Technische Universität München

7. Kernel Methods and Gaussian Processes

Motivation

- Usually learning algorithms assume that some kind of feature function is given
- Reasoning is then done on a feature vector of a given (finite) length
- But: some objects are hard to represent with a fixed-size feature vector, e.g. text documents, molecular structures, evolutionary trees
- Idea: use a way of measuring similarity **without** the need of features, e.g. the edit distance for strings
- This we will call a **kernel function**

Dual Representation

Many problems can be expressed using a **dual** formulation. Example (linear regression):

$$J(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{w}^T\phi(\mathbf{x}_n) - t_n)^2 + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} \qquad \phi(\mathbf{x}_n) \in \mathbb{R}^M$$

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if we write this in vector form, we get

$$J(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\Phi^T\Phi\mathbf{w} - \mathbf{t}^T\Phi\mathbf{w} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} \qquad \mathbf{t} \in \mathbb{R}^N$$

$$\Phi \in \mathbb{R}^{N\times M}$$

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$$\Phi \in \mathbb{R}^{N\times M}$$

and the solution is

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

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

However, we can express this result in a different way using the **matrix inversion lemma:**

$$(A + BCD)^{-1} = A^{-1} - A^{-1}B(C^{-1} + DA^{-1}B)^{-1}DA^{-1}$$

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

$$\mathbf{w} = \Phi^T \underbrace{(\Phi\Phi^T + \lambda I_N)^{-1}\mathbf{t}}_{=:\,\mathbf{a}}$$

"Dual Variables"

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$$\mathbf{w} = \Phi^T\underbrace{(\Phi\Phi^T + \lambda I_N)^{-1}\mathbf{t}}_{=:\,\mathbf{a}}$$

"Dual Variables"

Plugging $\mathbf{w} = \Phi^T\mathbf{a}$ into $J(\mathbf{w})$ gives:

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T\underbrace{\Phi\Phi^T}_{=:\,K}\Phi\Phi^T\mathbf{a} - \mathbf{a}^T\Phi\Phi^T\mathbf{t} + \mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T\Phi\Phi^T\mathbf{a}$$

Dual Representation

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$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T K K \mathbf{a} - \mathbf{a}^T K \mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T K \mathbf{a} \qquad K = \Phi\Phi^T$$

This is called the **dual formulation.**

Note: $\mathbf{a} \in \mathbb{R}^N \quad \mathbf{w} \in \mathbb{R}^M$

Dual Representation

Many problems can be expressed using a **dual** formulation. Example (linear regression):

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$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T KK\mathbf{a} - \mathbf{a}^T K\mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T K\mathbf{a}$$

This is called the **dual formulation.**

The solution to the dual problem is:

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

Dual Representation

Many problems can be expressed using a **dual** formulation. Example (linear regression):

$$J(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\Phi^T\Phi\mathbf{w} - \mathbf{t}^T\Phi\mathbf{w} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} \quad \mathbf{t} \in \mathbb{R}^N$$

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T K K \mathbf{a} - \mathbf{a}^T K \mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T K \mathbf{a}$$

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

This we can use to make **predictions**:

$$f(\mathbf{x}^*) = \mathbf{w}^T\phi(\mathbf{x}^*) = \mathbf{a}^T\Phi\phi(\mathbf{x}^*) = \mathbf{k}(\mathbf{x}^*)^T(K + \lambda I_N)^{-1}\mathbf{t}$$

(now $\mathbf{x}^*$ is unknown and $\mathbf{a}$ is given from training)

Dual Representation

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

where:

$$\mathbf{k}(\mathbf{x}^*) = \begin{pmatrix} \phi(\mathbf{x}_1)^T \phi(\mathbf{x}^*) \\ \vdots \\ \phi(\mathbf{x}_N)^T \phi(\mathbf{x}^*) \end{pmatrix} \quad K = \begin{pmatrix} \phi(\mathbf{x}_1)^T \phi(\mathbf{x}_1) & \dots & \phi(\mathbf{x}_1)^T \phi(\mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ \phi(\mathbf{x}_N)^T \phi(\mathbf{x}_1) & \dots & \phi(\mathbf{x}_N)^T \phi(\mathbf{x}_N) \end{pmatrix}$$

Thus, f is expressed only in terms of **dot products** between different pairs of $\phi(\mathbf{x})$, or in terms of the **kernel function**

$$k(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

Representation using the Kernel

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

Now we have to invert a matrix of size $N \times N$, before it was $M \times M$ where $M < N$, but:

By expressing everything with the kernel function, we can deal with very high-dimensional or even **infinite**-dimensional feature spaces!

Idea: Don't use features at all but simply define a **similarity** function expressed as the kernel!

Constructing Kernels

The straightforward way to define a kernel function is to first find a basis (=feature) function $\phi(\mathbf{x})$ and to define:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

This means, k is an inner product in some space $\mathcal{H}$, i.e:

1. Symmetry: $k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_j), \phi(\mathbf{x}_i) \rangle = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$
2. Linearity: $\langle a(\phi(\mathbf{x}_i) + \mathbf{z}), \phi(\mathbf{x}_j) \rangle = a \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle + a \langle \mathbf{z}, \phi(\mathbf{x}_j) \rangle$
3. Positive definite: $\langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_i) \rangle \geq 0$, equal if $\phi(\mathbf{x}_i) = \mathbf{0}$

Can we find conditions for k under which there is a (possibly infinite dimensional) basis function into $\mathcal{H}$, where k is an inner product?

Constructing Kernels

Theorem (Mercer): If k is

1. symmetric, i.e. $k(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_j, \mathbf{x}_i)$ and
2. positive definite, i.e.

$$K = \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \dots & k(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & \dots & k(\mathbf{x}_N, \mathbf{x}_N) \end{pmatrix}$$

"Gram Matrix"

is positive definite, then there exists a mapping $\phi(\mathbf{x})$ into a feature space $\mathcal{H}$ so that k can be expressed as an inner product in $\mathcal{H}$.

This means, we don't need to find $\phi(\mathbf{x})$ explicitly!

We can directly work with k "Kernel Trick"

Examples of Valid Kernels

- Polynomial Kernel:

$$k(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^T \mathbf{x}_j + c)^d \quad c > 0 \quad d \in \mathbb{N}$$

- Gaussian Kernel:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma^2)$$

- Kernel for sets:

$$k(A_1, A_2) = 2^{|A_1 \cap A_2|}$$

- Matern kernel:

$$k(r) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu r}}{l} \right)^{\nu} K_\nu \left(\frac{\sqrt{2\nu r}}{l} \right) \quad r = \|\mathbf{x}_i - \mathbf{x}_j\|, \nu > 0, l > 0$$

A Simple Example

Define a kernel function as

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}')^2 \qquad\qquad \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2$$

This can be written as:

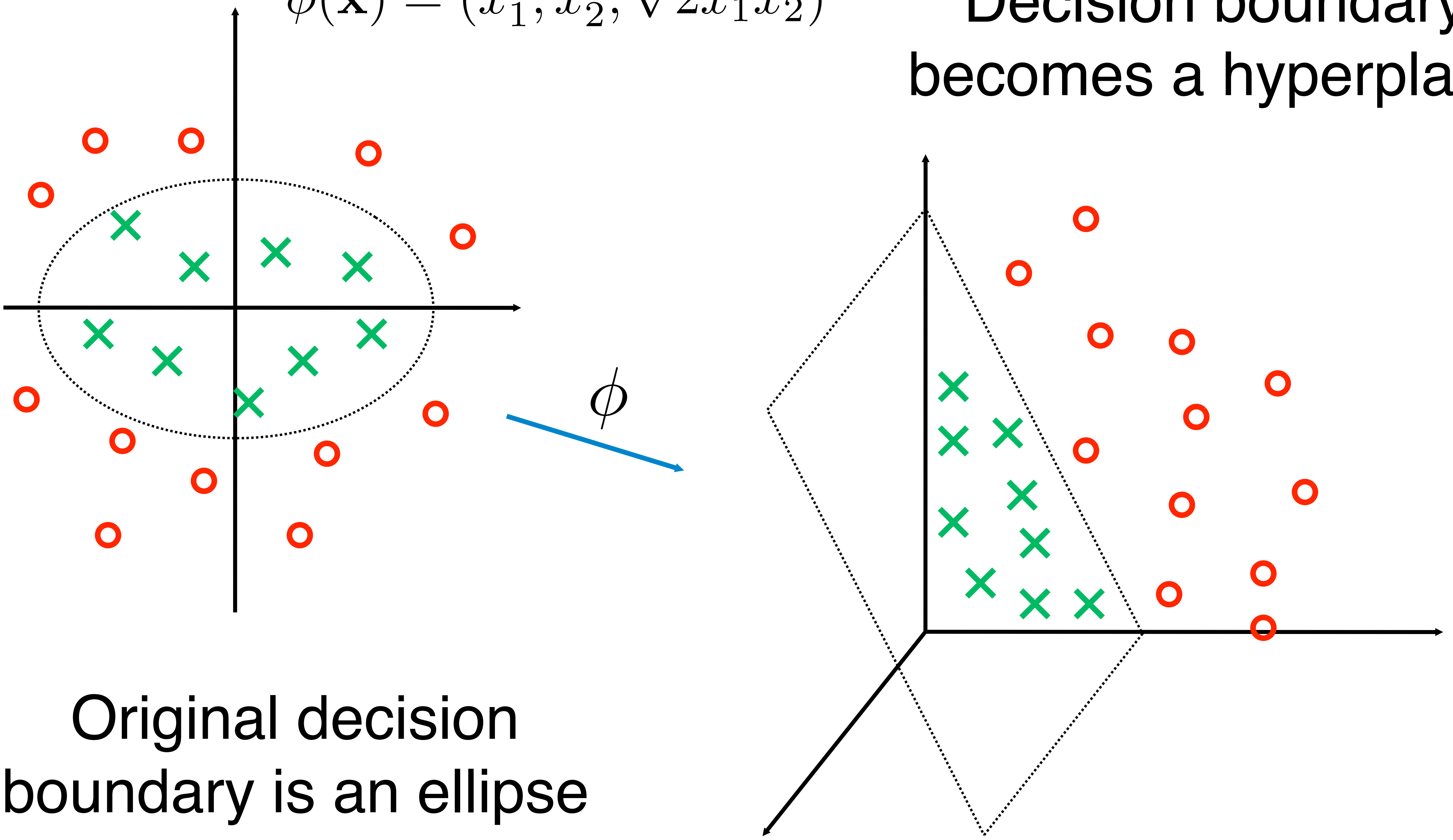
$$\begin{aligned}(x_1 x'_1 + x_2 x'_2)^2 &= x_1^2 x_1'^2 + 2 x_1 x'_1 x_2 x'_2 + x_2^2 x_2'^2 \\ &= (x_1^2, x_2^2, \sqrt{2} x_1 x_2)(x_1'^2, x_2'^2, \sqrt{2} x'_1 x'_2)^T \\ &= \phi(\mathbf{x})^T \phi(\mathbf{x}')\end{aligned}$$

It can be shown that this holds in general for

$$k(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^T \mathbf{x}_j)^d$$

Visualization of the Example

$$\phi(\mathbf{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$



Decision boundary becomes a hyperplane

Original decision boundary is an ellipse

Application Examples

Kernel Methods can be applied for many different problems, e.g.:

- Density estimation (unsupervised learning)
- Regression
- Principal Component Analysis (PCA)
- Classification

Most important Kernel Methods are

- Support Vector Machines
- Gaussian Processes

Kernelization

- Many existing algorithms can be converted into kernel methods
- This process is called “kernelization”

Idea:

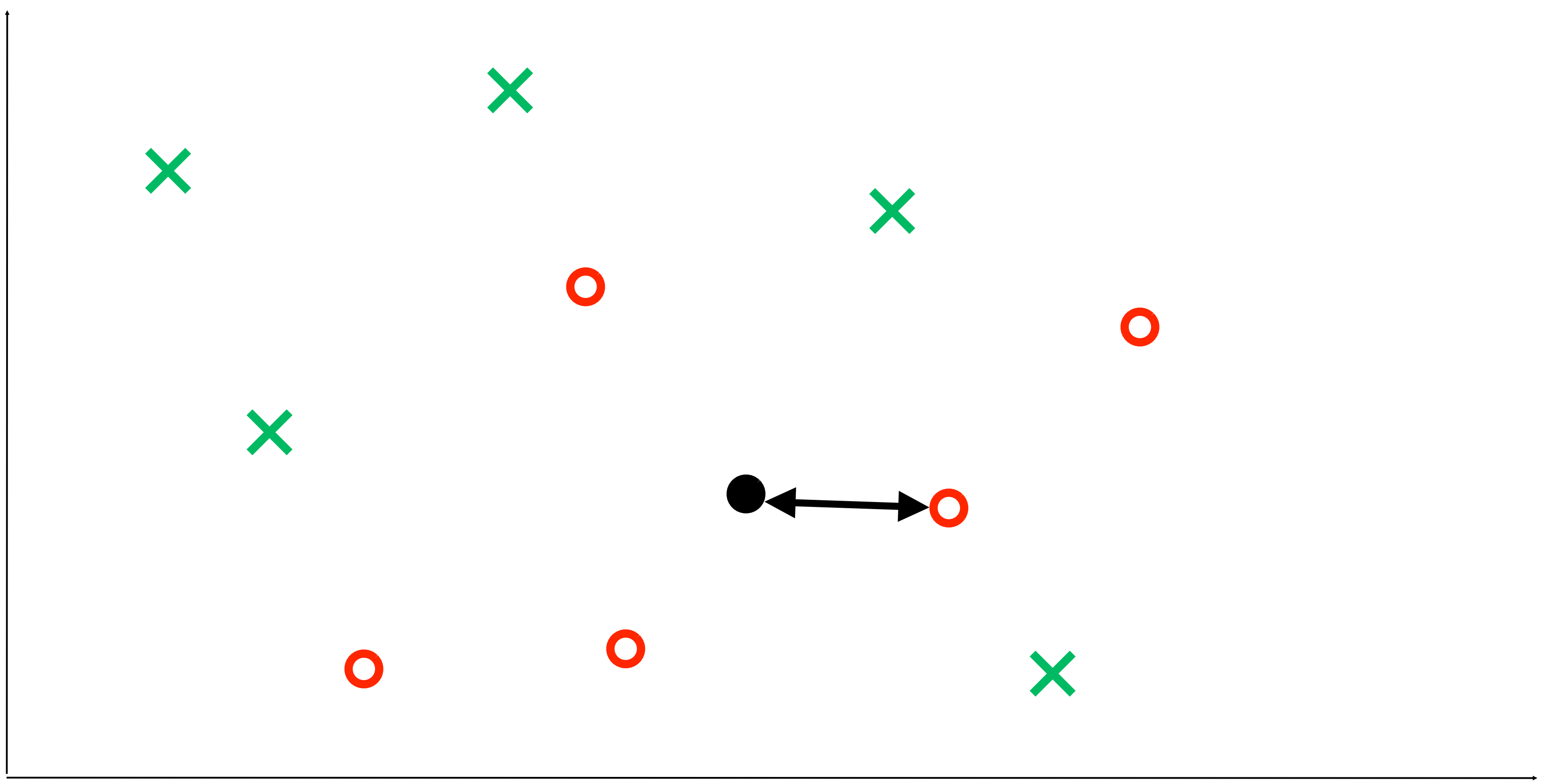
- express similarities of data points in terms of an inner product (dot product)
- replace all occurrences of that inner product by the kernel function

This is called the **kernel trick**

Example: Nearest Neighbor

- The NN classifier selects the label of the nearest neighbor in Euclidean distance

$$\|\mathbf{x}_i - \mathbf{x}_j\|^2 = \mathbf{x}_i^T \mathbf{x}_i + \mathbf{x}_j^T \mathbf{x}_j - 2\mathbf{x}_i^T \mathbf{x}_j$$



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- We can now replace the dot products by a valid Mercer kernel and we obtain:

$$d(\mathbf{x}_i, \mathbf{x}_j)^2 = k(\mathbf{x}_i, \mathbf{x}_i) + k(\mathbf{x}_j, \mathbf{x}_j) - 2k(\mathbf{x}_i, \mathbf{x}_j)$$

- This is a **kernelized** nearest-neighbor classifier
- We do not explicitly compute feature vectors!

Back to Linear Regression (Rep.)

We had the primal and the dual formulation:

$$J(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\Phi^T\Phi\mathbf{w} - \mathbf{t}^T\Phi\mathbf{w} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} \quad \mathbf{t} \in \mathbb{R}^N$$

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T K K \mathbf{a} - \mathbf{a}^T K \mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T K \mathbf{a}$$

with the dual solution:

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

This we can use to make **predictions**:

$$f(\mathbf{x}^*) = \mathbf{w}^T\phi(\mathbf{x}^*) = \mathbf{a}^T\Phi\phi(\mathbf{x}^*) = \mathbf{k}(\mathbf{x}^*)^T(K + \lambda I_N)^{-1}\mathbf{t}$$

Note: This is (only) the **most likely** prediction!

Observations

- 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 $\mathbf{w}$

Questions:

- 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

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

The marginal is

"Schur Complement"

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

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**!

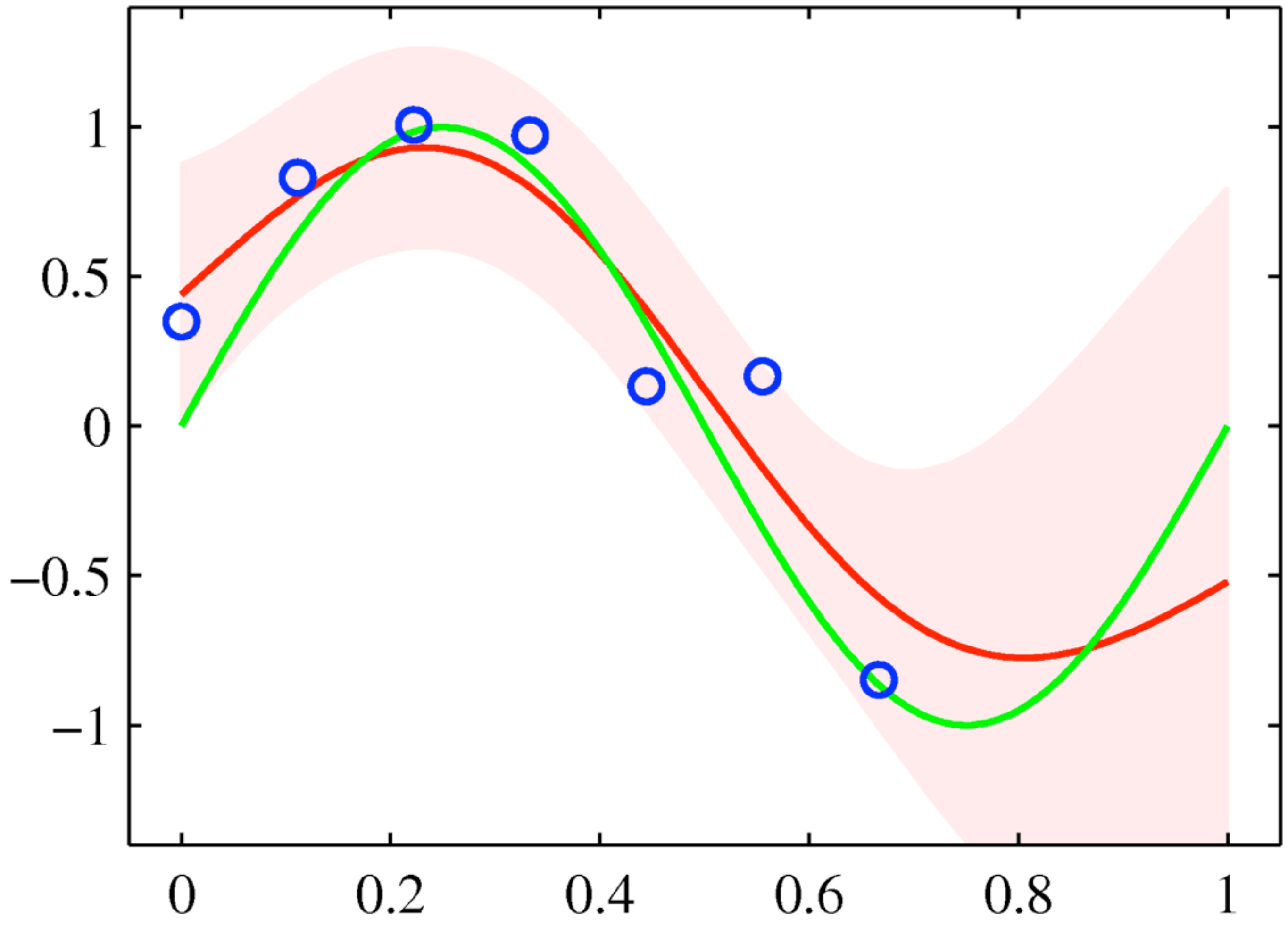
To specify a GP we need:

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.

The Covariance Function

The most used covariance function (kernel) is:

$$k(\mathbf{x}_p, \mathbf{x}_q) = \underbrace{\sigma_f^2}_{\text{signal variance}} \exp(-\frac{1}{\underbrace{2l^2}_{\text{length scale}}}(\mathbf{x}_p - \mathbf{x}_q)^2) + \underbrace{\sigma_n^2}_{\text{noise variance}} \delta_{pq}$$

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

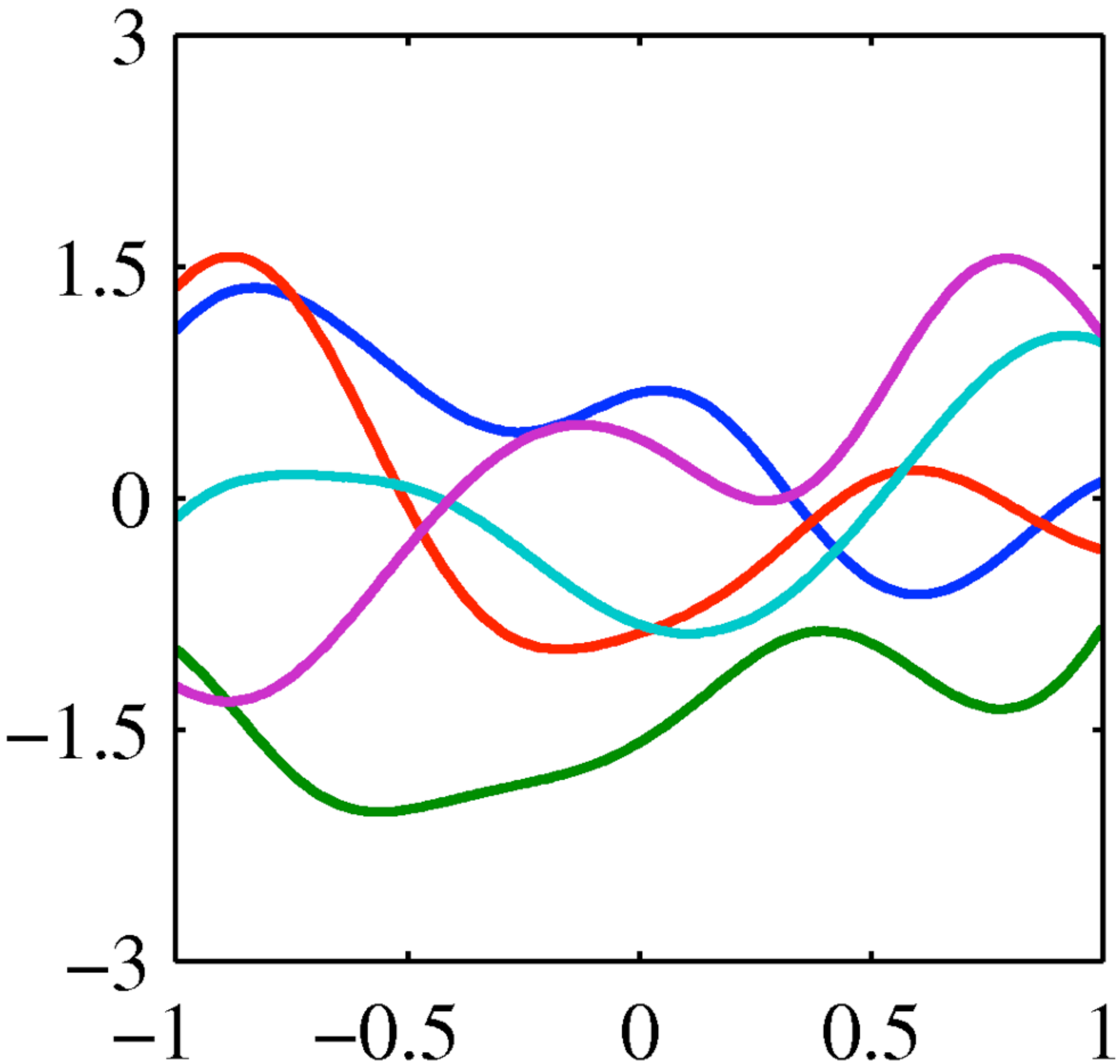
$$K_{ij} = k(\mathbf{x}_i^*, \mathbf{x}_j^*)$$

3. Generate a random Gaussian vector from

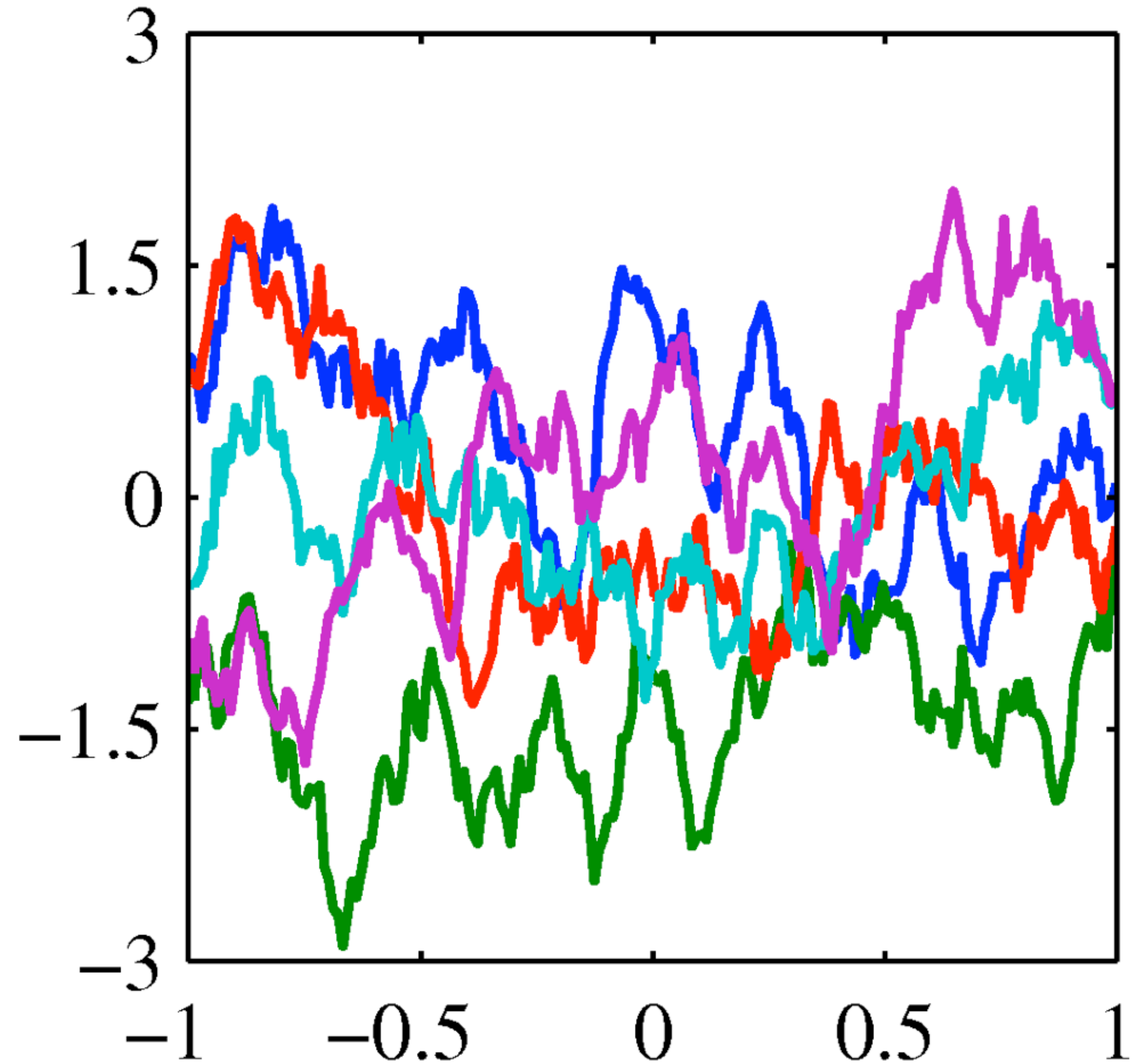
$$\mathbf{y}_* \sim \mathcal{N}(\mathbf{0}, K)$$

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 $\mathbf{x}_1, \dots, \mathbf{x}_N \quad y_1, \dots, y_N$

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

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

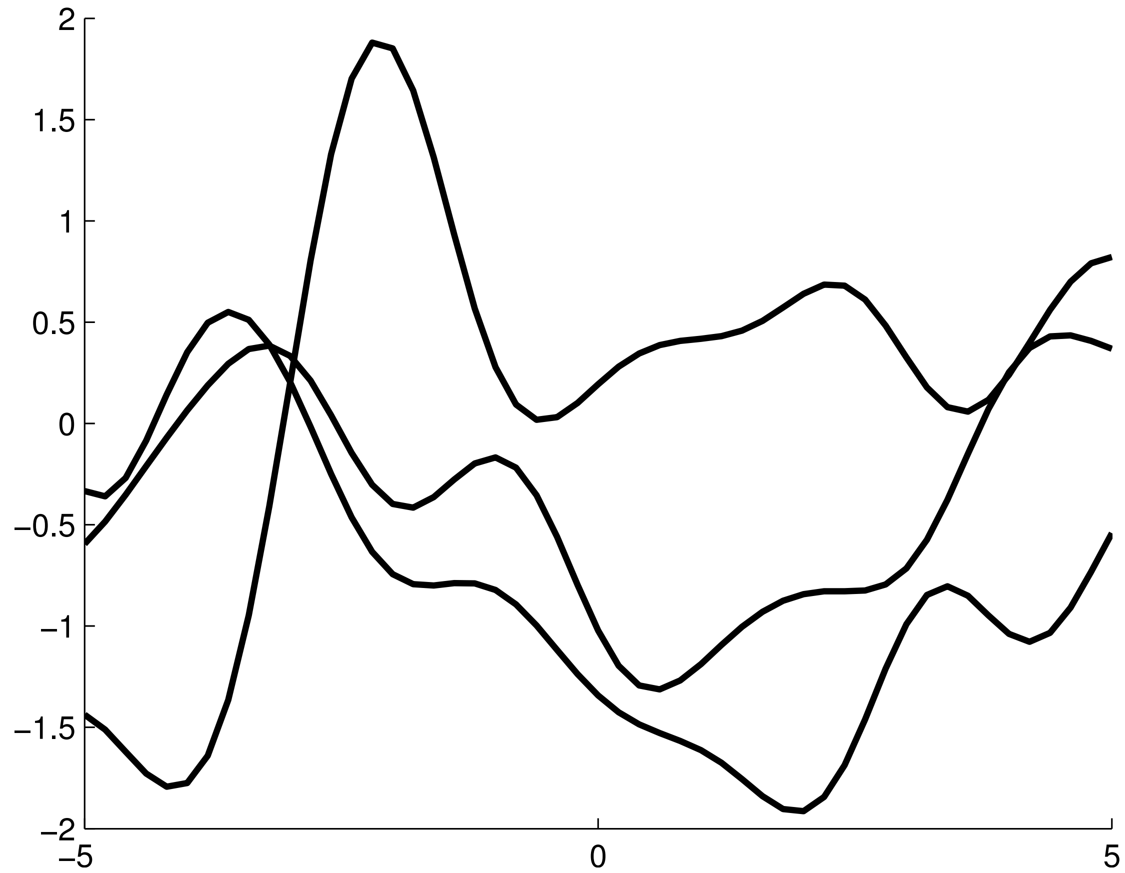
where

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

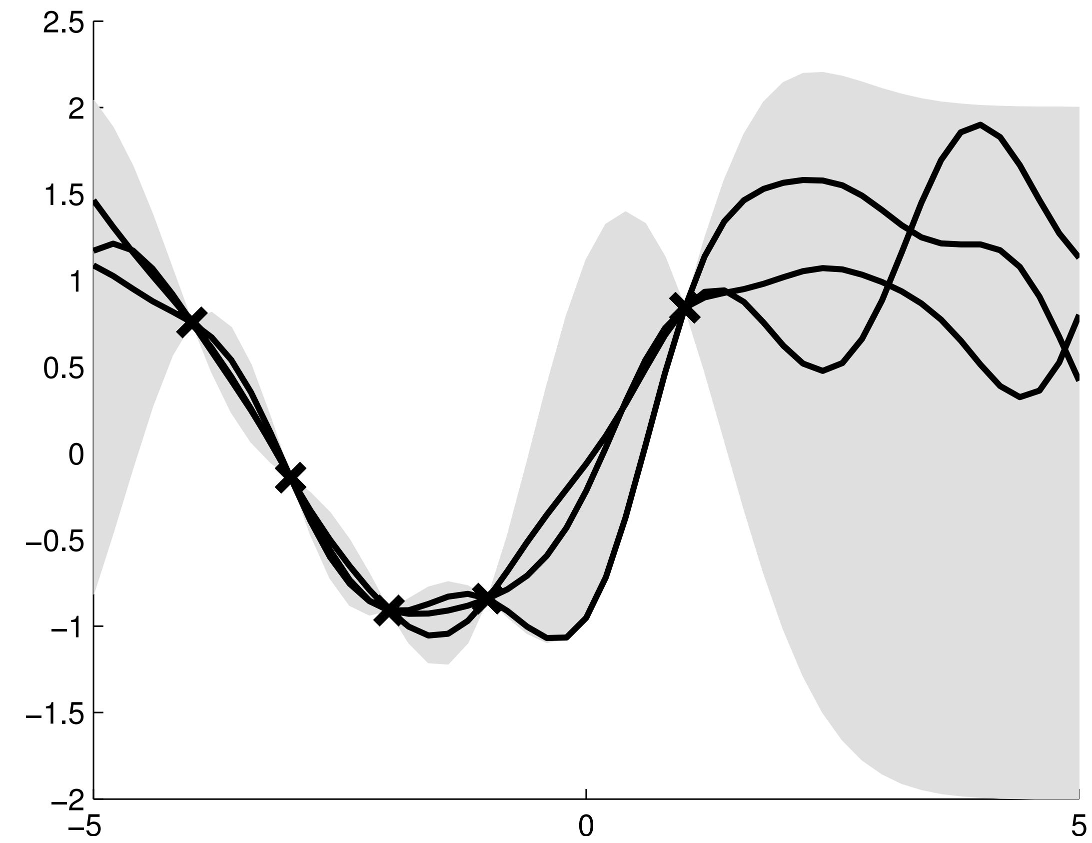
$$\Sigma_* = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^T K^{-1} \mathbf{k}_*$$

This defines the **predictive distribution.**

Example



Functions sampled from a Gaussian Process prior



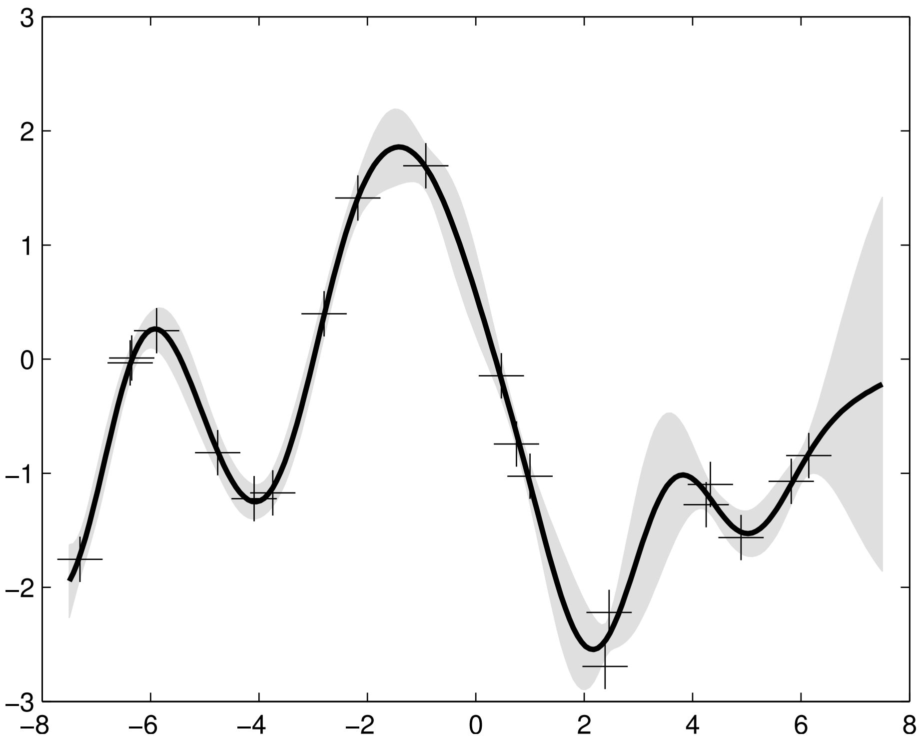
Functions sampled from the predictive distribution

The predictive distribution is itself a Gaussian process.

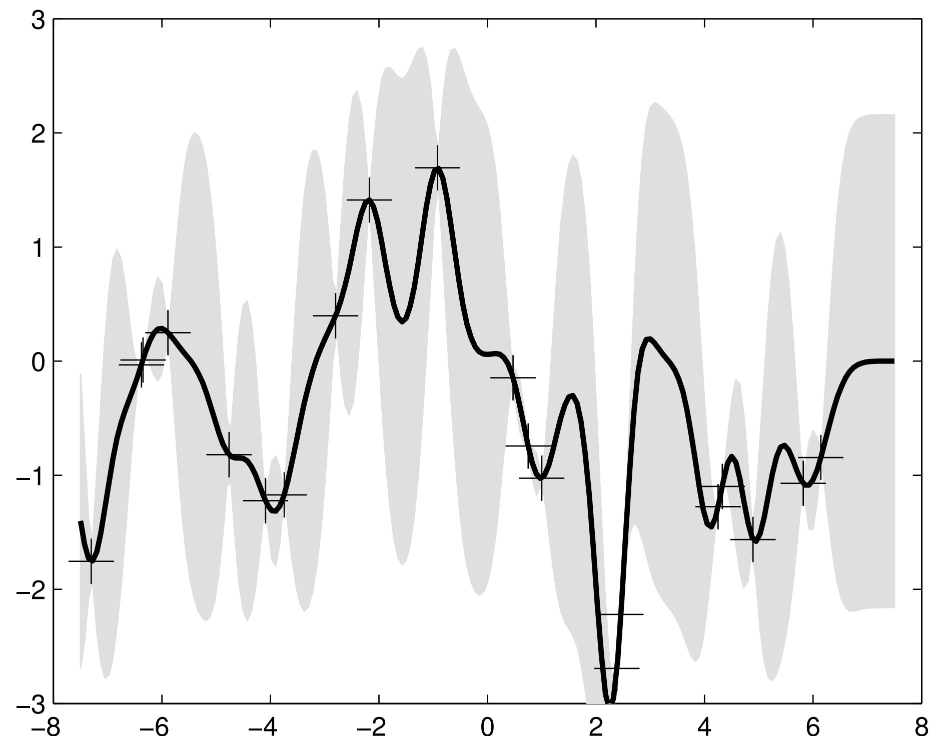
It represents the posterior after observing the data.

The covariance is low in the vicinity of data points.

Varying the Hyperparameters

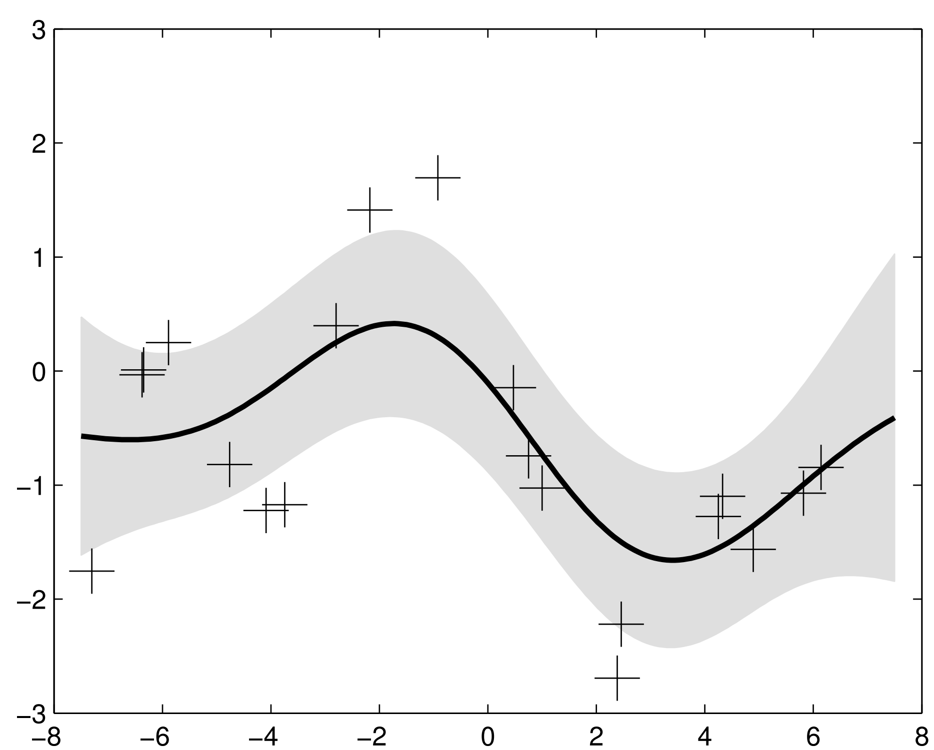


$$l = \sigma_f = 1, \quad \sigma_n = 0.1$$



$$l = 0.3, \quad \sigma_f = 1.08, \quad \sigma_n = 0.0005$$

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



$$l = 3 \quad \sigma_f = 1.16 \quad \sigma_n = 0.89$$

Remember: The Predictive Distribution

We obtain the **predictive distribution** by integrating over all possible model parameters ("inference"):

$$\underbrace{p(t^* \mid x^*, \mathbf{t}, \mathbf{x})}_{\text{Test data}} = \int \underbrace{p(t^* \mid x^*, \mathbf{w})}_{\text{Test data likelihood}} \underbrace{p(\mathbf{w} \mid \mathbf{x}, \mathbf{t})}_{\text{Parameter posterior}} d\mathbf{w}$$

This distribution can be computed in closed form, because both terms on the RHS are Gaussian.

From above we have $\boxed{p(\mathbf{w} \mid \mathbf{t}, \mathbf{x})} = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \Sigma)$

where $\quad \boldsymbol{\mu} = \sigma_1^{-2} \Sigma \Phi^T \mathbf{t}$

and $\quad \Sigma = \sigma_1^2 (\frac{\sigma_1^2}{\sigma_2^2} I_M + \Phi^T \Phi)^{-1}$

$$\Rightarrow \underbrace{\boldsymbol{\mu} = (\lambda I_M + \Phi^T \Phi)^{-1} \Phi^T \mathbf{t}}_{\text{MAP solution}}$$

Remember: The Predictive Distribution

Using the linear Gaussian model we get:

$$p(t^* \mid x^*; \mathbf{t}, \mathbf{x}) = \int p(t^* \mid x^*; \mathbf{w}) p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}) d\mathbf{w}$$

$$= \int \mathcal{N}(t^*; \phi(x^*)^T \mathbf{w}, \sigma) \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \Sigma) d\mathbf{w}$$

$$= \mathcal{N}(t^*; \phi(x^*)^T \boldsymbol{\mu}, \sigma_N^2(x^*))$$

where

$$\sigma_N^2(x) = \sigma^2 + \phi(x)^T \Sigma \phi(x)$$

Linear Regression GP

Question:

How does the predictive distribution of the near regression relate to Gaussian Process regression?

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Answer:

Linear regression is a special case of a GP where the kernel function is

$$k(\mathbf{x}_1, \mathbf{x}_2) = \sigma_2^2 \phi(\mathbf{x}_1)^T \phi(\mathbf{x}_2) + \sigma_1^2 \delta_{1,2}$$