

Advanced Machine Learning Lecture 4

Kernels & Gaussian Processes

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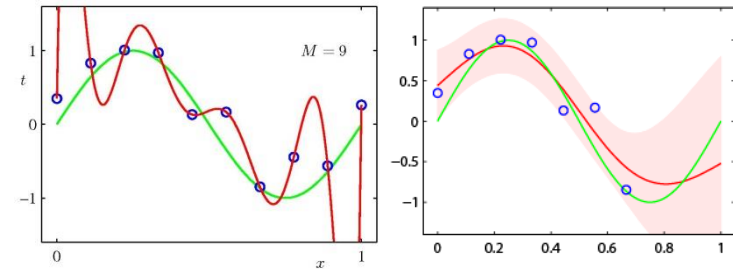
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This Lecture: *Advanced Machine Learning*

• Regression Approaches

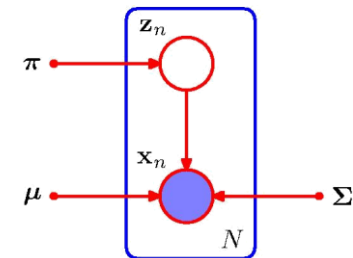
- Linear Regression
- Regularization (Ridge, Lasso)
- Kernels (Kernel Ridge Regression)
- Gaussian Processes

$$f : \mathcal{X} \rightarrow \mathbb{R}$$



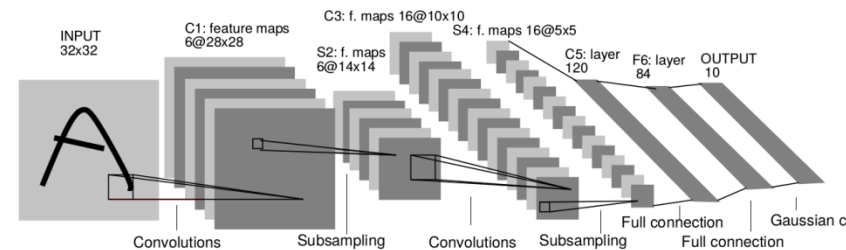
• Learning with Latent Variables

- EM and Generalizations
- Approximate Inference



• Deep Learning

- Neural Networks
- CNNs, RNNs, RBMs, etc.



Topics of This Lecture

- **Recap: Linear Regression**
- **Kernels**
 - Dual representations
 - Kernel Ridge Regression
 - Properties of kernels
- **Gaussian Processes**
 - Motivation
 - Gaussian Process definition
 - Squared exponential covariance function
 - Prediction with noise-free observations
 - Prediction with noisy observations
 - GP Regression
 - Influence of hyperparameters
- **Applications**

Recap: Loss Functions for Regression

- The squared loss is not the only possible choice
 - Poor choice when conditional distribution $p(t | \mathbf{x})$ is multimodal.

- Simple generalization: **Minkowski loss**

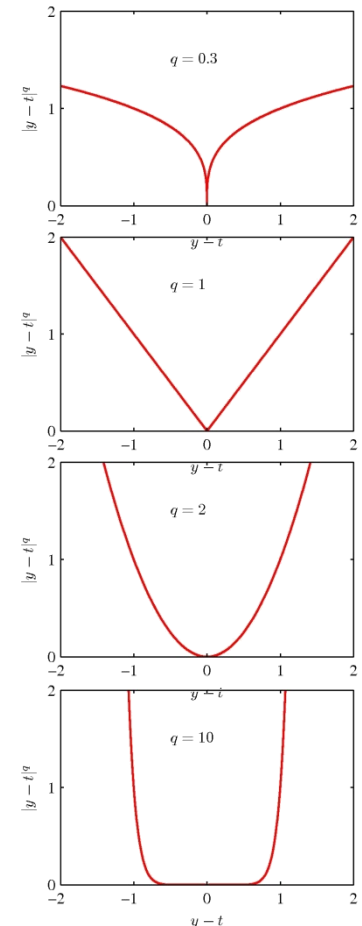
$$L(t, y(\mathbf{x})) = |y(\mathbf{x}) - t|^q$$

- **Expectation**

$$\mathbb{E}[L_q] = \iint |y(\mathbf{x}) - t|^q p(\mathbf{x}, t) dx dt$$

- **Minimum of $\mathbb{E}[L_q]$ is given by**

- **Conditional mean** for $q = 2$,
- **Conditional median** for $q = 1$,
- **Conditional mode** for $q = 0$.



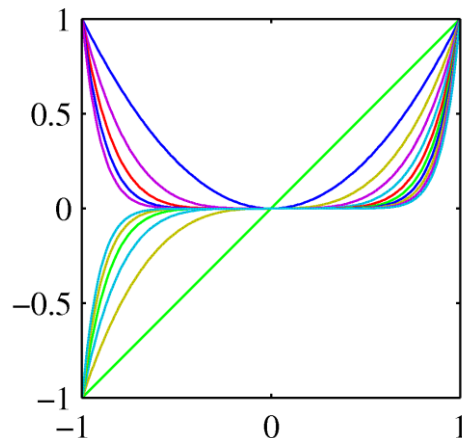
Recap: Linear Basis Function Models

- Generally, we consider models of the following form

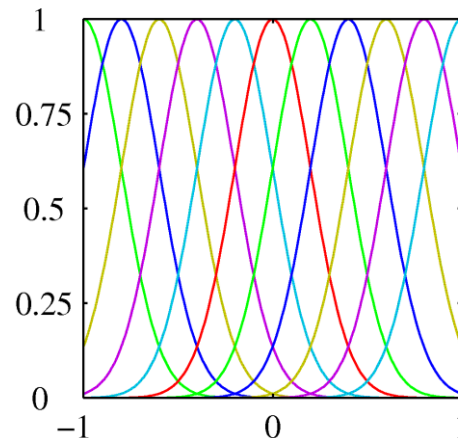
$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

- where $\phi_j(\mathbf{x})$ are known as *basis functions*.
- In the simplest case, we use linear basis functions: $\phi_d(\mathbf{x}) = x_d$.

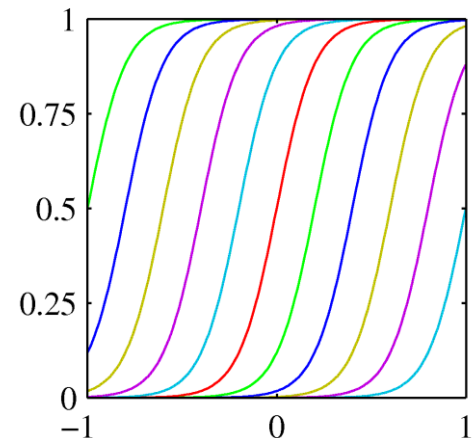
- Other popular basis functions



Polynomial



Gaussian

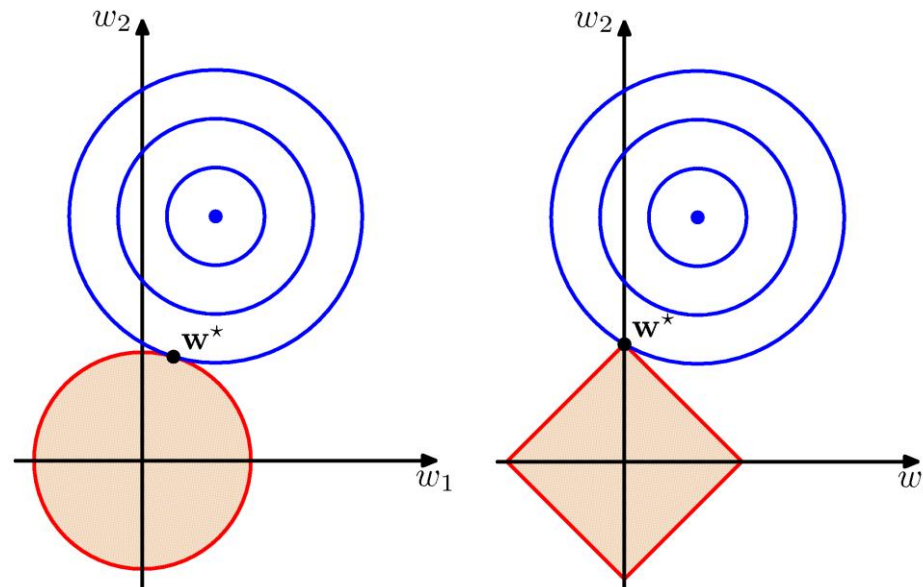


Sigmoid

Recap: Regularized Least-Squares

- Consider more general regularization functions

➤ “L_q norms”:
$$\frac{1}{2} \sum_{n=1}^N \{t_n - \mathbf{w}^T \phi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2} \sum_{j=1}^M |w_j|^q$$



- Effect: **Sparsity** for $q \leq 1$.
 - Minimization tends to set many coefficients to zero

Recap: Lasso as Bayes Estimation

- L_1 regularization (“The Lasso”)

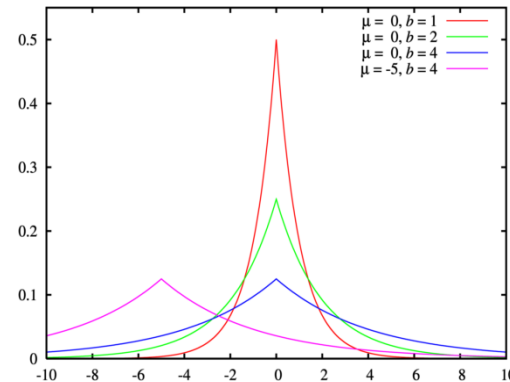
$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w}} \frac{1}{2} \sum_{n=1}^N \{t_n - \mathbf{w}^T \phi(\mathbf{x}_n)\}^2 + \lambda \sum_{j=1}^M |w_j|$$

- Interpretation as Bayes Estimation

➤ We can think of $|w_j|^q$ as the log-prior density for w_j .

- Prior for Lasso ($q = 1$): Laplacian distribution

$$p(\mathbf{w}) = \frac{1}{2\tau} \exp \{-|\mathbf{w}|/\tau\} \quad \text{with} \quad \tau = \frac{1}{\lambda}$$



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 - Dual representations
 - Kernel Ridge Regression
 - Properties of kernels
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Introduction to Kernel Methods

- Dual representations

- Many linear models for regression and classification can be reformulated in terms of a dual representation, where predictions are based on linear combinations of a **kernel function** evaluated at training data points.
- For models that are based on a fixed nonlinear feature space mapping $\phi(\mathbf{x})$, the kernel function is given by

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$$

- We will see that by substituting the inner product by the kernel, we can achieve interesting extensions of many well-known algorithms...

Dual Representations: Derivation

- Consider a regularized linear regression model

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

with the solution

$$\mathbf{w} = -\frac{1}{\lambda} \sum_{n=1}^N \{ \mathbf{w}^T \phi(\mathbf{x}_n) - t_n \} \phi(\mathbf{x}_n)$$

- We can write this as a linear combination of the $\phi(\mathbf{x}_n)$ with coefficients that are functions of \mathbf{w} :

$$\mathbf{w} = \sum_{n=1}^N a_n \phi(\mathbf{x}_n) = \Phi^T \mathbf{a}$$

with
$$a_n = -\frac{1}{\lambda} \{ \mathbf{w}^T \phi(\mathbf{x}_n) - t_n \}$$

Dual Representations: Derivation

- Dual definition

- Instead of working with \mathbf{w} , we can formulate the optimization for \mathbf{a} by substituting $\mathbf{w} = \Phi^T \mathbf{a}$ into $J(\mathbf{w})$:

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

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

- Define the **kernel matrix** $\mathbf{K} = \Phi \Phi^T$ with elements

$$K_{nm} = \phi(\mathbf{x}_n)^T \phi(\mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m)$$

- Now, the sum-of-squares error can be written as

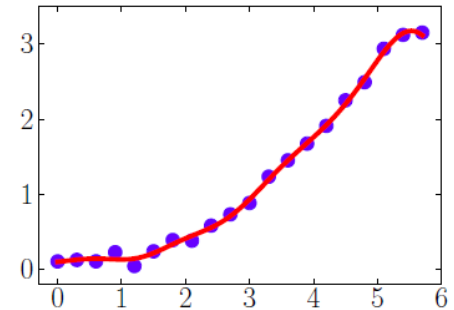
$$J(\mathbf{a}) = \frac{1}{2} \mathbf{a}^T \mathbf{K} \mathbf{K} \mathbf{a} - \mathbf{a}^T \mathbf{K} \mathbf{t} + \frac{1}{2} \mathbf{t}^T \mathbf{t} + \frac{\lambda}{2} \mathbf{a}^T \mathbf{K} \mathbf{a}$$

Kernel Ridge Regression

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

- Solving for \mathbf{a} , we obtain

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



- Prediction for a new input \mathbf{x} :

- Writing $\mathbf{k}(\mathbf{x})$ for the vector with elements $k_n(\mathbf{x}) = k(\mathbf{x}_n, \mathbf{x})$

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) = \mathbf{a}^T \Phi \phi(\mathbf{x}) = \mathbf{k}(\mathbf{x})^T (\mathbf{K} + \lambda \mathbf{I}_N)^{-1} \mathbf{t}$$

⇒ *The dual formulation allows the solution to be entirely expressed in terms of the kernel function $k(\mathbf{x}, \mathbf{x}')$.*

⇒ The resulting form is known as **Kernel Ridge Regression** and allows us to perform non-linear regression.

Why use $k(\mathbf{x}, \mathbf{x}')$ instead of $\phi(\mathbf{x})^T \phi(\mathbf{x}')$?

1. Memory usage

- Storing $\phi(\mathbf{x}_1), \dots, \phi(\mathbf{x}_N)$ requires $O(NM)$ memory.
- Storing $k(\mathbf{x}_1, \mathbf{x}_1), \dots, k(\mathbf{x}_N, \mathbf{x}_N)$ requires $O(N^2)$ memory.

2. Speed

- We might find an expression for $k(\mathbf{x}_i, \mathbf{x}_j)$ that is faster to evaluate than first forming $\phi(\mathbf{x})$ and then computing $\phi(\mathbf{x})^T \phi(\mathbf{x}')$.
- Example: comparing angles ($x \in [0, 2\pi]$):

$$\begin{aligned}\langle \phi(x_i), \phi(x_j) \rangle &= \langle [\cos(x_i), \sin(x_i)], [\cos(x_j), \sin(x_j)] \rangle \\ &= \cos(x_i) \cos(x_j) + \sin(x_i) \sin(x_j)\end{aligned}$$

$$k(x_i, x_j) := \cos(x_i - x_j)$$

Why use $k(\mathbf{x}, \mathbf{x}')$ instead of $\phi(\mathbf{x})^T \phi(\mathbf{x}')$?

3. Flexibility

- There are kernel functions $k(\mathbf{x}_i, \mathbf{x}_j)$ for which we know that a feature transformation ϕ exists, but we don't know what ϕ is.
- This allows us to work with far more general similarity functions.
- We can define kernels on strings, trees, graphs, ...

4. Dimensionality

- Since we no longer need to explicitly compute $\phi(\mathbf{x})$, we can work with high-dimensional (even infinite-dim.) feature spaces.
- *In the following, we take a closer look at the background behind kernels and at how to use them...*

Properties of Kernels

- **Definition (Positive Definite Kernel Function)**
 - Let \mathcal{X} be a non-empty set. A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called **positive definite kernel function**, iff
 - k is symmetric, i.e. $k(x, x') = k(x', x)$ for all $x, x' \in \mathcal{X}$, and
 - for any set of points $x_1, \dots, x_n \in \mathcal{X}$, the matrix

$$K_{ij} = (k(x_i, x_j))_{i,j}$$

is positive (semi-)definite, i.e. for all vectors $\mathbf{x} \in \mathbb{R}^n$:

$$\sum_{i,j=1}^N \mathbf{x}_i K_{ij} \mathbf{x}_j \geq 0$$

Hilbert Spaces

- **Definition (Hilbert Space)**

- A **Hilbert Space** \mathcal{H} is a vector space H with an *inner product* $\langle \cdot, \cdot \rangle_{\mathcal{H}}$, e.g. a mapping

$$\langle \cdot, \cdot \rangle_{\mathcal{H}} : H \times H \rightarrow \mathbb{R}$$

which is

- **symmetric:** $\langle v, v' \rangle_{\mathcal{H}} = \langle v', v \rangle_{\mathcal{H}}$ for all $v, v' \in H$,
- **positive definite:** $\langle v, v \rangle_{\mathcal{H}} \geq 0$ for all $v \in H$,
where $\langle v, v \rangle_{\mathcal{H}} = 0$ only for $v = \mathbf{0} \in H$.
- **bilinear:** $\langle av, v' \rangle_{\mathcal{H}} = a \langle v, v' \rangle_{\mathcal{H}}$ for $v \in H, a \in \mathbb{R}$
 $\langle v + v', v'' \rangle_{\mathcal{H}} = \langle v, v'' \rangle_{\mathcal{H}} + \langle v', v'' \rangle_{\mathcal{H}}$

- We can treat a Hilbert space like some \mathbb{R}^n , if we only use concepts like *vectors, angles, distances*.
- **Note:** $\dim \mathcal{H} = \infty$ is possible!

Properties of Kernels

- **Theorem**

- *Let $k: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a positive definite kernel function. Then there exists a Hilbert Space \mathcal{H} and a mapping $\varphi: \mathcal{X} \rightarrow \mathcal{H}$ such that*

$$k(x, x') = \langle (\phi(x), \phi(x')) \rangle_{\mathcal{H}}$$

- *where $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is the inner product in \mathcal{H} .*

- **Translation**

- **Take any set \mathcal{X} and any function $k: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$.**
- **If k is a positive definite kernel, then we can use k to learn a (soft) maximum-margin classifier for the elements in \mathcal{X} !**

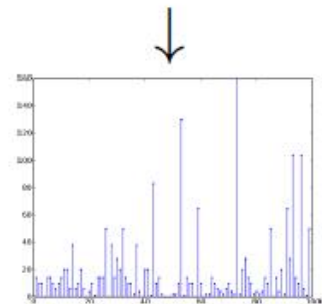
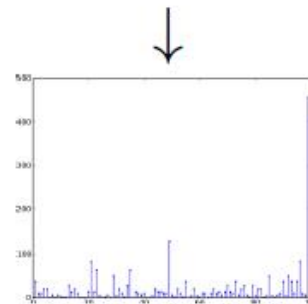
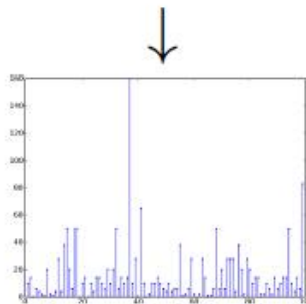
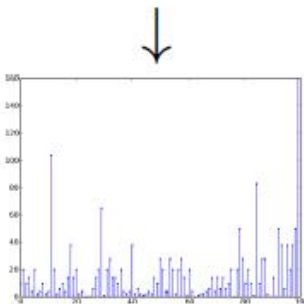
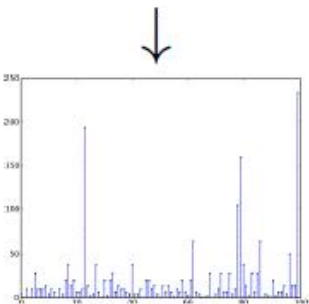
- **Note**

- \mathcal{X} can be any set, e.g. $\mathcal{X} = \text{"all videos on YouTube"}$ or $\mathcal{X} = \text{"all permutations of } \{1, \dots, k\}$ ", or $\mathcal{X} = \text{"the internet"}$.

Example: Bag of Visual Words Representation

- General framework in visual recognition
 - Create a codebook (vocabulary) of prototypical image features
 - Represent images as histograms over codebook activations
 - Compare two images by any histogram kernel, e.g. χ^2 kernel

$$k_{\chi^2}(h, h') = \exp \left(-\frac{1}{\gamma} \sum_j \frac{(h_j - h'_j)^2}{h_j + h'_j} \right)$$



The “Kernel Trick”

Any algorithm that uses data only in the form of inner products can be *kernelized*.

- How to kernelize an algorithm
 - Write the algorithm only in terms of inner products.
 - Replace all inner products by kernel function evaluations.
- ⇒ The resulting algorithm will do the same as the linear version, but in the (hidden) feature space \mathcal{H} .
- Caveat: working in \mathcal{H} is not a guarantee for better performance. A good choice of k and model selection are important!

Outlook

- **Kernels are a widely used concept in Machine Learning**
 - They are the basis for Support Vector Machines from ML1.
 - We will see several other *kernelized* algorithms in this lecture...
- **Examples**
 - Gaussian Processes
 - Support Vector Regression
 - Kernel PCA
 - Kernel k-Means
 - ...
- **Let's first examine the role of kernels in probabilistic discriminative models.**
 - ⇒ This will lead us to **Gaussian Processes**.

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- Recap: Linear Regression
- Kernels
 - Dual representations
 - Kernel Ridge Regression
 - Properties of kernels
- **Gaussian Processes**
 - **Motivation**
 - **Gaussian Process definition**
 - **Squared exponential covariance function**
 - **Prediction with noise-free observations**
 - **Prediction with noisy observations**
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Gaussian Processes

- So far...

- Considered linear regression models of the form

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

- where \mathbf{w} is a vector of parameters

$\phi(\mathbf{x})$ is a vector of fixed non-linear basis functions.

- We showed that a prior distribution over \mathbf{w} induced a prior distribution over functions $y(\mathbf{x}, \mathbf{w})$.
- Given a training set, we evaluated the posterior distribution over $\mathbf{w} \Rightarrow$ corresponding posterior over regression functions.
- This implies a predictive distribution $p(t | \mathbf{x})$ for new inputs \mathbf{x} .

- Gaussian process viewpoint

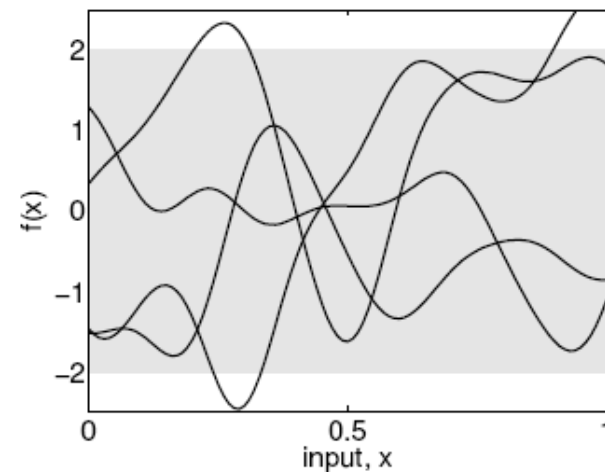
- Dispense with the parametric model and instead define a prior probability distribution over functions directly.

Gaussian Process

- **Gaussian distribution**
 - Probability distribution over scalars / vectors.
- **Gaussian process** (generalization of Gaussian distrib.)
 - Describes properties of functions.
 - Function: Think of a function as a long vector where each entry specifies the function value $f(\mathbf{x}_i)$ at a particular point \mathbf{x}_i .
 - Issue: How to deal with infinite number of points?
 - If you ask only for properties of the function at a finite number of points...
 - Then inference in Gaussian Process gives you the same answer if you ignore the infinitely many other points.
- **Definition**
 - A **Gaussian process (GP)** is a collection of random variables any finite number of which has a joint Gaussian distribution.

Gaussian Process

- Example prior over functions $p(f)$
 - Represents our prior belief about functions before seeing any data.
 - Although specific functions don't have mean of zero, the mean of $f(x)$ values for any fixed x is zero (here).
 - Favors smooth functions
 - I.e. functions cannot vary too rapidly
 - Smoothness is induced by the **covariance function** of the Gaussian Process.
 - Learning in Gaussian processes
 - Is mainly defined by finding suitable properties of the covariance function.



Linear Regression Revisited

- Let's return to the linear regression example and re-derive the predictive distribution by working in terms of distributions over functions $y(\mathbf{x}, \mathbf{w})$...

- Linear Regression Model

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

- Consider a prior distribution over \mathbf{w} given by

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I})$$

- For any given value of \mathbf{w} , the definition induces a particular function of \mathbf{x} .
- The probability distribution over \mathbf{w} therefore induces a probability distribution over functions $y(\mathbf{x})$.

Linear Regression Revisited

- **Linear Regression (cont'd)**

- We want to evaluate this function at specific values of \mathbf{x} , e.g. at the training data points $\mathbf{x}_1, \dots, \mathbf{x}_N$.
- We are therefore interested in the joint distribution of function values $y(\mathbf{x}_1), \dots, y(\mathbf{x}_N)$, which we denote by the vector \mathbf{y} .

$$\mathbf{y} = \Phi \mathbf{w}$$

- We know that \mathbf{y} is a linear combination of Gaussian distributed variables and is therefore itself Gaussian.
- ⇒ Only need to find its mean and covariance.

$$\mathbb{E}[\mathbf{y}] = \Phi \mathbb{E}[\mathbf{w}] = \mathbf{0}$$

$$\text{cov}[\mathbf{y}] = \mathbb{E}[\mathbf{y}\mathbf{y}^T] = \Phi \mathbb{E}[\mathbf{w}\mathbf{w}^T] \Phi^T = \frac{1}{\alpha} \Phi \Phi^T = \mathbf{K}$$

- with the kernel matrix $\mathbf{K} = \{k(\mathbf{x}_n, \mathbf{x}_m)\}_{nm}$.

Gaussian Process

- This model is a particular example of a Gaussian Process.
 - Linear regression with a zero-mean, isotropic Gaussian prior on \mathbf{w} .
- General definition
 - A **Gaussian Process** is defined as a probability distribution over functions $y(\mathbf{x})$ such that the set of values of $y(\mathbf{x})$ evaluated at an arbitrary set of points $\mathbf{x}_1, \dots, \mathbf{x}_N$ have a Gaussian distribution.
 - A key point about GPs is that the joint distribution over N variables y_1, \dots, y_N is completely specified by the second-order statistics, namely mean and covariance.

Gaussian Process

- A Gaussian process is completely defined by

- Mean function $m(\mathbf{x})$ and

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})]$$

- Covariance function $k(\mathbf{x}, \mathbf{x}')$

$$k(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))]$$

- We write the Gaussian process (GP)

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

Gaussian Process

- **Property**

- Defined as a collection of random variables, which implies **consistency**.

- **Consistency means**

- If the GP specifies e.g. $(y_1, y_2) \sim \mathcal{N}(\mu, \Sigma)$

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$$

- Then it must also specify $y_1 \sim \mathcal{N}(\mu_1, \Sigma_{11})$

- I.e. examination of a larger set of variables does not change the distribution of a smaller set.

Gaussian Process: Example

- **Example:**

- Bayesian linear regression model: $f(\mathbf{x}) = \phi(\mathbf{x})^T \mathbf{w}$
- With Gaussian prior: $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \Sigma_p)$

⇒ **Mean:**

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

⇒ **Covariance:**

$$\begin{aligned} \mathbb{E}[f(\mathbf{x})f(\mathbf{x}')] &= \phi(\mathbf{x})^T \mathbb{E}[\mathbf{w}\mathbf{w}^T] \phi(\mathbf{x}') \\ &= \phi(\mathbf{x})^T \Sigma_p \phi(\mathbf{x}') \\ &= \tilde{\phi}(\mathbf{x})^T \tilde{\phi}(\mathbf{x}') \quad \text{where} \quad \tilde{\phi}(\mathbf{x}) = \Sigma_p^{\frac{1}{2}} \phi(\mathbf{x}) \end{aligned}$$

Gaussian Process: Squared Exponential

- Typical covariance function

- Squared exponential (SE)

- Covariance function specifies the covariance between pairs of random variables

$$\text{cov}[f(\mathbf{x}_p), f(\mathbf{x}_q)] = k(\mathbf{x}_p, \mathbf{x}_q) = \exp \left\{ -\frac{1}{2} |\mathbf{x}_p - \mathbf{x}_q|^2 \right\}$$

- Remarks

- Covariance between the **outputs** is written as a function between the **inputs**.
- The squared exponential covariance function corresponds to a Bayesian linear regression model with an **infinite** number of basis functions.
- For any positive definite covariance function $k(.,.)$, there exists a (possibly infinite) expansion in terms of basis functions.

Gaussian Process: Prior over Functions

- **Distribution over functions:**

- Specification of covariance function implies distribution over functions.
- I.e. we can draw samples from the distribution of functions evaluated at a (finite) number of points.

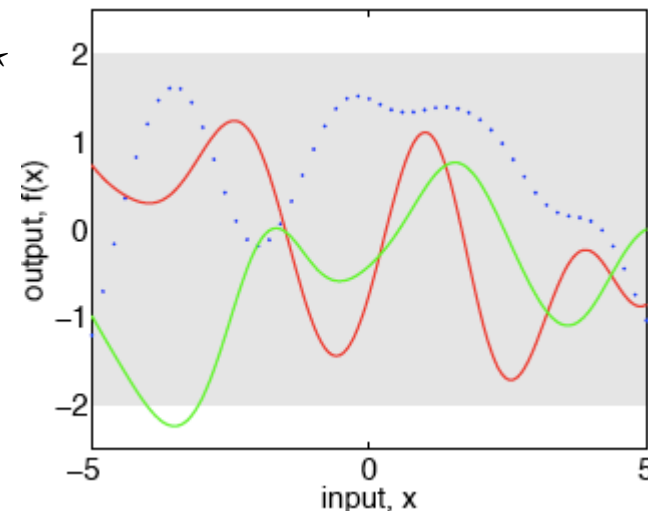
- **Procedure**

- We choose a number of input points X_*
- We write the corresponding covariance matrix (e.g. using SE) element-wise:

$$K(X_*, X_*)$$

- Then we generate a random Gaussian vector with this covariance matrix:

$$f_* \sim \mathcal{N}(\mathbf{0}, K(X_*, X_*))$$



**Example of 3 functions
sampled**

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Prediction with Noise-free Observations

- Assume our observations are noise-free:

$$\{(\mathbf{x}_n, f_n) \mid n = 1, \dots, N\}$$

- **Joint distribution** of the training outputs \mathbf{f} and test outputs \mathbf{f}_* **according to the prior:**

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

- $K(X, X_*)$ contains covariances for all pairs of training and test points.
- To get the **posterior** (after including the observations)
 - We need to restrict the above prior to contain only those functions which agree with the observed values.
 - Think of generating functions from the prior and rejecting those that disagree with the observations (obviously prohibitive).

Prediction with Noise-free Observations

- Calculation of posterior: simple in GP framework
 - Corresponds to conditioning the joint Gaussian prior distribution on the observations:

$$\mathbf{f}_\star | X_\star, X, \mathbf{f} \sim \mathcal{N}(\bar{\mathbf{f}}_\star, \text{cov}[\mathbf{f}_\star]) \quad \bar{\mathbf{f}}_\star = \mathbb{E}[\mathbf{f}_\star | X, X_\star, \mathbf{t}]$$

- with:

$$\begin{aligned} \bar{\mathbf{f}}_\star &= K(X_\star, X)K(X, X)^{-1}\mathbf{f} \\ \text{cov}[\mathbf{f}_\star] &= K(X_\star, X_\star) - K(X_\star, X)K(X, X)^{-1}K(X, X_\star) \end{aligned}$$

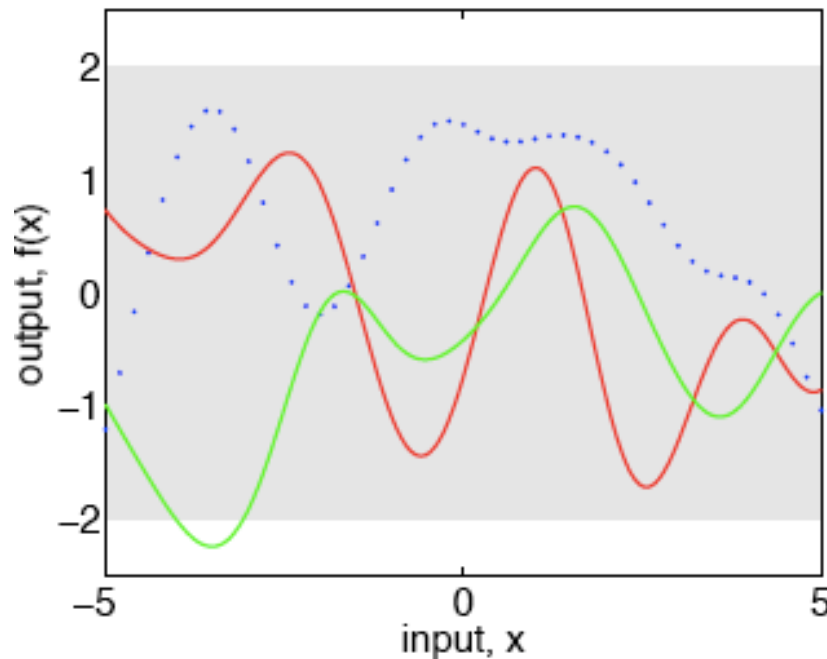
- This uses the general property of Gaussians that

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix} \Rightarrow \begin{aligned} \boldsymbol{\mu}_{a|b} &= \boldsymbol{\mu}_a + \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}(\mathbf{x}_b - \boldsymbol{\mu}_b) \\ \boldsymbol{\Sigma}_{a|b} &= \boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}\boldsymbol{\Sigma}_{ba} \end{aligned}$$

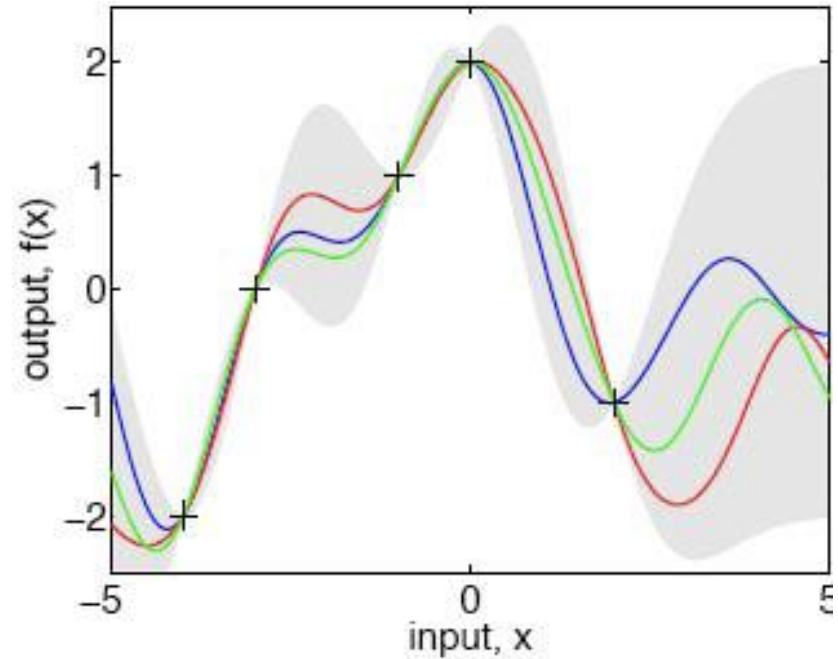
Prediction with Noise-free Observations

- Example:

Prior



Posterior using 5
noise-free observations



Topics of This Lecture

- Recap: Linear Regression
- Kernels
 - Dual representations
 - Kernel Ridge Regression
 - Properties of kernels
- **Gaussian Processes**
 - Motivation
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Prediction with Noisy Observations

- Typically, we assume noise in the observations

$$t = f(\mathbf{x}) + \epsilon \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

- The prior on the noisy observations becomes

$$\text{COV}[y_p, y_q] = k(\mathbf{x}_p, \mathbf{x}_q) + \sigma_n^2 \delta_{pq}$$

- Written in compact form:

$$\text{COV}[\mathbf{y}] = K(X, X) + \sigma_n^2 I$$

- Joint distribution of the observed values and the test locations under the prior is then:

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

Prediction with Noisy Observations

- Calculation of posterior:

- Corresponds to **conditioning the joint Gaussian prior distribution on the observations:**

$$\mathbf{f}_\star | X_\star, X, \mathbf{t} \sim \mathcal{N}(\bar{\mathbf{f}}_\star, \text{cov}[\mathbf{f}_\star]) \quad \bar{\mathbf{f}}_\star = \mathbb{E}[\mathbf{f}_\star | X, X_\star, \mathbf{t}]$$

- **with:**

$$\bar{\mathbf{f}}_\star = K(X_\star, X) (K(X, X) + \sigma_n^2 I)^{-1} \mathbf{t}$$

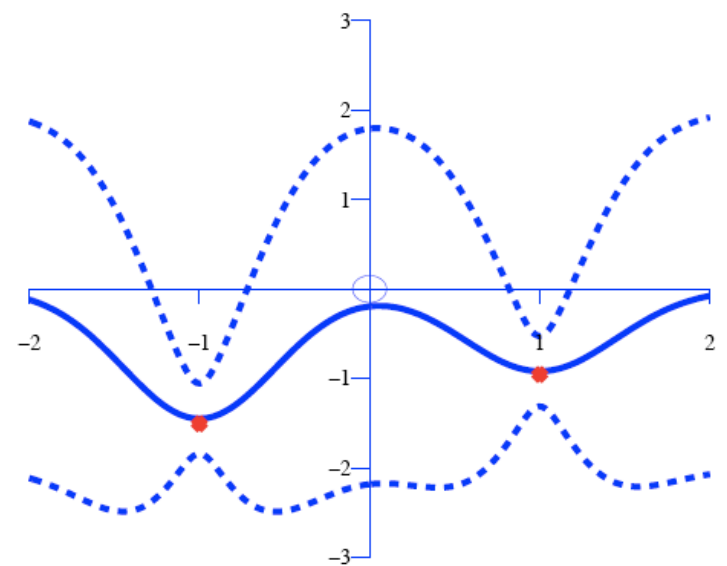
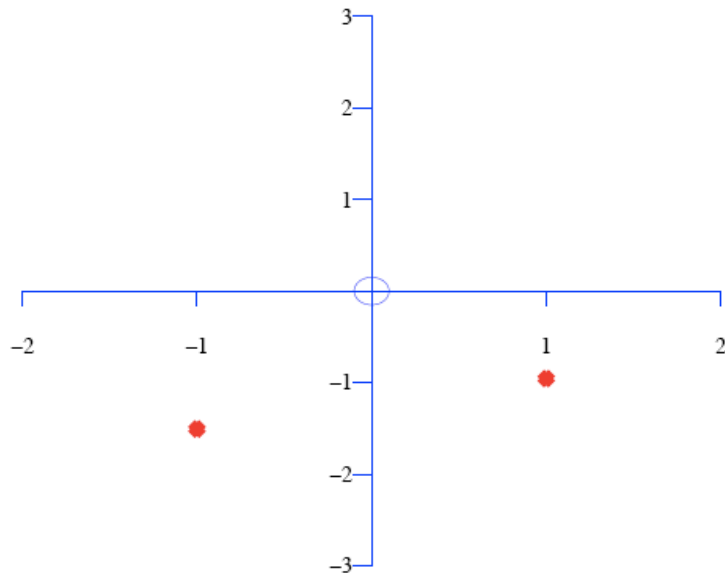
$$\text{cov}[\mathbf{f}_\star] = K(X_\star, X_\star) - K(X_\star, X) (K(X, X) + \sigma_n^2 I)^{-1} K(X, X_\star)$$

⇒ **This is the key result that defines Gaussian process regression!**

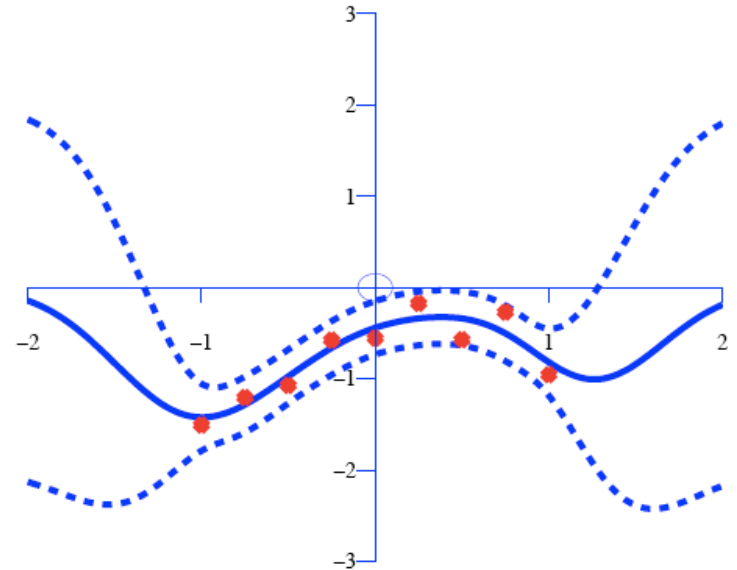
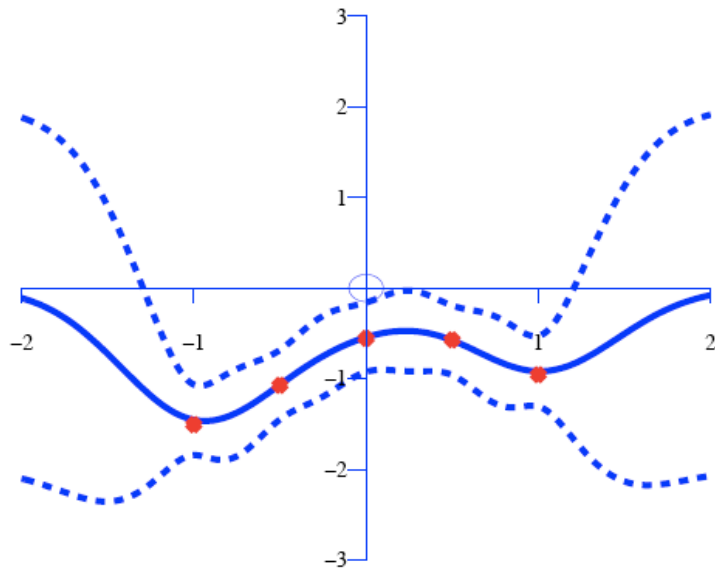
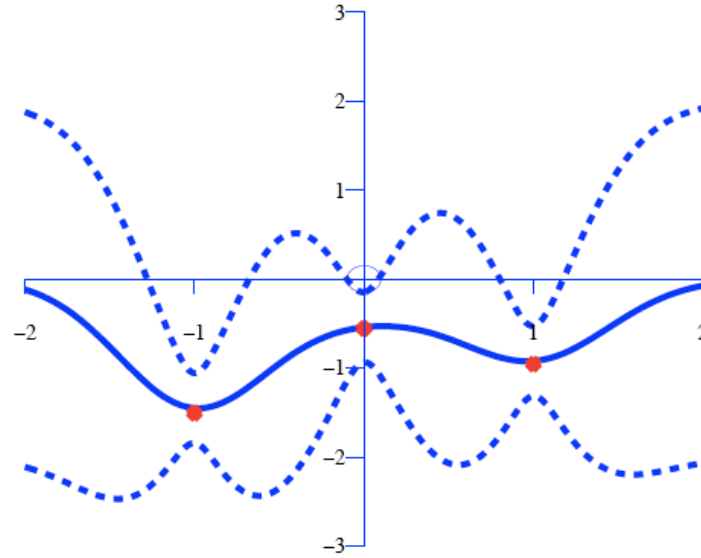
- The predictive distribution is a Gaussian whose mean and variance depend on the test points X_\star and on the kernel $k(\mathbf{x}, \mathbf{x}')$, evaluated on the training data X .

Gaussian Process Regression

- Example



Gaussian Process Regression



Discussion

- **Key result:** $\mathbf{f}_* | X_*, X, \mathbf{t} \sim \mathcal{N}(\bar{\mathbf{f}}_*, \text{cov}[\mathbf{f}_*])$ with

$$\bar{\mathbf{f}}_* = K(X_*, X) (K(X, X) + \sigma_n^2 I)^{-1} \mathbf{t}$$

$$\text{cov}[\mathbf{f}_*] = K(X_*, X_*) - K(X_*, X) (K(X, X) + \sigma_n^2 I)^{-1} K(X, X_*)$$

- **Observations**

- The mean can be written in linear form

$$\bar{f}(\mathbf{x}_*) = k(\mathbf{x}_*, X) \underbrace{[K(X, X) + \sigma_n^2 I]^{-1} \mathbf{t}}_{\boldsymbol{\alpha}} = \sum_{n=1}^N \alpha_n k(\mathbf{x}_*, \mathbf{x}_n).$$

- This form is commonly encountered in the kernel literature (\rightarrow SVM)

- The variance is the difference between two terms

$$V(\mathbf{x}_*) = \underbrace{k(\mathbf{x}_*, \mathbf{x}_*)}_{\text{Prior variance}} - \underbrace{k(\mathbf{x}_*, X) [K(X, X) + \sigma_n^2 I]^{-1} k(X, \mathbf{x}_*)}_{\text{Explanation of data } X}$$

Prior variance

Explanation of data X

Computational Complexity

- Computational complexity

- Central operation in using GPs involves **inverting a matrix of size $N \times N$** (the kernel matrix $K(X, X)$):

$$\bar{\mathbf{f}}_{\star} = K(X_{\star}, X) \left(K(X, X) + \sigma_n^2 I \right)^{-1} \mathbf{t}$$

$$\text{cov}[\mathbf{f}_{\star}] = K(X_{\star}, X_{\star}) - K(X_{\star}, X) \left(K(X, X) + \sigma_n^2 I \right)^{-1} K(X, X_{\star})$$

⇒ Effort in $\mathcal{O}(N^3)$ for N data points!

- Compare this with the basis function model (→ **Lecture 3**)

$$p(f_{\star} | \mathbf{x}_{\star}, X, \mathbf{t}) \sim \mathcal{N} \left(\frac{1}{\sigma_n^2} \phi(\mathbf{x}_{\star})^T \mathbf{S}^{-1} \Phi(X) \mathbf{t}, \phi(\mathbf{x}_{\star})^T \mathbf{S}^{-1} \phi(\mathbf{x}_{\star}) \right)$$

$$\mathbf{S} = \frac{1}{\sigma_n^2} \Phi(X) \Phi(X)^T + \Sigma_p^{-1}$$

⇒ Effort in $\mathcal{O}(M^3)$ for M basis functions.

Computational Complexity

- Complexity of GP model
 - Training effort: $\mathcal{O}(N^3)$ through matrix inversion
 - Test effort: $\mathcal{O}(N^2)$ through vector-matrix multiplication
- Complexity of basis function model
 - Training effort: $\mathcal{O}(M^3)$
 - Test effort: $\mathcal{O}(M^2)$
- Discussion
 - If the number of basis functions M is smaller than the number of data points N , then the basis function model is more efficient.
 - However, advantage of GP viewpoint is that we can consider covariance functions that can only be expressed by an **infinite number of basis functions**.
 - Still, exact GP methods become infeasible for large training sets.

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Influence of Hyperparameters

- Most covariance functions have some free parameters.

- Example:

$$k_y(\mathbf{x}_p, \mathbf{x}_q) = \sigma_f^2 \exp \left\{ -\frac{(\mathbf{x}_p - \mathbf{x}_q)^2}{2 \cdot l^2} \right\} + \sigma_n^2 \delta_{pq}$$

- Parameters: (l, σ_f, σ_n)
 - Signal variance: σ_f^2
 - Range of neighbor influence (called “length scale”): l
 - Observation noise: σ_n^2

Influence of Hyperparameters

$$k_y(\mathbf{x}_p, \mathbf{x}_q) = \sigma_f^2 \exp \left\{ -\frac{(\mathbf{x}_p - \mathbf{x}_q)^2}{2 \cdot l^2} \right\} + \sigma_n^2 \delta_{pq}$$

- Examples for different settings of the length scale

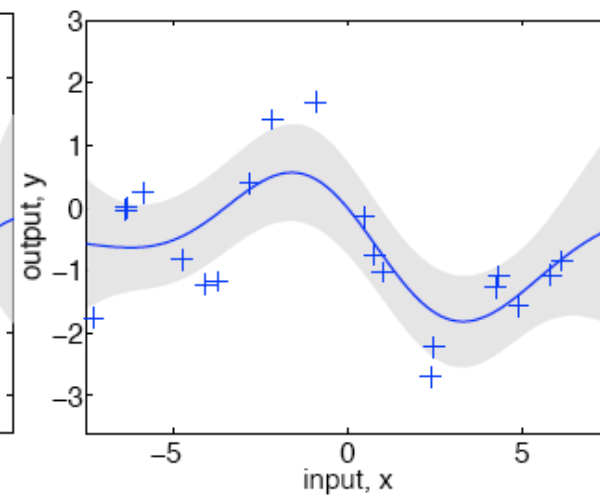
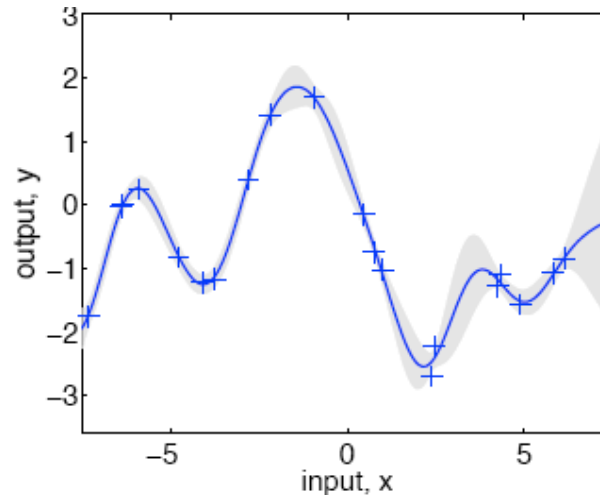
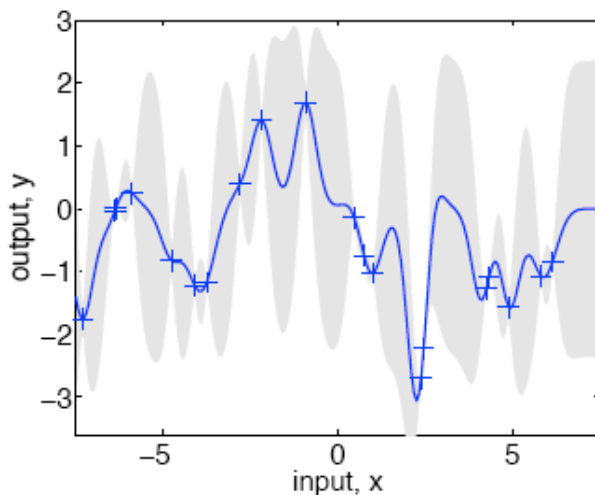
$$(l, \sigma_f, \sigma_n) =$$

(σ parameters set by optimizing the marginal likelihood)

$$= (0.3, 1.08, 0.00005)$$

$$= (1, 1, 0.1)$$

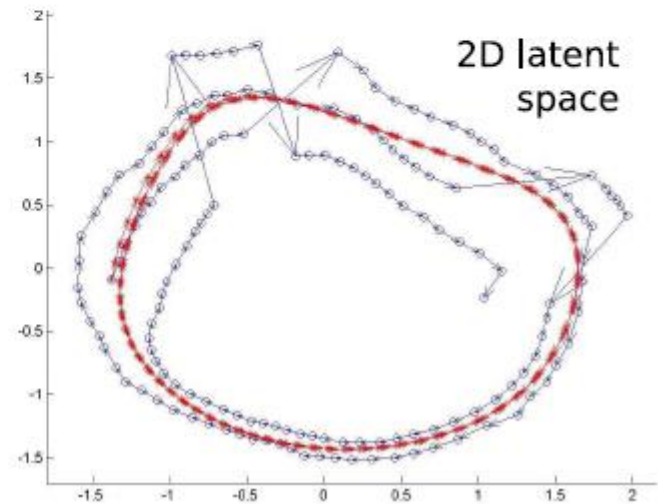
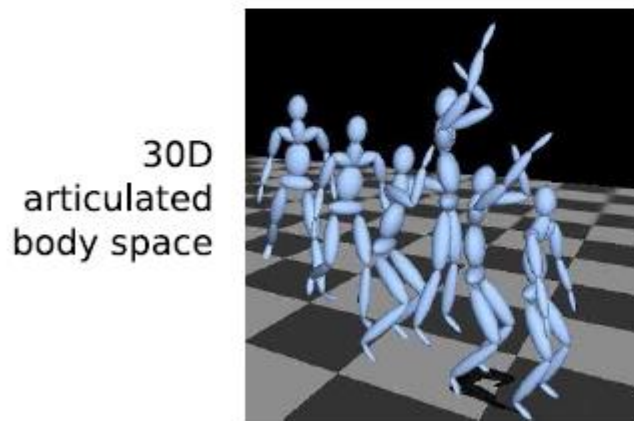
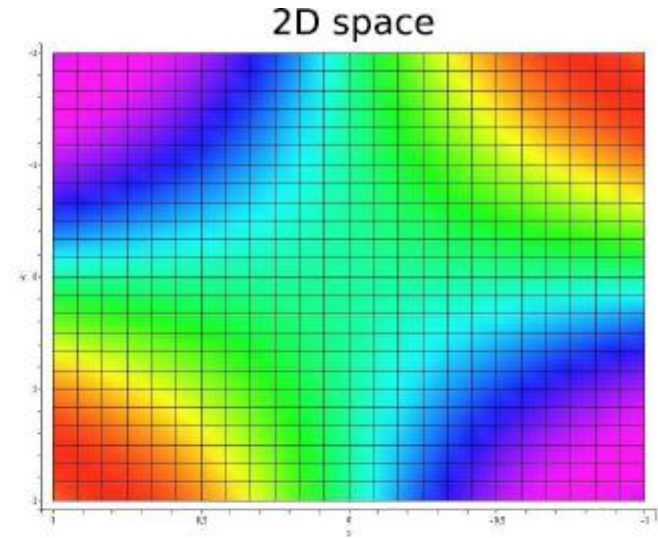
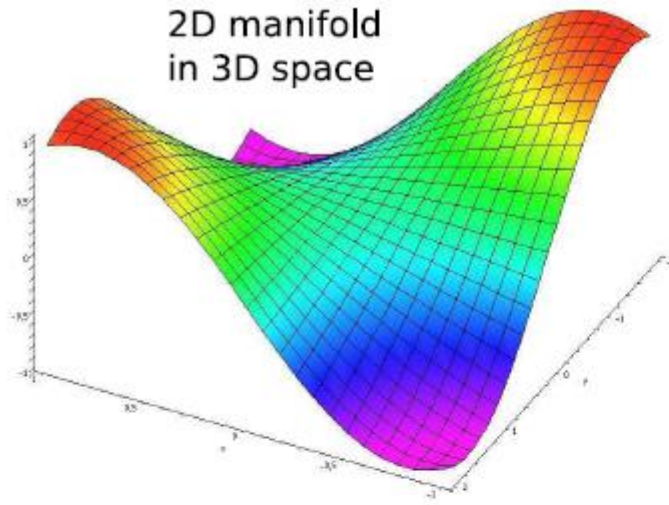
$$= (3.0, 1.16, 0.89)$$



Topics of This Lecture

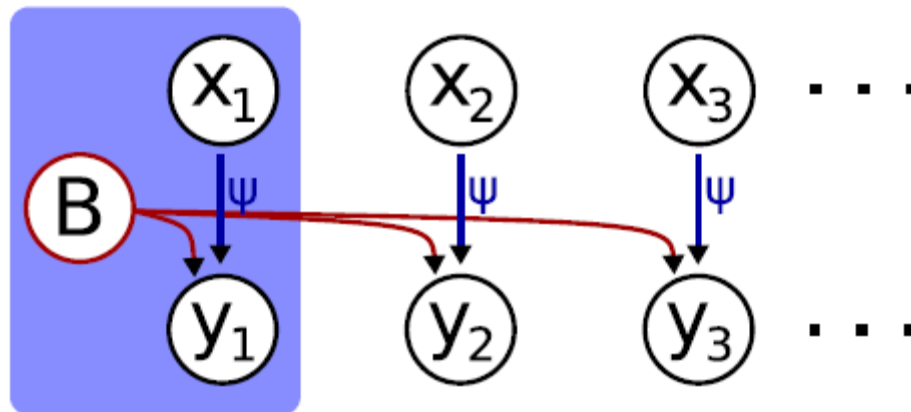
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Application: Non-Linear Dimensionality Reduction



Gaussian Process Latent Variable Model

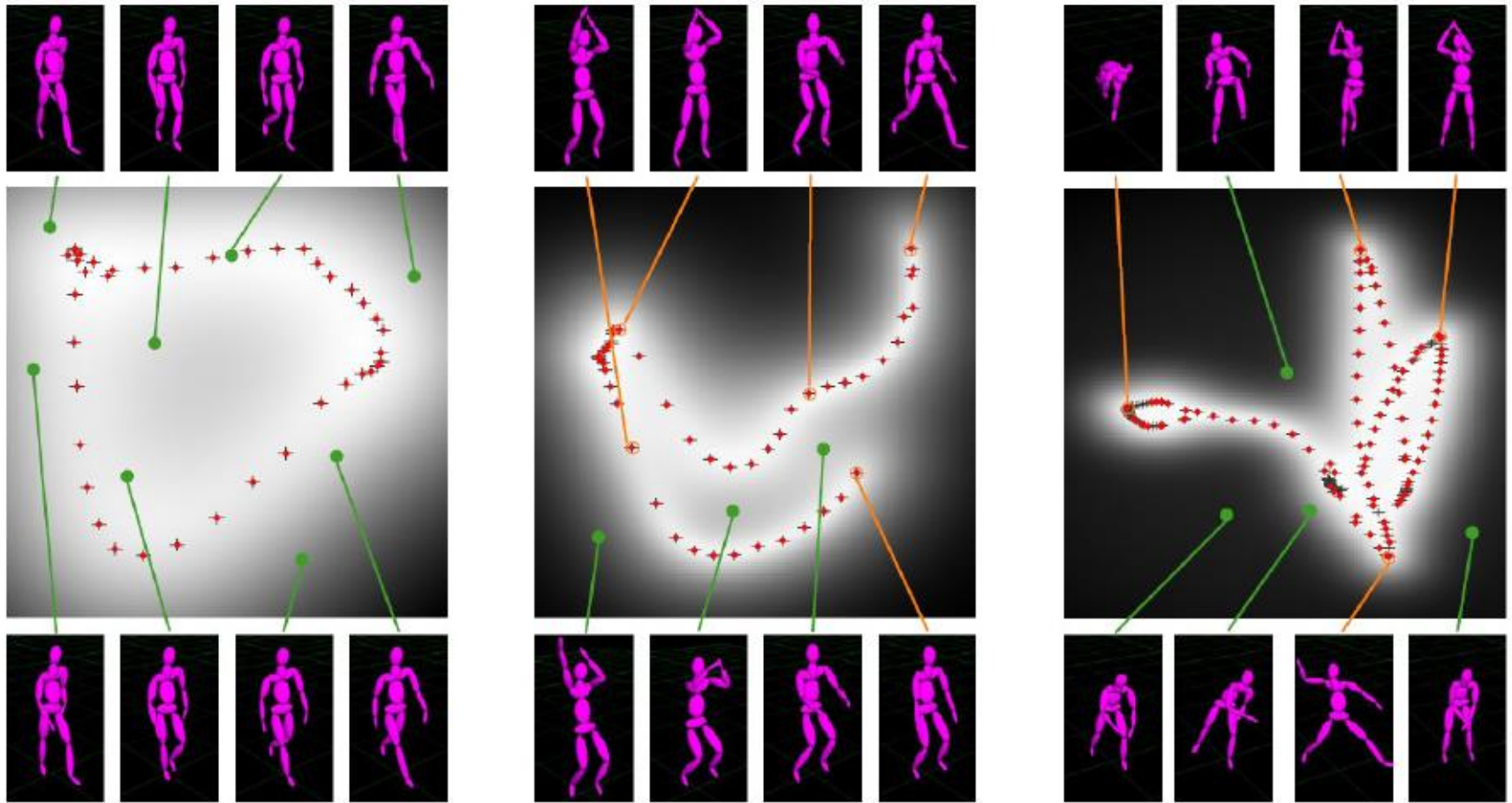
- At each time step t , we express our observations y as a combination of basis functions ψ of latent variables x .



$$y_t = \sum_j b_j \psi_j(\mathbf{x}_t) + \delta_t$$

- This is modeled as a Gaussian process...

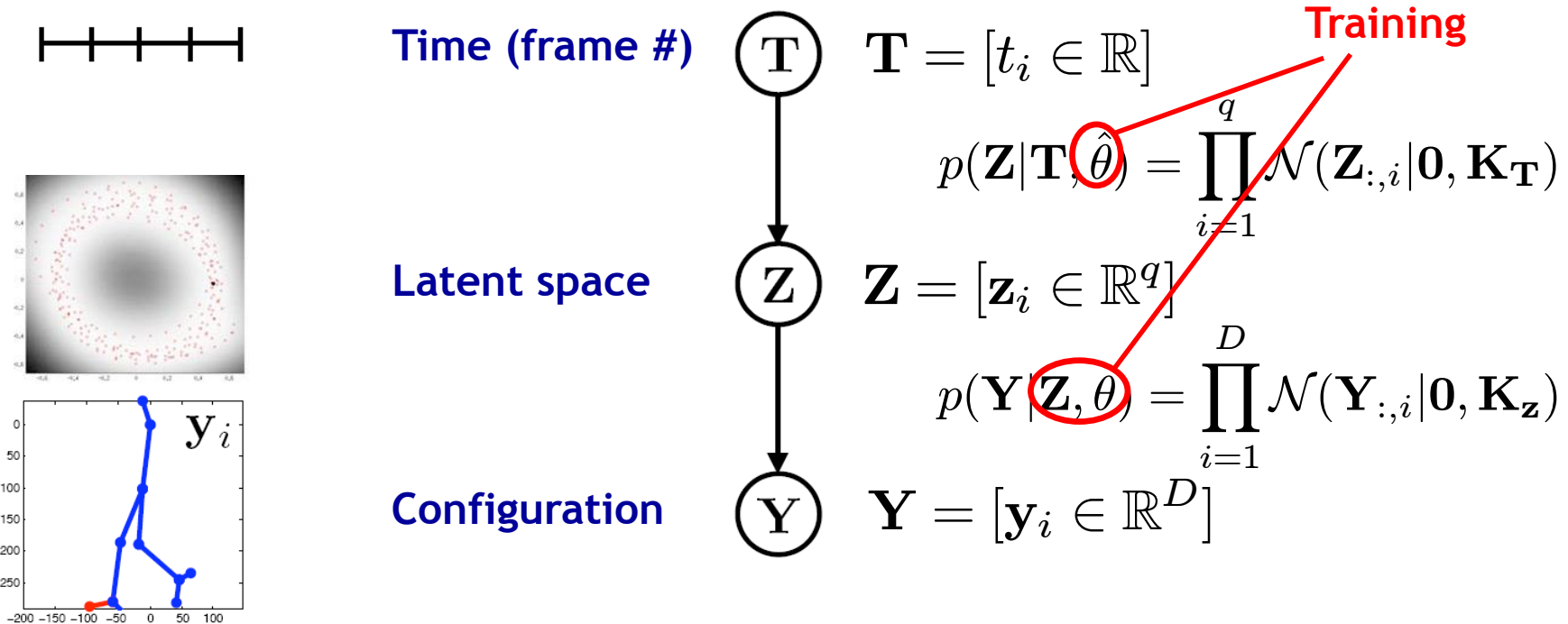
Example: Style-based Inverse Kinematics



Learned GPLVMs using a *walk*, a *jump shot* and a *baseball pitch*

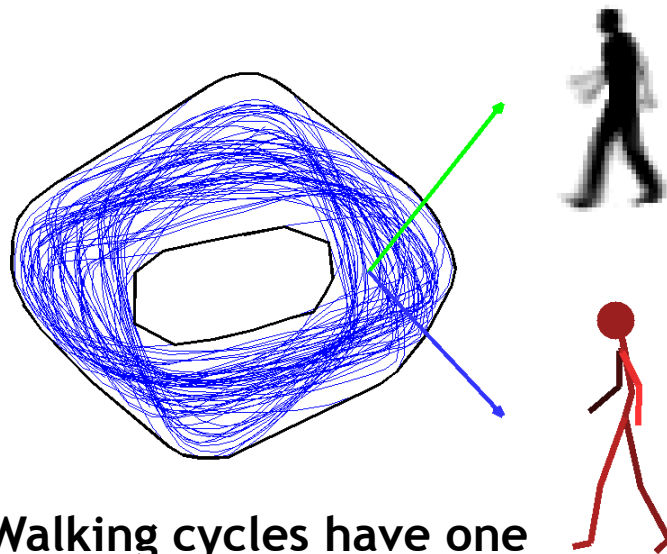
Application: Modeling Body Dynamics

- Task: estimate full body pose in m video frames.
 - High-dimensional \mathbf{Y} *
 - Model body dynamics using hierarchical Gaussian process latent variable model (hGPLVM) [Lawrence & Moore, ICML 2007].

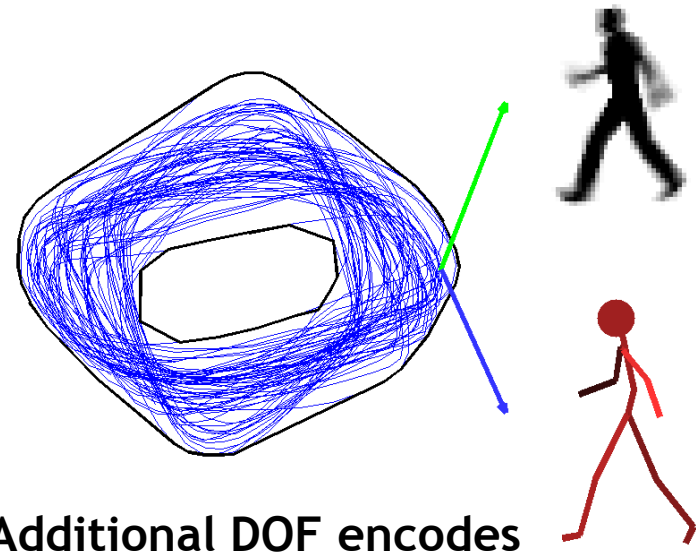


Articulated Motion in Latent Space (different work)

- Gaussian Process regression from latent space to
 - Pose [\rightarrow] = $p(\text{Pose} | z)$ to recover original pose from latent space]
 - Silhouette [\rightarrow] = $p(\text{Silhouette} | z)$ to do inference on silhouettes]

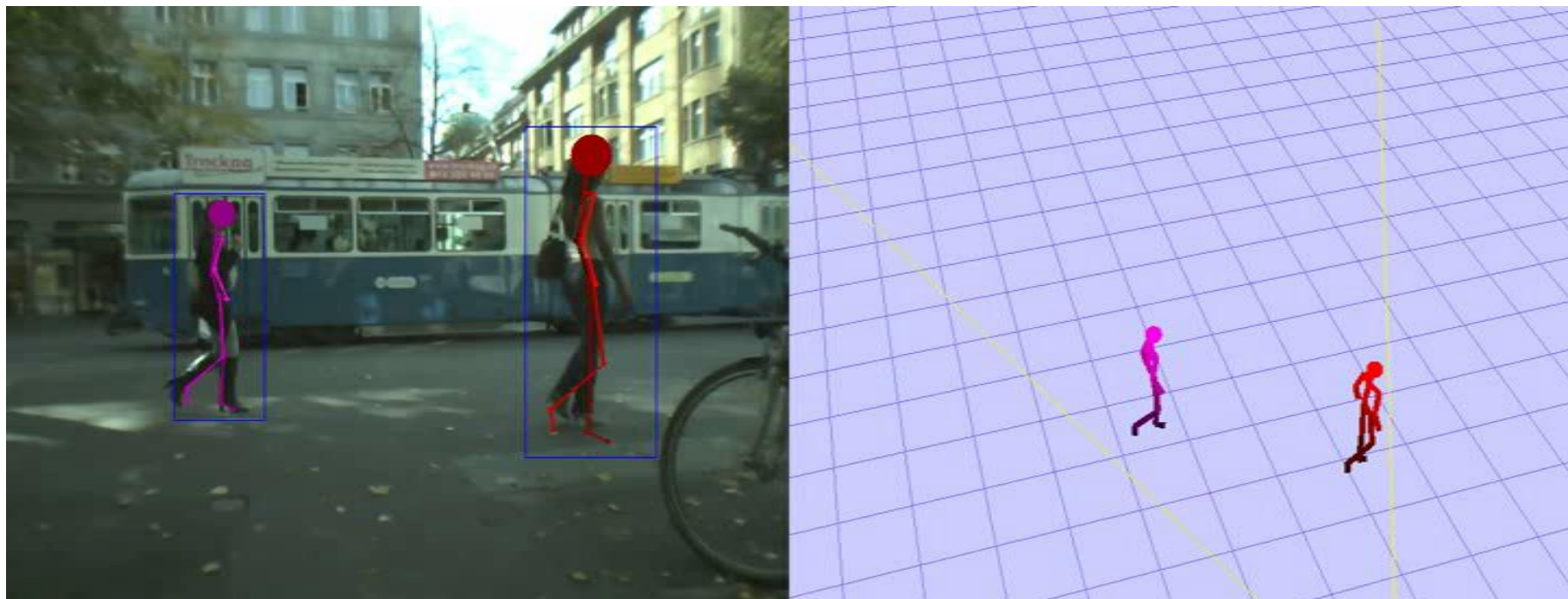


Walking cycles have one main (periodic) DOF



Additional DOF encodes „walking style“

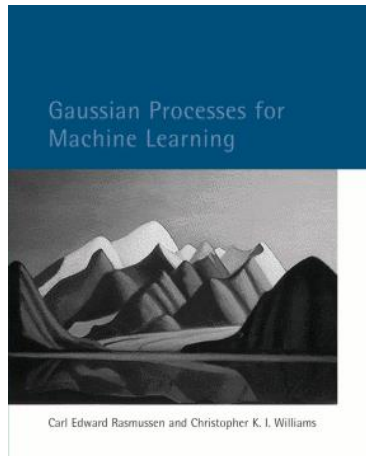
Results



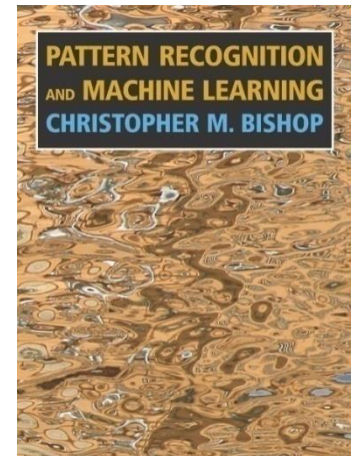
454 frames (~35 sec)
23 Pedestrians
20 detected by multi-body tracker

References and Further Reading

- **Kernels and Gaussian Processes are (shortly) described in Chapters 6.1 and 6.4 of Bishop's book.**



Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006



Carl E. Rasmussen, Christopher K.I. Williams
Gaussian Processes for Machine Learning
MIT Press, 2006

- **A better introduction can be found in Chapters 1 and 2 of the book by Rasmussen & Williams (also available online: <http://www.gaussianprocess.org/gpml/>)**