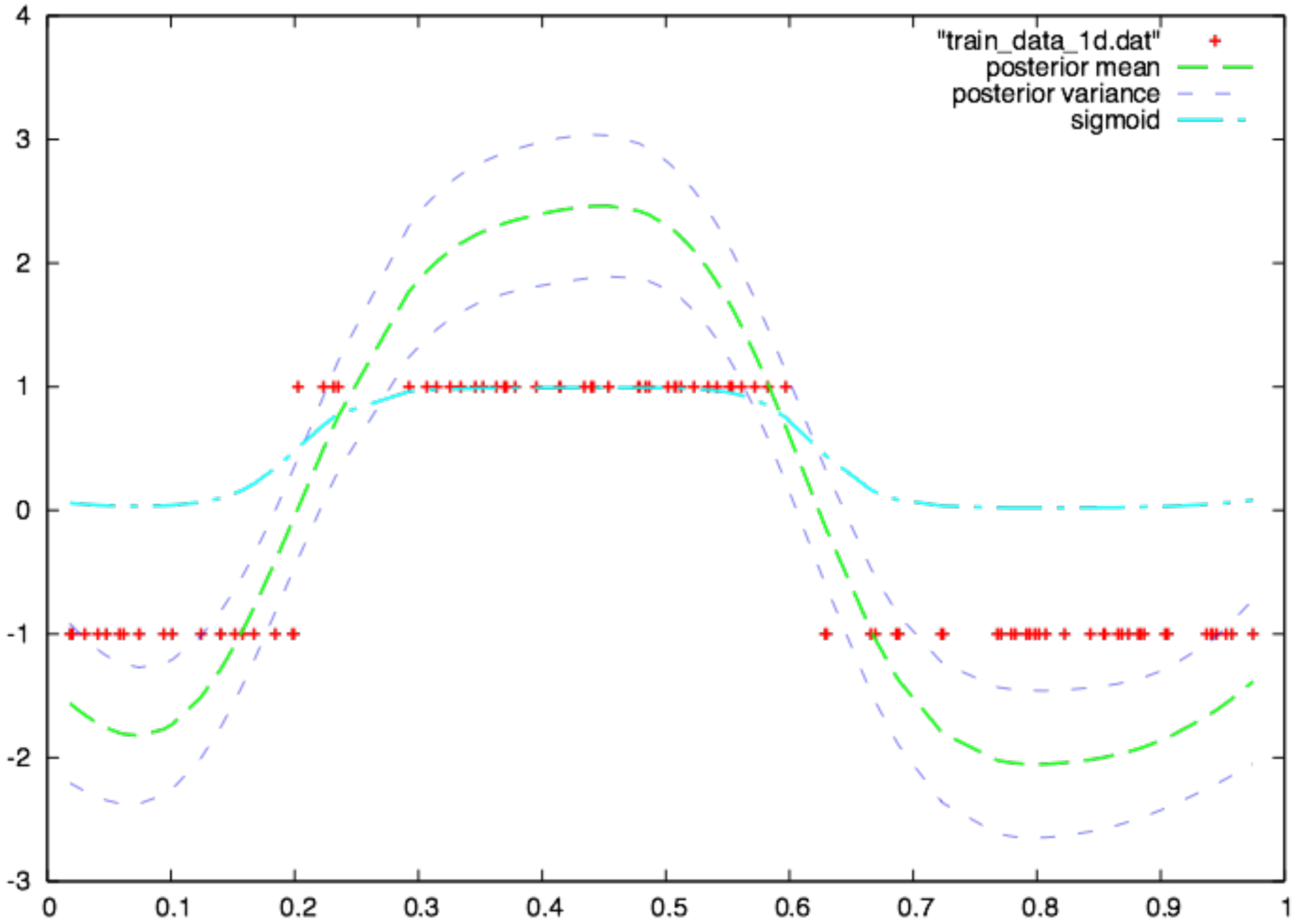
likelihood (sigmoid)

$$p(\mathbf{f} \mid X, \mathbf{y}) = \frac{p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid X)}{p(\mathbf{y} \mid X)}$$

prior

normalizer

A Simple Example



- Red: Two-class training data
- Green: mean function of $p(\mathbf{f} \mid X, \mathbf{y})$
- Light blue: sigmoid of the mean function

But There Is A Problem...

$$p(\mathbf{f} \mid X, \mathbf{y}) = \frac{p(\mathbf{y} \mid \mathbf{f})p(\mathbf{f} \mid X)}{p(\mathbf{y} \mid X)}$$

- The likelihood term is not a Gaussian!
- This means, we can not compute the posterior in closed form.
- There are several different solutions in the literature, e.g.:
    - Laplace approximation
    - Expectation Propagation
    - Variational methods

Laplace Approximation

$$p(\mathbf{f} \mid X, \mathbf{y}) \approx q(\mathbf{f} \mid X, \mathbf{y}) = \mathcal{N}(\mathbf{f} \mid \hat{\mathbf{f}}, A^{-1})$$

where $\hat{\mathbf{f}} = \arg\max_{\mathbf{f}} p(\mathbf{f} \mid X, \mathbf{y})$

and $A = -\nabla\nabla \log p(\mathbf{f} \mid X, \mathbf{y})|_{\mathbf{f}=\hat{\mathbf{f}}}$

second-order Taylor expansion

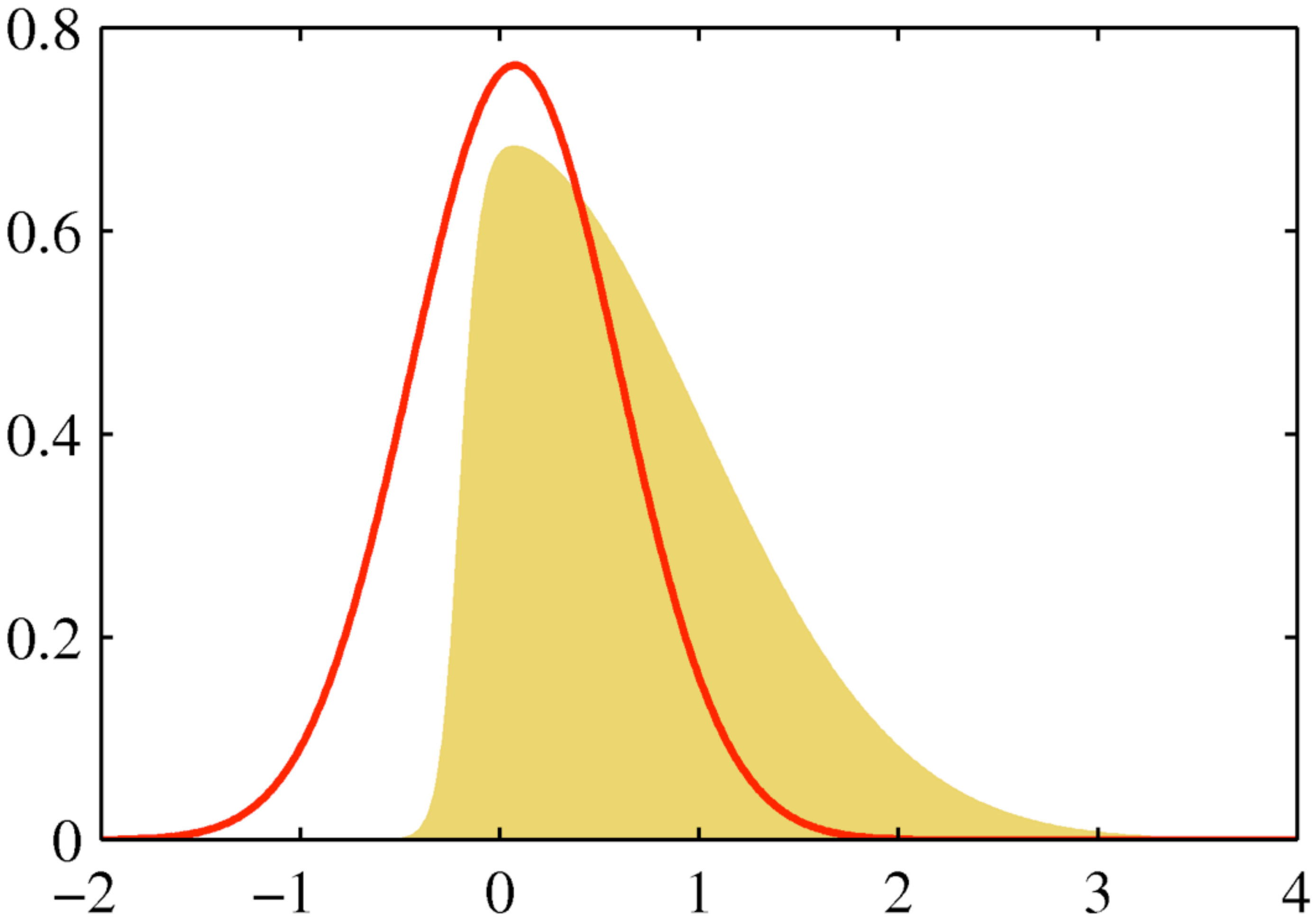
To compute $\hat{\mathbf{f}}$ an iterative approach using Newton’s method has to be used.

The Hessian matrix A can be computed as

$$A = K^{-1} + W$$

where $W = -\nabla\nabla \log p(\mathbf{y} \mid \mathbf{f})$ is a diagonal matrix which depends on the sigmoid function.

Laplace Approximation



- Yellow: a non-Gaussian posterior
- Red: a Gaussian approximation, the mean is the mode of the posterior, the variance is the negative second derivative at the mode

Predictions

Now that we have $p(\mathbf{f} \mid X, \mathbf{y})$ we can compute:

$$p(f_* \mid X, \mathbf{y}, \mathbf{x}_*) = \int p(f_* \mid X, \mathbf{x}_*, \mathbf{f}) p(\mathbf{f} \mid X, \mathbf{y}) d\mathbf{f}$$

From the regression case we have:

$$p(f_* \mid X, \mathbf{x}_*, \mathbf{f}) = \mathcal{N}(f_* \mid \mu_*, \Sigma_*)$$

where $\mu_* = \mathbf{k}_*^T K^{-1} \mathbf{f}$ $\qquad$ $\Sigma_* = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^T K^{-1} \mathbf{k}_*$

Linear in $\mathbf{f}$

This reminds us of a property of Gaussians that we saw earlier!

Gaussian Properties (Rep.)

If we are given this:

I. $$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \mu, \Sigma_1)$$

II. $$p(\mathbf{y} \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid A\mathbf{x} + \mathbf{b}, \Sigma_2)$$

Then it follows (properties of Gaussians):

III. $$p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid A\mu + \mathbf{b}, \Sigma_2 + A\Sigma_1 A^T)$$

IV. $$p(\mathbf{x} \mid \mathbf{y}) = \mathcal{N}(\mathbf{x} \mid \Sigma(A^T\Sigma_2^{-1}(\mathbf{y} - \mathbf{b}) + \Sigma_1^{-1}\mathbf{y}), \Sigma)$$

where

$$\Sigma = (\Sigma_1^{-1} + A^T\Sigma_s^{-1}A)^{-1}$$

Applying this to Laplace

$$\mathbb{E}[f_* \mid X, \mathbf{y}, \mathbf{x}_*] = \mathbf{k}(\mathbf{x}_*)^T K^{-1} \hat{\mathbf{f}}$$

$$\mathbb{V}[f_* \mid X, \mathbf{y}, \mathbf{x}_*] = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^T (K + W^{-1})^{-1} \mathbf{k}_*$$

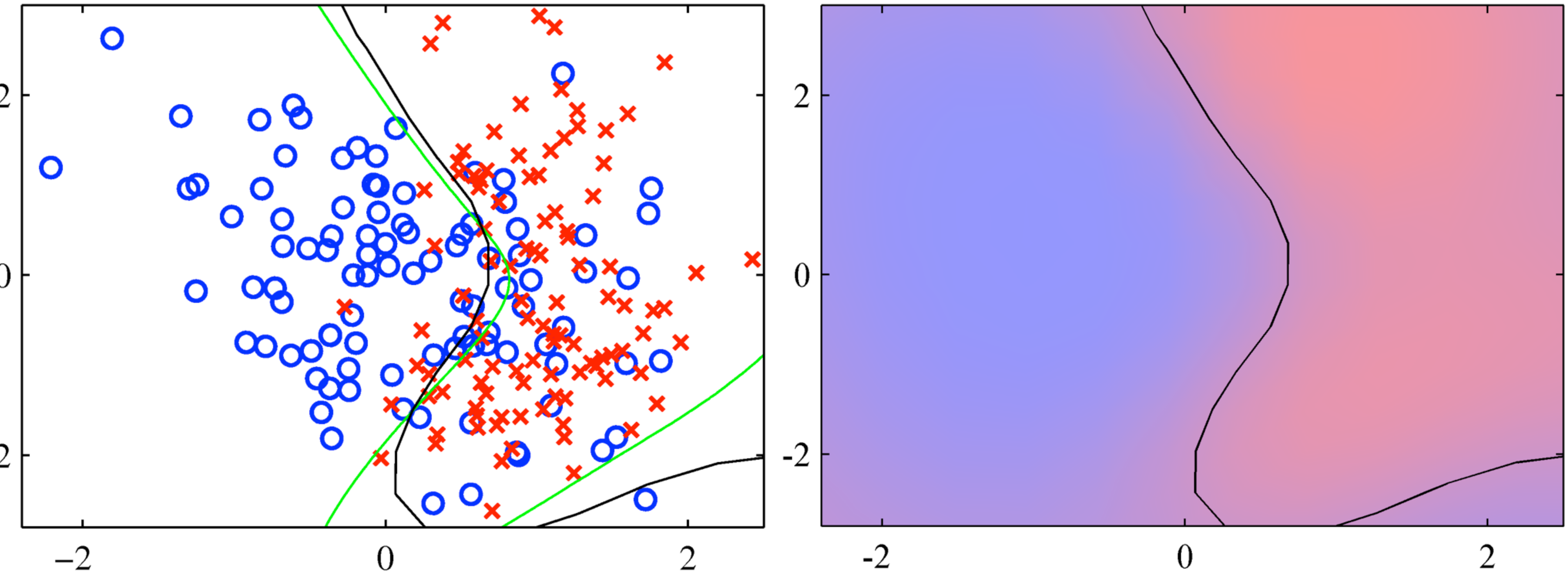
It remains to compute

$$p(y_* = +1 \mid X, \mathbf{y}, \mathbf{x}_*) = \int p(y_* \mid f_*) p(f_* \mid X, \mathbf{y}, \mathbf{x}_*) df_*$$

Depending on the kind of sigmoid function we

- can compute this in closed form (cumulative Gaussian sigmoid)
- have to use sampling methods or analytical approximations (logistic sigmoid)

A Simple Example



- Two-class problem (training data in red and blue)
- Green line: optimal decision boundary
- Black line: GP classifier decision boundary
- Right: posterior probability

Summary

- Gaussian Processes are Normal distributions over functions
- To specify a GP we need a covariance function (kernel) and a mean function
- For regression we can compute the predictive distribution in closed form
- For classification, we use a sigmoid and have to approximate the latent posterior
- More on Gaussian Processes: http://videolectures.net/epsrcws08_rasmussen_lgp/