# Advanced Machine Learning
# Summer 2019

## Part 4 – Linear Regression III
### 10.04.2019

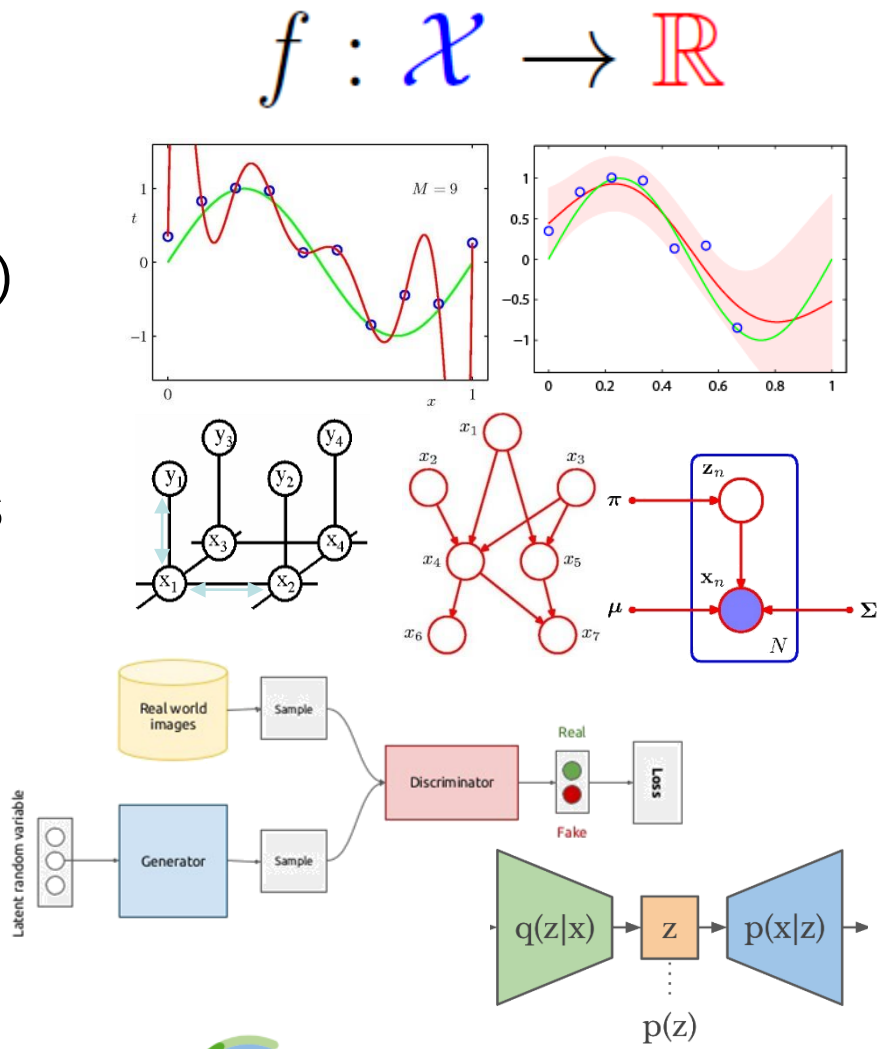
Prof. Dr. Bastian Leibe

RWTH Aachen University, Computer Vision Group
http://www.vision.rwth-aachen.de

Visual Computing Institute | RWTH AACHEN UNIVERSITY

# Course Outline

- Regression Techniques
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
- Deep Reinforcement Learning
- Probabilistic Graphical Models
  - Bayesian Networks
  - Markov Random Fields
  - Inference (exact & approximate)
- Deep Generative Models
  - Generative Adversarial Networks
  - Variational Autoencoders



# Topics of This Lecture

- Recap: Linear Regression
- Bias-Variance Trade-Off
- Kernels
  - Dual representations
  - Kernel Ridge Regression
  - Properties of kernels
- Other Kernel Methods
  - Kernel PCA
  - Kernel k-Means Clustering

# Recap: Other Loss Functions for Regression

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

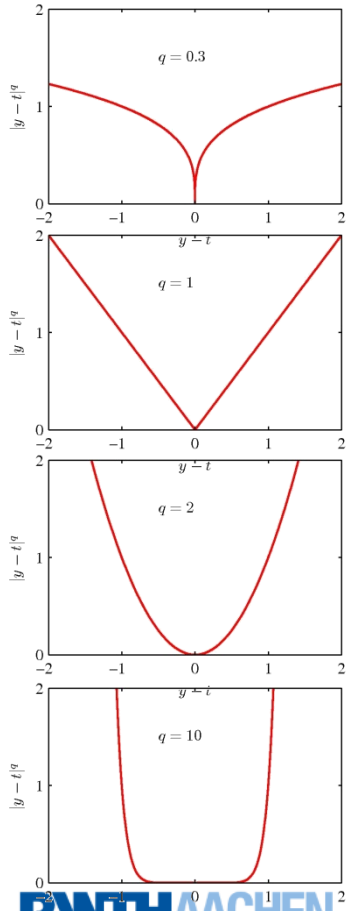
- Simple generalization: Minkowski loss

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

  - Expectation

$$\mathbb{E}[L_q] = \int\int |y(\mathbf{x}) - t|^q p(\mathbf{x}, t) \mathrm{d}\mathbf{x} \mathrm{d}t$$

- 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

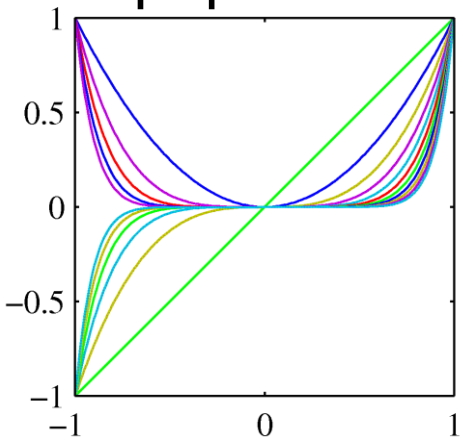
- Generally, we consider models of the following form

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

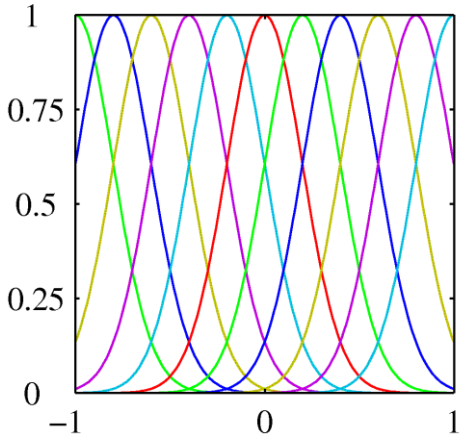
  – where $\phi_j(\mathbf{x})$ are known as *basis functions*.

  – In the simplest case, we use linear basis functions: $\phi_d(\mathbf{x}) = x_d$.

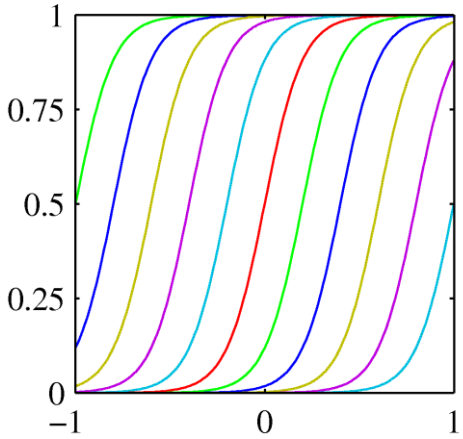
- Other popular basis functions




Polynomial




Gaussian

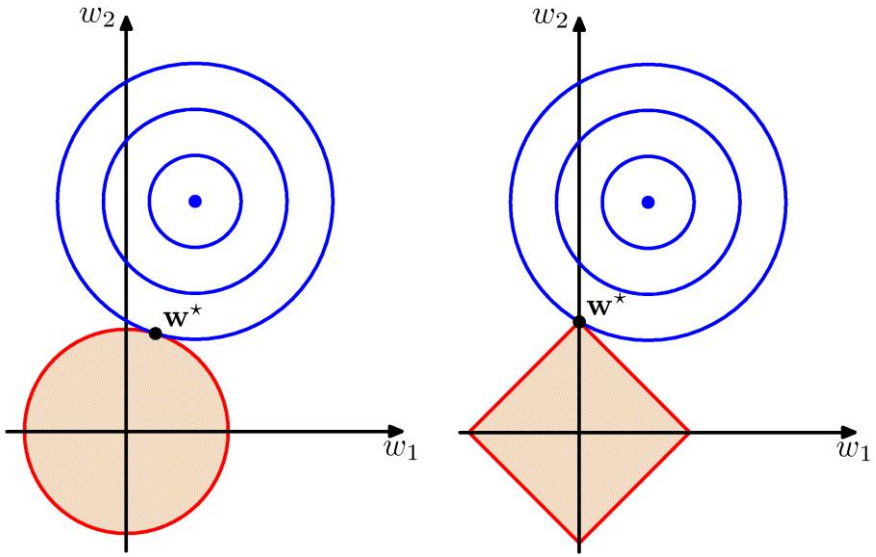



Sigmoid

# Recap: Regularized Least-Squares

- Consider more general regularization functions
  - "$L_q$ norms":

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




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



Image source: C.M. Bishop, 2006

# 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

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

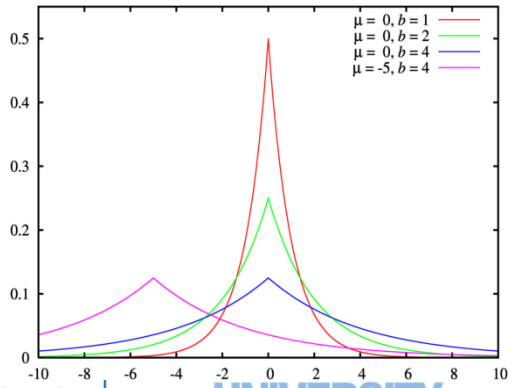



Image source: Wikipedia

# Topics of This Lecture

- Recap: Linear Regression
- Bias-Variance Decomposition
- Kernels
  - Dual representations
  - Kernel Ridge Regression
  - Properties of kernels
- Other Kernel Methods
  - Kernel PCA
  - Kernel k-Means Clustering

# Recap: Loss Functions for Regression

- Derivation: Expand the square term as follows

$$\begin{aligned}\{y(\mathbf{x}) - t\}^2 &= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}] + \mathbb{E}[t|\mathbf{x}] - t\}^2 \\ &= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 + \{\mathbb{E}[t|\mathbf{x}] - t\}^2 \\ &\quad + 2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\}\end{aligned}$$

- Substituting into the loss function $\mathbb{E}[L] = \iint \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\, \mathrm{d}\mathbf{x}\, \mathrm{d}t$
  - The cross-term vanishes, and we end up with

$$\mathbb{E}[L] = \int \underbrace{\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2}\, p(\mathbf{x})\, \mathrm{d}\mathbf{x} + \int \underbrace{\mathrm{var}\,[t|\mathbf{x}]}\, p(\mathbf{x})\, \mathrm{d}\mathbf{x}$$

Optimal least-squares predictor given by the conditional mean

Intrinsic variability of target data ⇒ Irreducible minimum value of the loss function

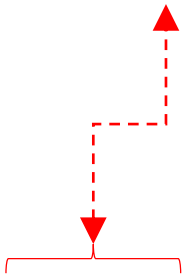
# Bias-Variance Decomposition

- Recall the *expected squared loss*,

$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \iint \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

  – where

$$h(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}] = \int t p(t|\mathbf{x})\,\mathrm{d}t.$$



- The second term of $\mathbb{E}[L]$ corresponds to the noise inherent in the random variable $t$.

- *What about the first term?*

# Bias-Variance Decomposition

- Suppose we were given multiple data sets, each of size $N$.
  - Any particular data set $\mathcal{D}$ will give a particular function $y(\mathbf{x};\mathcal{D})$
  - We then have

$$\begin{aligned}
&\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2 \\
&= \{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] + \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 \\
&= \{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2 + \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 \\
&\quad +2\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}.
\end{aligned}$$

- Taking the expectation over $\mathcal{D}$ yields

$$\begin{aligned}
&\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2\right] \\
&= \underbrace{\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right]}_{\text{variance}}.
\end{aligned}$$



Slide adapted from C.M. Bishop, 2006

# Bias-Variance Decomposition

- Thus we can write

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

– where

$$(\text{bias})^2 = \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$\text{variance} = \int \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right] p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

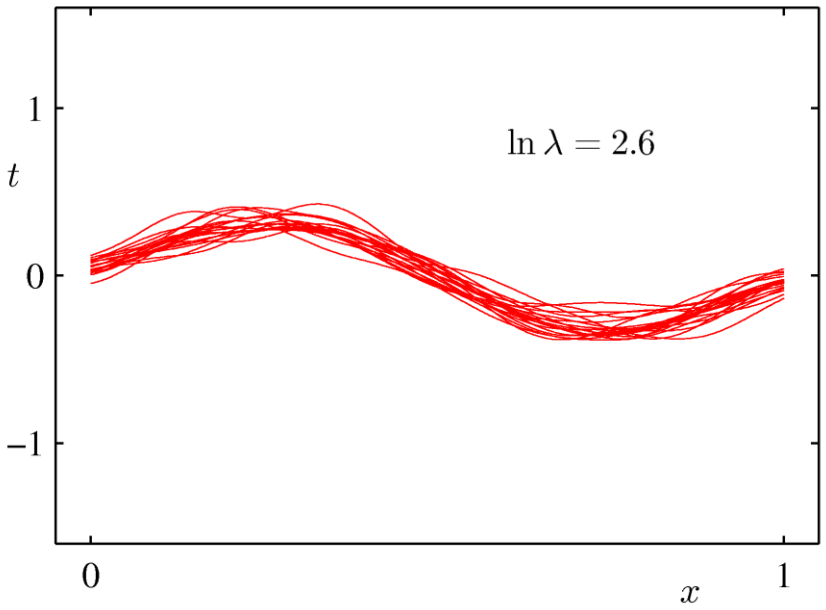
$$\text{noise} = \iint \{h(\mathbf{x}) - t\}^2 p(\mathbf{x},t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

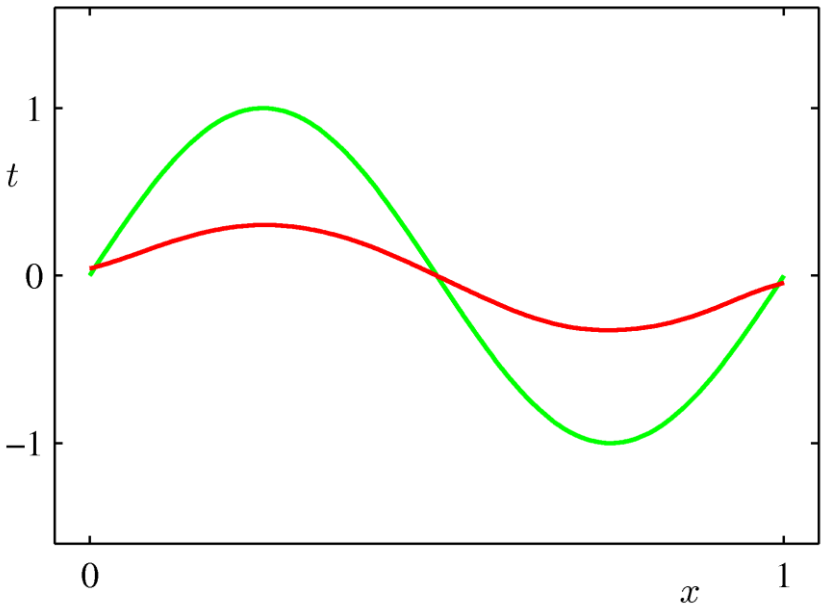


Slide adapted from C.M. Bishop, 2006

# Bias-Variance Decomposition

- Example
  - 25 data sets from the sinusoidal, varying the degree of regularization, $\lambda$.



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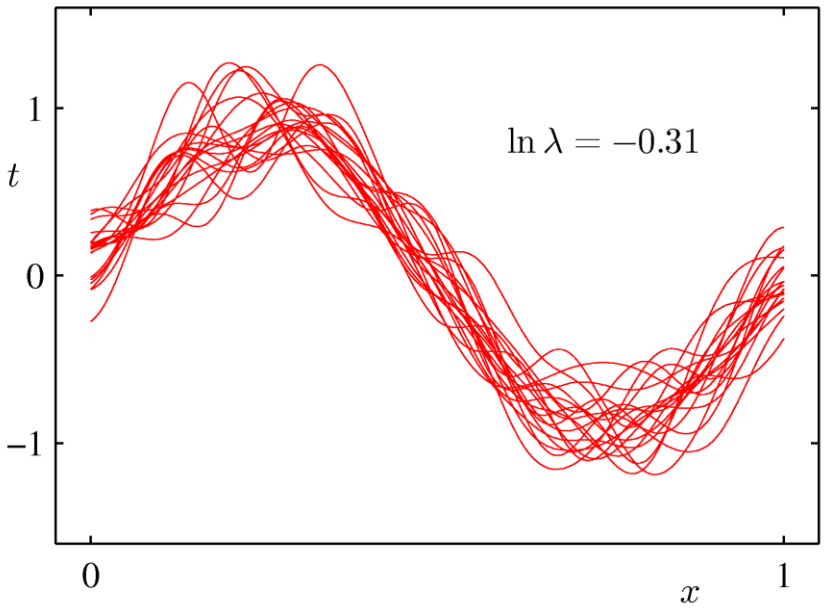


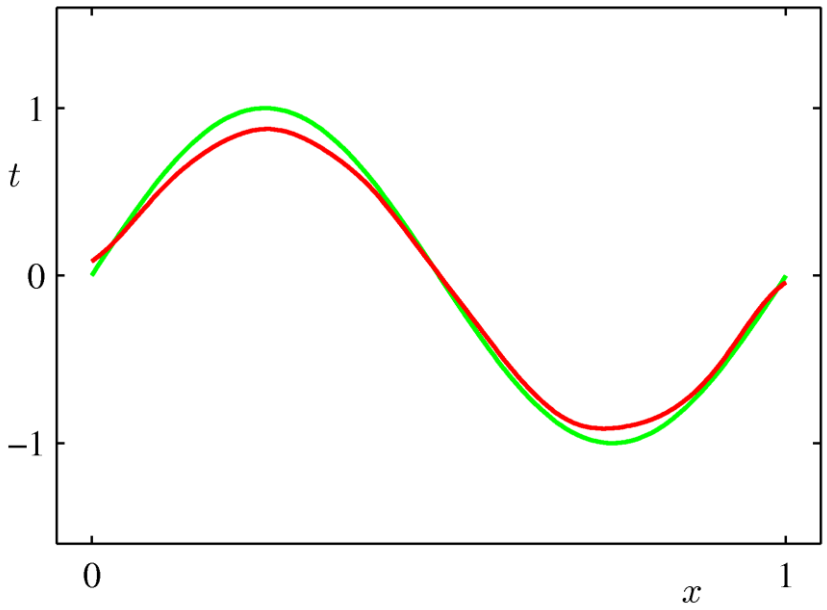

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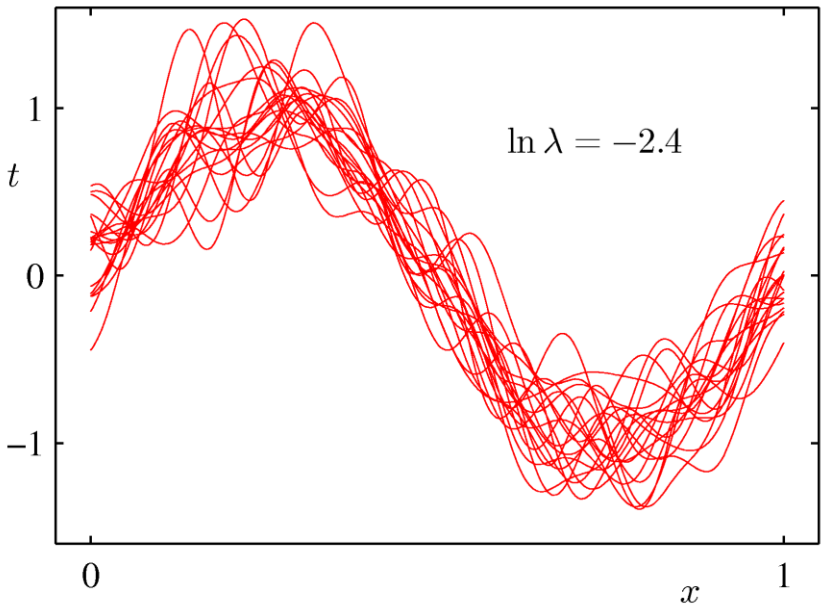
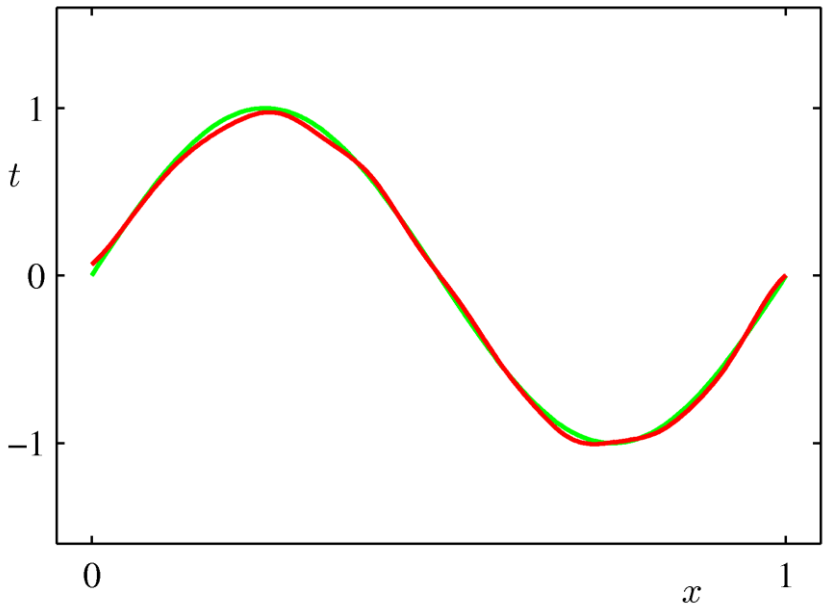
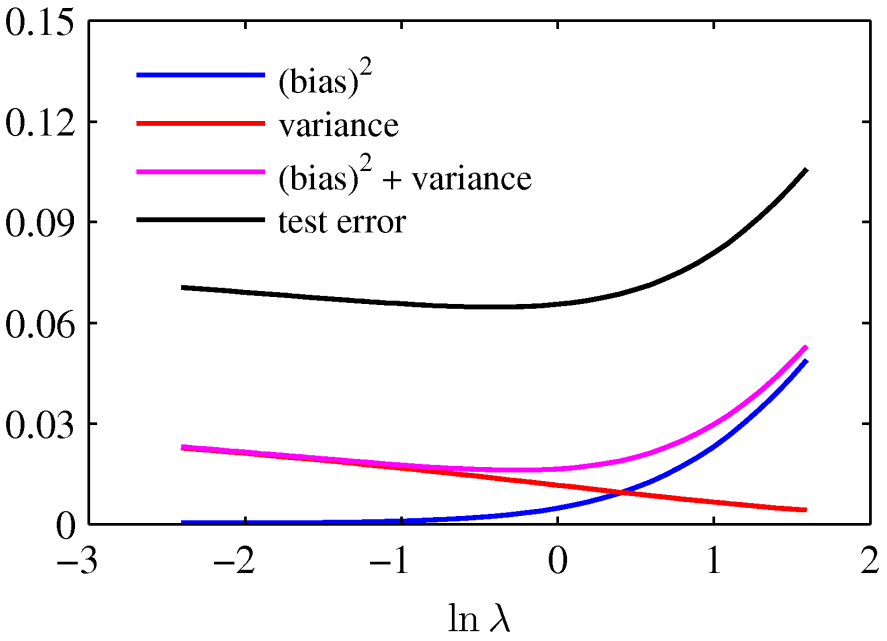


# The Bias-Variance Trade-Off

- Result from these plots
  - An over-regularized model (large $\lambda$) will have a high bias.
  - An under-regularized model (small $\lambda$) will have a high variance.




- We can compute an estimate for the generalization capability this way (magenta curve)!
  - *Can you see where the problem is with this?*

  ⇒ Computation is based on average w.r.t. ensembles of data sets.

  ⇒ Unfortunately of little practical value…



Slide adapted from C.M. Bishop, 2006

Image source: C.M. Bishop, 2006

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- Kernels
  - Dual representations
  - Kernel Ridge Regression
  - Properties of kernels
- Other Kernel Methods
  - Kernel PCA
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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 $\mathbf{w} = \mathbf{\Phi}^T\mathbf{a}$ 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 $\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^T$ 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

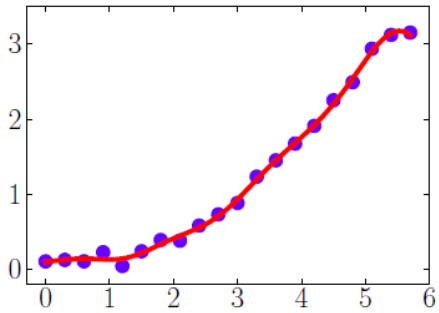
$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}^T\mathbf{K}\mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T\mathbf{K}\mathbf{a}$$

# 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.



Image source: Christoph Lampert

# 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 ($x \in [0, 2\pi]$):

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



Slide credit: Christoph Lampert

# 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 $\phi$ exists, but we don't know what $\phi$ 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 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 $x_1, \ldots, x_n \in \mathcal{X}$, the matrix

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

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

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



Slide credit: Christoph Lampert

# Hilbert Spaces

- Definition (Hilbert Space)
  - A Hilbert Space $\mathcal{H}$ is a vector space $H$ with an *inner product* $\langle . , . \rangle_{\mathcal{H}}$, e.g. a mapping
    $$\langle ., . \rangle_{\mathcal{H}} : H \times H \rightarrow \mathbb{R}$$
    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 $\langle . , . \rangle_{\mathcal{H}}$ *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. $\mathcal{X}$ = *"all videos on YouTube"* or $\mathcal{X}$ = *"all permutations of* {1, . . . , *k*}", or $\mathcal{X}$ = *"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. $\chi^2$ 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.

$\Rightarrow$ 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
  - …

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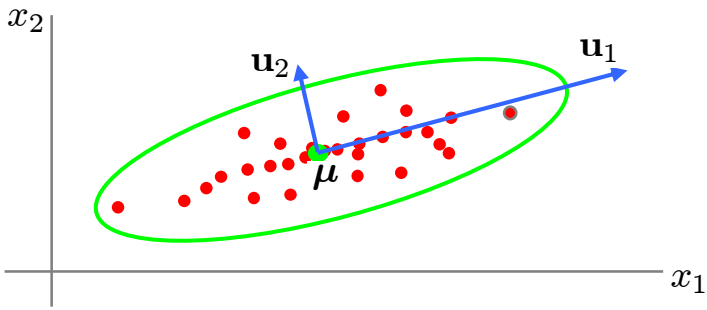
# Recap: PCA

- PCA procedure
  - Given samples $\mathbf{x}_n \in \mathbb{R}^d$, PCA finds the directions of maximal covariance. Without loss of generality assume that $\sum_n \mathbf{x}_n = \mathbf{0}$.
  - The PCA directions $\mathbf{e}_1,\ldots,\mathbf{e}_d$ are the eigenvectors of the covariance matrix

$$C = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^T$$

    sorted by their eigenvalue.




  - We can express $\mathbf{x}_n$ in PCA space by $F(\mathbf{x}_n) = \sum_{k=1}^{K} \langle \mathbf{x}_n, \mathbf{e}_k \rangle \mathbf{e}_k$
  - Lower-dim. coordinate mapping:

$$\mathbf{x}_n \mapsto \begin{pmatrix} \langle \mathbf{x}_n, \mathbf{e}_1 \rangle \\ \langle \mathbf{x}_n, \mathbf{e}_2 \rangle \\ \ldots \\ \langle \mathbf{x}_n, \mathbf{e}_K \rangle \end{pmatrix} \in \mathbb{R}^K$$



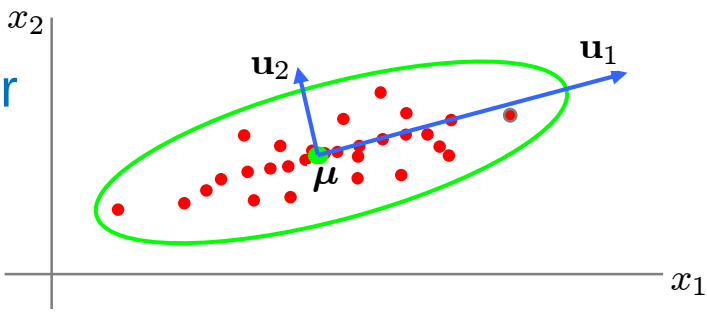
Slide credit: Christoph Lampert

# Kernel-PCA

- Kernel-PCA procedure
  - Given samples $\mathbf{x}_n \in \mathcal{X}$, kernel $\mathcal{X} \times \mathcal{X} \to \mathbb{R}$ with an implicit feature map $\phi$: $\mathcal{X} \to \mathcal{H}$. Perform PCA in the Hilbert space $\mathcal{H}$.
  - The kernel-PCA directions $\mathbf{e}_1,\ldots,\mathbf{e}_d$ are the eigenvectors of the covariance operator

$$C = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{\phi}(\mathbf{x}_n)\boldsymbol{\phi}(\mathbf{x}_n)^T$$

sorted by their eigenvalue.




  - Lower-dim. coordinate mapping:

$$\mathbf{x}_n \mapsto \begin{pmatrix} \langle \boldsymbol{\phi}(\mathbf{x}_n), \mathbf{e}_1 \rangle \\ \langle \boldsymbol{\phi}(\mathbf{x}_n), \mathbf{e}_2 \rangle \\ \ldots \\ \langle \boldsymbol{\phi}(\mathbf{x}_n), \mathbf{e}_K \rangle \end{pmatrix} \in \mathbb{R}^K$$

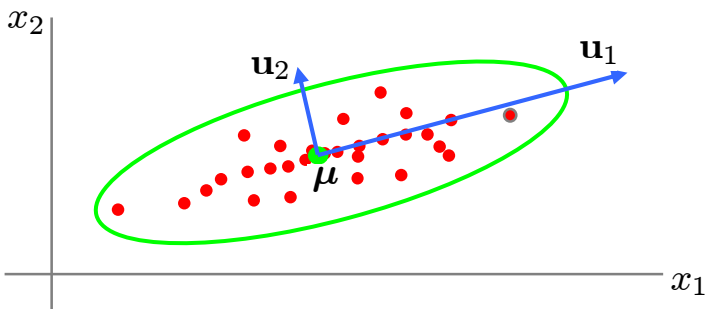


Slide credit: Christoph Lampert

# Kernel-PCA

- Kernel-PCA procedure
  - Given samples $\mathbf{x}_n \in \mathcal{X}$, kernel $\mathcal{X} \times \mathcal{X} \to \mathbb{R}$ with an implicit feature map $\phi$: $\mathcal{X} \to \mathcal{H}$. Perform PCA in the Hilbert space $\mathcal{H}$.
  - Equivalently, we can use the eigenvectors $\mathbf{e}'_k$ and eigenvalues $\lambda_k$ of the kernel matrix

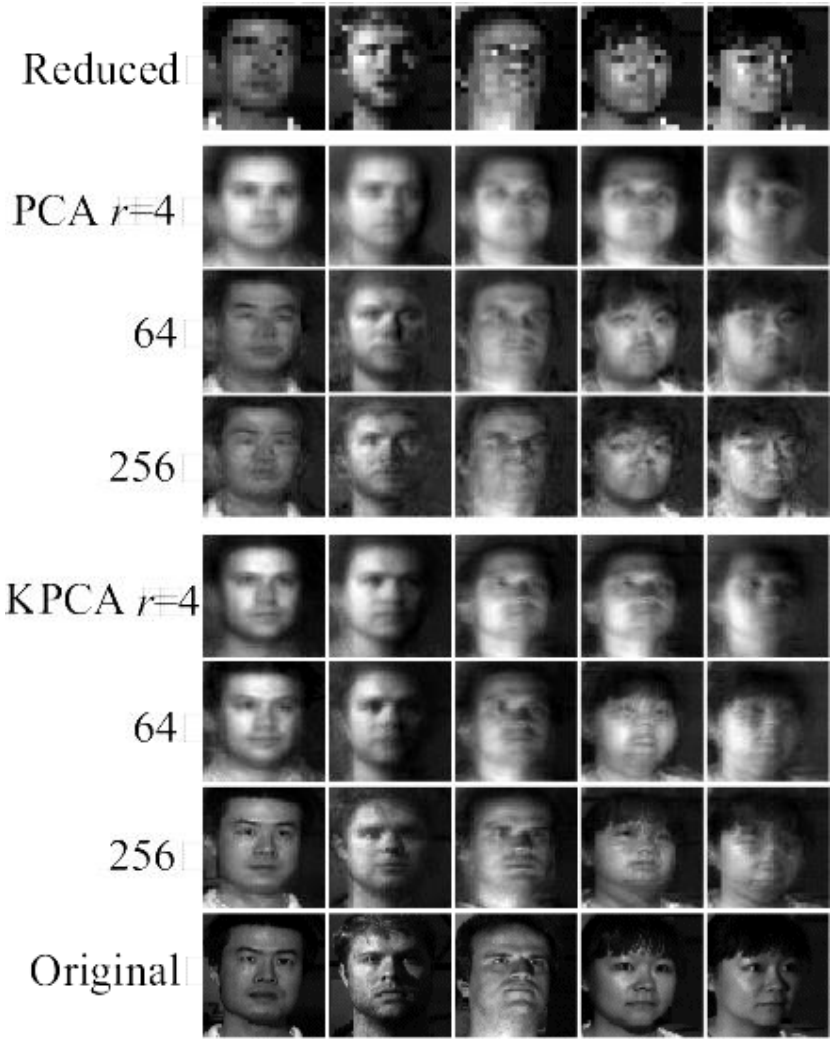
$$\begin{aligned} K &= \left(\langle \boldsymbol{\phi}(\mathbf{x}_m), \boldsymbol{\phi}(\mathbf{x}_n) \rangle\right)_{m,n=1,\ldots,N} \\ &= \left(k(\mathbf{x}_m, \mathbf{x}_n)\right)_{m,n=1,\ldots,N} \end{aligned}$$




  - Coordinate mapping: $\mathbf{x}_n \mapsto (\sqrt{\lambda_1}\mathbf{e}'_1, \ldots, \sqrt{\lambda_K}\mathbf{e}'_K)$

# Example: Image Superresolution

- Training procedure
  - Collect high-res face images
  - Use KPCA with RBF-kernel to learn non-linear subspaces
- For new low-res image:
  - Scale to target high resolution
  - Project to closest point in face subspace




Reconstruction in $r$ dimensions

Kim, Franz, Schölkopf, Iterative Kernel Principal Component Analysis for Image Modelling, IEEE Trans. PAMI, Vol. 27(9), 2005.

# Kernel k-Means Clustering

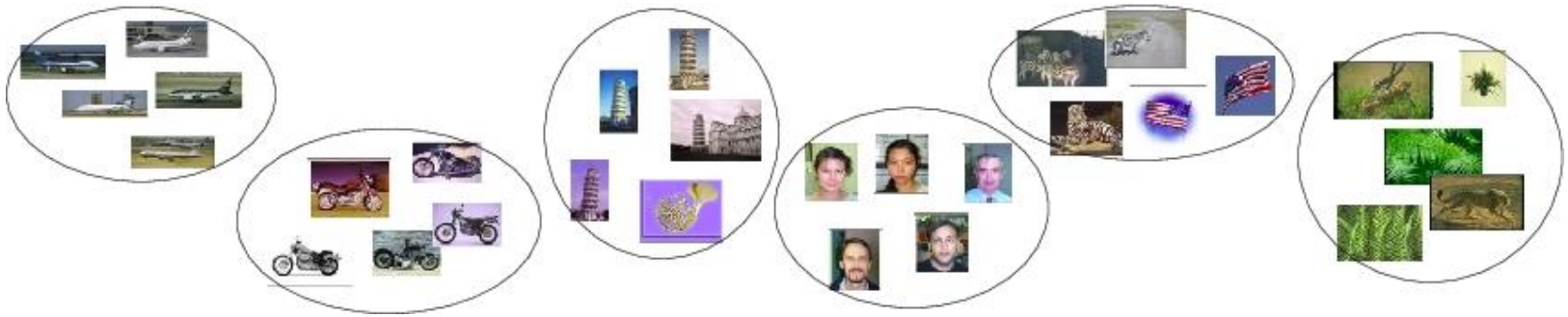
- Kernel PCA is more than just non-linear versions of PCA
  - PCA maps $\mathbb{R}^d$ to $\mathbb{R}^{d'}$, e.g. to remove noise dimensions.
  - Kernel-PCA maps $\mathcal{X} \rightarrow \mathbb{R}^{d'}$, so it provides a vectorial representation also of non-vectorial data!

  $\Rightarrow$ *We can use this to apply algorithms that only work in vector spaces to data that is not in a vector representation.*

- Example: k-Means clustering
  - Given $x_1, \ldots, x_n \in \mathcal{X}$.
  - Choose a kernel function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$.
  - Apply kernel-PCA to obtain vectorial $v_1, \ldots, v_n \in \mathbb{R}^{d'}$.
  - Cluster $v_1, \ldots, v_n \in \mathbb{R}^{d'}$ using *K*-Means.

  $\Rightarrow$ $x_1, \ldots, x_n$ are now clustered based on the similarity defined by *k*.

# Example: Unsupervised Object Categorization



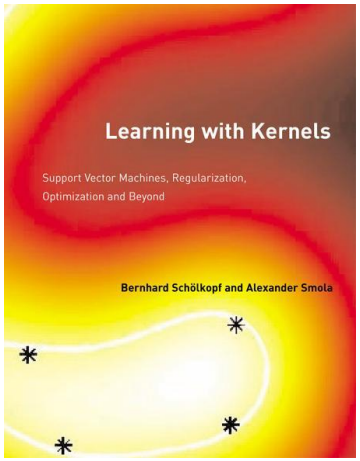
- Automatically group images that show similar objects
  - Represent images by bag-of-word histograms
  - Perform Kernel k-Means Clustering

  $\Rightarrow$ Observation: Clusters get better if we use a good image kernel (e.g., $\chi^2$) instead of plain k-Means (linear kernel).

T. Tuytelaars, C. Lampert, M. Blaschko, W. Buntine, Unsupervised object discovery: a comparison, IJCV, 2009.]

# References and Further Reading

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

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Pattern Recognition and Machine Learning
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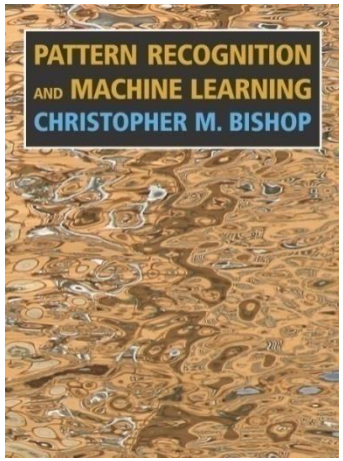
B. Schölkopf, A. Smola
Learning with Kernels
MIT Press, 2002
http://www.learning-with-kernels.org/




- More information on Kernel PCA can be found in Chapter 12.3 of Bishop's book. You can also look at Schölkopf & Smola (some chapters available online).