

These are the slides of the lecture

Pattern Recognition
Winter term 2020/21
Friedrich-Alexander University of Erlangen-Nuremberg.

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Erlangen, January 8, 2021
Prof. Dr.-Ing. Andreas Maier

Pattern Recognition (PR)

Prof. Dr.-Ing. Andreas Maier

Pattern Recognition Lab (CS 5), Friedrich-Alexander-Universität Erlangen-Nürnberg

Winter Term 2020/21



Kernels



Motivation

Linear decision boundaries in its current form have serious limitations:

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- non-linearly separable data cannot be classified
- noisy data cause problems
- formulation deals with vectorial data only

Possible solution:

- Map data into a higher dimensional feature space using a **non-linear feature transform**, then use a linear classifier.

Dual Representation

- The SVM decision boundary can be rewritten in dual form:

$$f(\mathbf{x}) = \boldsymbol{\alpha}^T \mathbf{x} + \alpha_0 = \sum_i \lambda_i y_i \mathbf{x}_i^T \mathbf{x} + \alpha_0$$

where we have used the identity:

$$\boldsymbol{\alpha} = \sum_i \lambda_i y_i \mathbf{x}_i .$$

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- The Lagrange dual problem is given by the **optimization problem**:

$$\begin{aligned} &\text{maximize} && -\frac{1}{2} \sum_i \sum_j \lambda_i \lambda_j y_i y_j \cdot \mathbf{x}_i^T \mathbf{x}_j + \sum_i \lambda_i \\ &\text{subject to} && \boldsymbol{\lambda} \succeq 0, \quad \sum_i \lambda_i y_i = 0 \end{aligned}$$

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Conclusion: feature vectors \mathbf{x}_i , \mathbf{x}_j , and \mathbf{x} only appear in **inner products**, both in the learning and the classification phase.

Inner Product and the Perceptron

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Feature Transforms

We select a feature transform $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^D$, $D \geq d$, such that the resulting features $\phi(\mathbf{x}_i)$, $i = 1, 2, \dots, m$, are linearly separable.

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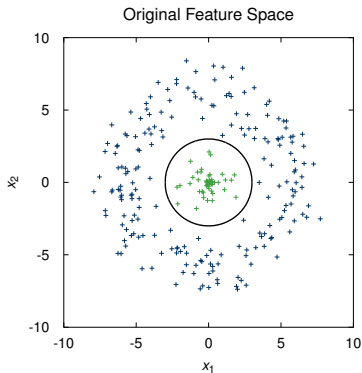


Fig.: Application of the feature transform $\phi(\mathbf{x}) = (x_1^2, x_2^2)^T$.

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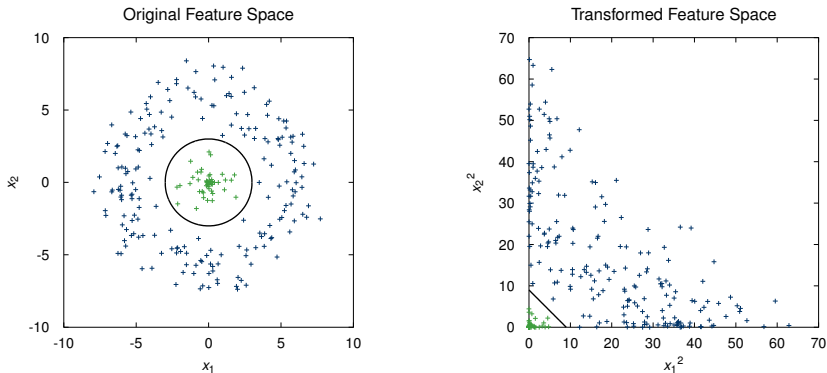


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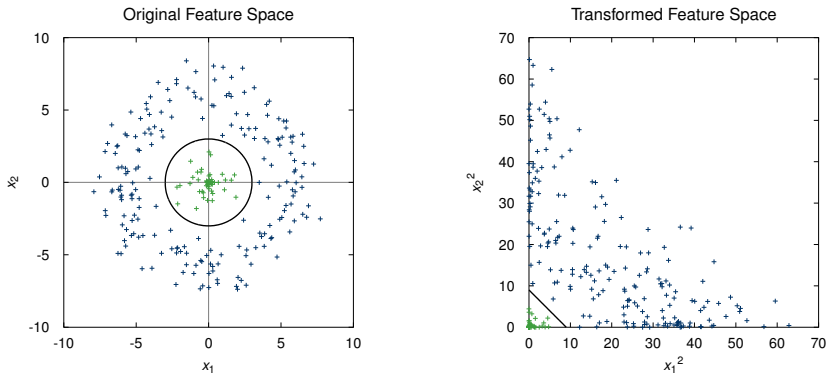


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Feature Transforms (cont.)

Second Example: data is not centered

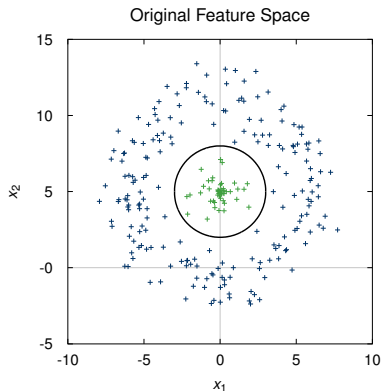


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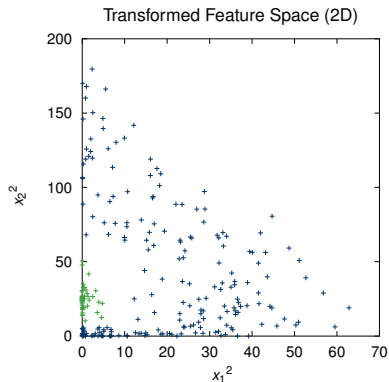
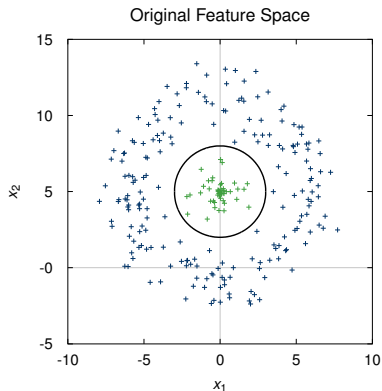


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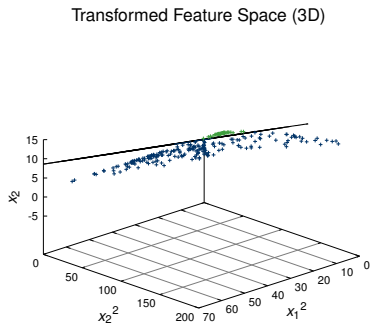
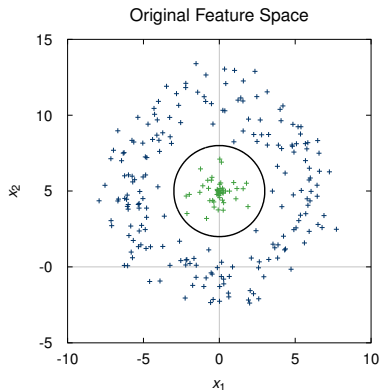


Fig.: Application of the feature transform $\phi(\mathbf{x}) = (x_1^2, x_2^2, x_2)^T$.

Feature Transforms (cont.)

Example

Assume the decision boundary is given by the quadratic function

$$f(\mathbf{x}) = a_0 + a_1 x_1^2 + a_2 x_2^2 + a_3 x_1 x_2 + a_4 x_1 + a_5 x_2.$$

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Obviously this is not a linear decision boundary.

By the following mapping, we get features that have a linear decision boundary:

$$\phi(\mathbf{x}) = \begin{pmatrix} x_1^2 \\ x_2^2 \\ x_1 \cdot x_2 \\ x_1 \\ x_2 \end{pmatrix}$$

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Conclusion: Distances can be computed by just evaluating inner products.

Feature Transforms (cont.)

These feature transforms can be easily incorporated into SVMs:

- Decision boundary:

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Kernel Functions

Definition

A *kernel function* $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a symmetric function that maps a pair of features to a real number. For a kernel function the following property holds:

$$k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$$

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Note:

Usually the evaluation of the kernel function is much easier than the computation of transformed features followed by the inner product.

Kernel Functions (cont.)

Definition

For a given set of feature vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m$, we define the *kernel matrix*

$$\mathbf{K} = [K_{i,j}]_{i,j=1,2,\dots,m}, \quad \text{where} \quad K_{i,j} = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle.$$

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The entries of the matrix are similarity measures for transformed feature pairs.

Kernel Functions (cont.)

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Kernel Functions (cont.)

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Question:

Can we compute for any kernel function $k(\mathbf{x}, \mathbf{x}')$ a feature mapping ϕ such that the kernel function can be written as an inner product?

Kernel Functions (cont.)

Theorem (Mercer's Theorem)

For any symmetric function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ that is square integrable on its domain and which satisfies

$$\int_{\mathcal{X} \times \mathcal{X}} f(\mathbf{x}) f(\mathbf{x}') k(\mathbf{x}, \mathbf{x}') d\mathbf{x} d\mathbf{x}' \geq 0$$

for all square integrable functions f , there exist transforms $\phi_i : \mathcal{X} \rightarrow \mathbb{R}$ and $\lambda_i \geq 0$ such that:

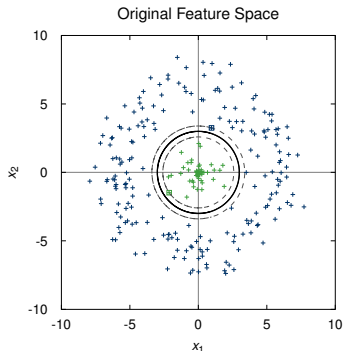
$$k(\mathbf{x}, \mathbf{x}') = \sum_i \lambda_i \phi_i(\mathbf{x}) \phi_i(\mathbf{x}')$$

for all \mathbf{x} and \mathbf{x}' .

Kernel Functions (cont.)

The Kernel Trick

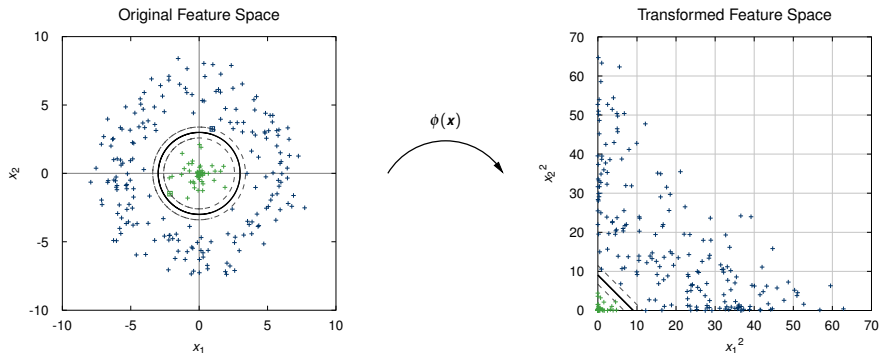
In *any* algorithm that is formulated in terms of a positive semidefinite kernel k , we can derive an alternative algorithm by replacing the kernel function k by another positive semidefinite kernel k' .



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Kernel SVMs with Soft Margins

Linear kernel $\langle \mathbf{x}, \mathbf{x}' \rangle$:

- the complexity parameter C controls the number of support vectors and
- hence the width of the margin and
- the orientation of the decision boundary

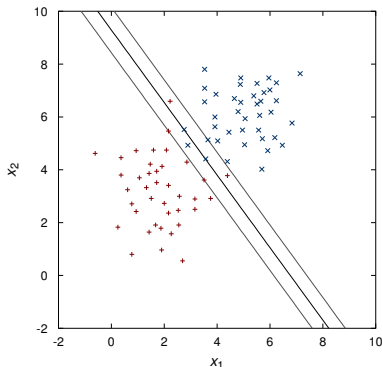


Fig.: $C = 10$: 8 support vectors, 3 misclassifications

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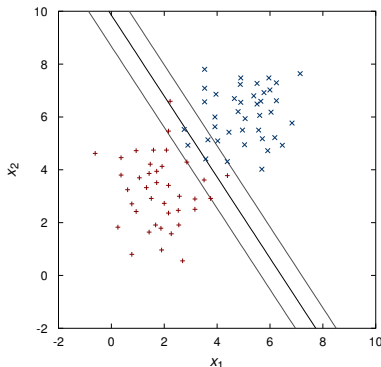


Fig.: $C = 1$: 11 support vectors, 4 misclassifications

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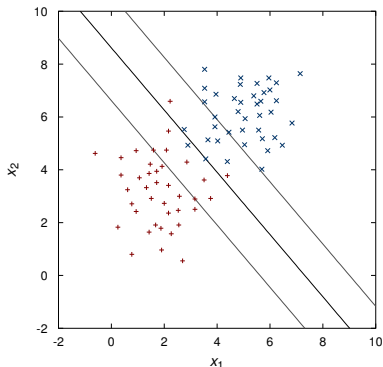


Fig.: $C = 0.1$: 17 support vectors, 3 misclassifications

Kernel SVMs with Soft Margins (cont.)

Polynomial kernel $\langle \mathbf{x}, \mathbf{x}' \rangle^2$:

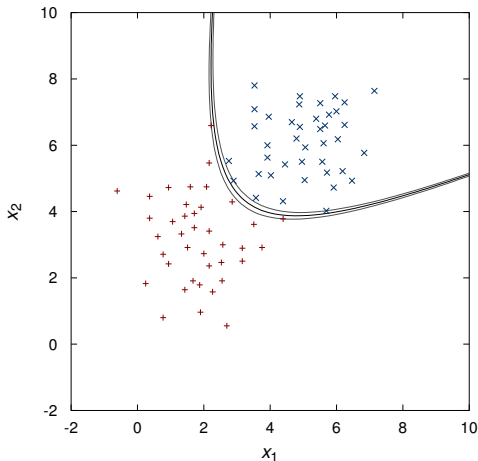


Fig.: $C = 10$: 4 support vectors, 0 misclassifications

Kernel SVMs with Soft Margins (cont.)

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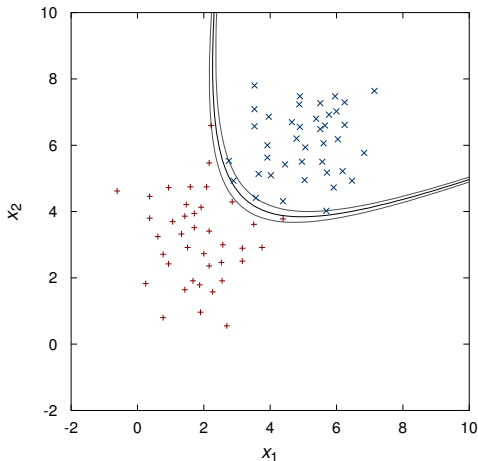


Fig.: $C = 1$: 5 support vectors, 0 misclassifications

Kernel SVMs with Soft Margins (cont.)

Gaussian RBF kernel $e^{-0.1 \cdot \langle \mathbf{x}, \mathbf{x}' \rangle^2}$:

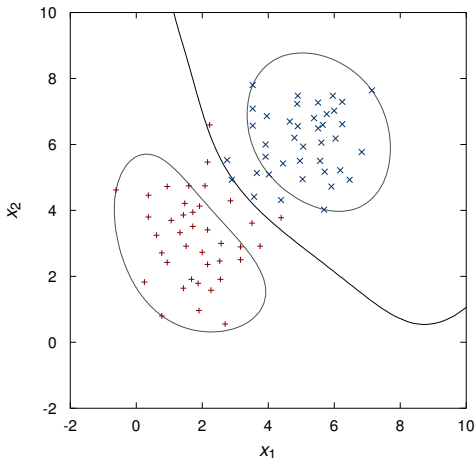


Fig.: $C = 10$: 18 support vectors, 3 misclassifications

Kernel SVMs with Soft Margins (cont.)

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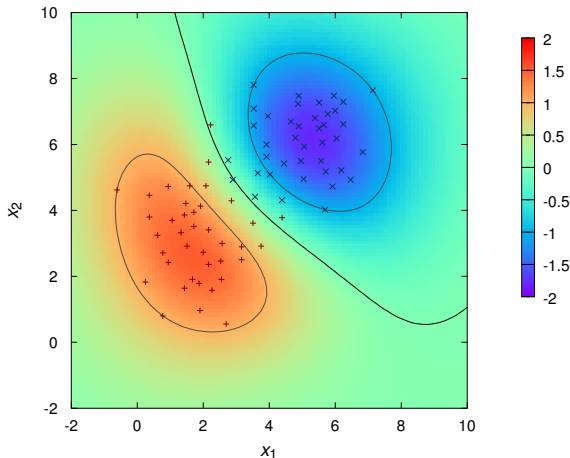


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**Pattern
Recognition
Lab**



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TECHNISCHE FAKULTÄT

Next Time in

Pattern Recognition



Kernel PCA

PCA revisited

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PCA revisited

- Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m \in \mathbb{R}^d$ be the feature vectors with zero mean.
- Compute the **scatter matrix** (covariance matrix):

$$\Sigma = \frac{1}{m} \sum_{i=1}^m \mathbf{x}_i \mathbf{x}_i^T \in \mathbb{R}^{d \times d}$$

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- **Sort** eigenvectors with decreasing eigenvalues.

Kernel PCA

PCA revisited

- Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m \in \mathbb{R}^d$ be the feature vectors with zero mean.
- Compute the **scatter matrix** (covariance matrix):

$$\Sigma = \frac{1}{m} \sum_{i=1}^m \mathbf{x}_i \mathbf{x}_i^T \in \mathbb{R}^{d \times d}$$

- Compute the **eigenvectors** and **eigenvalues**:

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- **Sort** eigenvectors with decreasing eigenvalues.
- Subsequent **projection** of features to the eigenvectors.

Kernel PCA (cont.)

Facts from linear algebra:

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- The eigenvectors \mathbf{e}_i span the same space as the feature vectors.

Kernel PCA (cont.)

Facts from linear algebra:

- The eigenvectors \mathbf{e}_i span the same space as the feature vectors.
- Each eigenvector \mathbf{e}_i can be written as a linear combination of feature vectors:

$$\mathbf{e}_i = \sum_k \alpha_{i,k} \mathbf{x}_k$$

Kernel PCA (cont.)

The eigenvector/-value problem for the PCA computation can now be rewritten:

$$\Sigma \mathbf{e}_i = \lambda_i \mathbf{e}_i$$

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$$\sum_{j,k} \alpha_{i,k} \mathbf{x}_j \mathbf{x}_j^T \mathbf{x}_k = m \cdot \lambda_i \sum_k \alpha_{i,k} \mathbf{x}_k$$

Kernel PCA (cont.)

- The following equations have to be fulfilled for all projections on \mathbf{x}_l for all indices l :

$$\sum_{j,k} \alpha_{i,k} \mathbf{x}_l^T \mathbf{x}_j \mathbf{x}_j^T \mathbf{x}_k = m \cdot \lambda_i \sum_k \alpha_{i,k} \mathbf{x}_l^T \mathbf{x}_k$$

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- Wow – now all feature vectors show up in terms of inner products and the kernel trick can be applied, if *transformed* features $\phi(\mathbf{x})$ have zero mean.

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- Wow** – now all feature vectors show up in terms of inner products and the kernel trick can be applied, if *transformed* features $\phi(\mathbf{x})$ have zero mean.
- For *any* kernel $k(\mathbf{x}, \mathbf{x}')$, we get the key equation for Kernel PCA:

$$\sum_{j,k} \alpha_{i,k} \cdot k(\mathbf{x}_l, \mathbf{x}_j) \cdot k(\mathbf{x}_j, \mathbf{x}_k) = m \cdot \lambda_i \cdot \sum_k \alpha_{i,k} \cdot k(\mathbf{x}_l, \mathbf{x}_k)$$

Kernel PCA (cont.)

This can be written in **matrix notation** using the symmetric, positive semi-definite kernel matrix $\mathbf{K} \in \mathbb{R}^{m \times m}$ and the vector $\alpha_i = (\alpha_{i,1}, \alpha_{i,2}, \dots, \alpha_{i,m})^T$:

$$\begin{aligned} \mathbf{K}^2 \alpha_i &= m \cdot \lambda_i \mathbf{K} \alpha_i \\ \mathbf{K}(\mathbf{K} \alpha_i) &= m \cdot \lambda_i (\mathbf{K} \alpha_i) \end{aligned}$$

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This is equivalent to

$$\mathbf{K}(\mathbf{K} \alpha_i - m \cdot \lambda_i \alpha_i) = 0$$

- $\mathbf{K} \alpha_i$ is an eigenvector of \mathbf{K}
- α_i is an eigenvector of \mathbf{K}

Kernel PCA (cont.)

The coefficient vector α_i for the principal components can be computed by solving the eigenvalue/-vector problem for i :

$$K\alpha_i = m\lambda_i \alpha_i$$

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Note:

- Kernel PCA (and thus the classical PCA as well) can be computed by solving an eigenvector/-value problem for an $(m \times m)$ -matrix, where m is the cardinality of the training feature set.

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$$c = \phi(\mathbf{x})^T \mathbf{e}_i = \sum_k \alpha_{i,k} \phi(\mathbf{x})^T \phi(\mathbf{x}_k) = \sum_k \alpha_{i,k} k(\mathbf{x}, \mathbf{x}_k)$$

Kernel PCA (cont.)

It is assumed that the transformed features have **zero mean**:

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Kernel PCA (cont.)

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This can be enforced by the **normalization step**:

$$\tilde{\phi}(\mathbf{x}_i) = \phi(\mathbf{x}_i) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k)$$

Kernel PCA

Implication for the components of the centered kernel matrix $\tilde{\mathbf{K}}$:

$$\tilde{K}_{i,j} = \tilde{\phi}(\mathbf{x}_i)^T \tilde{\phi}(\mathbf{x}_j)$$

Kernel PCA

Implication for the components of the **centered kernel matrix** $\tilde{\mathbf{K}}$:

$$\begin{aligned}\tilde{K}_{i,j} &= \tilde{\phi}(\mathbf{x}_i)^T \tilde{\phi}(\mathbf{x}_j) \\ &= \left(\phi(\mathbf{x}_i) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k) \right)^T \left(\phi(\mathbf{x}_j) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k) \right)\end{aligned}$$

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Implication for the components of the **centered kernel matrix** $\tilde{\mathbf{K}}$:

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 \tilde{K}_{i,j} &= \tilde{\phi}(\mathbf{x}_i)^T \tilde{\phi}(\mathbf{x}_j) \\
 &= \left(\phi(\mathbf{x}_i) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k) \right)^T \left(\phi(\mathbf{x}_j) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k) \right) \\
 &= \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_k) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k)^T \phi(\mathbf{x}_j) + \\
 &\quad + \frac{1}{m^2} \sum_{k,l=1}^m \phi(\mathbf{x}_k)^T \phi(\mathbf{x}_l)
 \end{aligned}$$

Kernel PCA

Implication for the components of the **centered kernel matrix** \tilde{K} :

$$\begin{aligned}
 \tilde{K}_{i,j} &= \tilde{\phi}(\mathbf{x}_i)^T \tilde{\phi}(\mathbf{x}_j) \\
 &= \left(\phi(\mathbf{x}_i) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k) \right)^T \left(\phi(\mathbf{x}_j) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k) \right) \\
 &= \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_k) - \frac{1}{m} \sum_{k=1}^m \phi(\mathbf{x}_k)^T \phi(\mathbf{x}_j) + \\
 &\quad + \frac{1}{m^2} \sum_{k,l=1}^m \phi(\mathbf{x}_k)^T \phi(\mathbf{x}_l) \\
 &= K_{i,j} - \frac{1}{m} \sum_{k=1}^m K_{i,k} - \frac{1}{m} \sum_{k=1}^m K_{k,j} + \frac{1}{m^2} \sum_{k,l=1}^m K_{k,l}
 \end{aligned}$$

Kernel PCA (cont.)

Example: classical vs. kernel PCA

Consider $m = 50$ images with 1024^2 pixels. The pixels define 1024^2 -dimensional feature vectors:

$$\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{50} \in \mathbb{R}^{2^{20}}$$

Kernel PCA (cont.)

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The kernel PCA using the linear kernel

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

requires the eigenvalue/-vector decomposition of the (50×50) kernel matrix.

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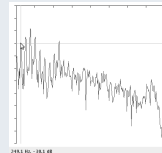
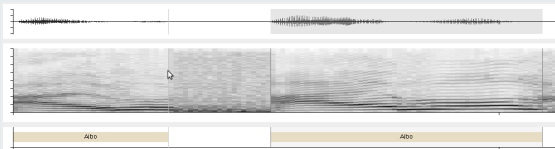
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The classical PCA requires the eigenvalue/-vector decomposition of a $(2^{20} \times 2^{20})$ matrix.

Kernels for Feature Sequences

Example: string kernels

- In speech recognition we do not have feature vectors but sequences of feature vectors.
- In order to use kernel methods we need a kernel for time series.



Kernels for Feature Sequences (cont.)

Example: string kernels (cont.)

- Feature vectors are considered in $\mathbb{R}^d = \mathcal{X}$.
- Sequences of feature vectors are elements of \mathcal{X}^* .
- **Problem:** How to define a kernel over the sequence space \mathcal{X}^* ?

Implications:

- PCA on feature sequences – COOL!
- SVM for feature sequences – EVEN COOLER!

Kernels for Feature Sequences (cont.)

Example: string kernels (cont.)

Comparison of sequences via *dynamic time warping* (DTW):

Given the feature sequences $(p, q \in \{1, 2, \dots\})$:

$$\langle \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_p \rangle \in \mathcal{X}^*$$

$$\langle \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_q \rangle \in \mathcal{X}^*$$

Kernels for Feature Sequences (cont.)

Example: string kernels (cont.)

- Distance is computed by DTW:

$$D(\langle \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_p \rangle, \langle \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_q \rangle) = \frac{1}{p} \sum_{k=1}^p \|\mathbf{x}_{v(k)} - \mathbf{y}_{w(k)}\|_2$$

where v, w define the mapping of indices to indices.

Kernels for Feature Sequences (cont.)

Example: string kernels (cont.)

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where v, w define the mapping of indices to indices.

- The DTW kernel can be defined as:

$$k(\mathbf{x}, \mathbf{y}) = e^{-D(\langle \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_p \rangle, \langle \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_q \rangle)}$$

Fisher Kernels

Now we design kernels building on probability density functions $p(\mathbf{x}; \theta)$.

- Fisher score:

$$\mathbf{J}_{\theta}(\mathbf{x}) = -\frac{\partial}{\partial \theta} \log p(\mathbf{x}; \theta)$$

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$$I(\mathbf{x}) = E_{\mathbf{x}}[\mathbf{J}_{\theta}(\mathbf{x})\mathbf{J}_{\theta}^T(\mathbf{x})]$$

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Note:

The Fisher information matrix is the curvature of the Kullback-Leibler divergence.

Fisher Kernels (cont.)

The Fisher kernel can be defined in **two different ways**:

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{J}_{\theta}^T(\mathbf{x}) \mathbf{J}_{\theta}(\mathbf{x}')$$

or

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{J}_{\theta}^T(\mathbf{x}) \mathbf{I}^{-1}(\mathbf{x}) \mathbf{J}_{\theta}(\mathbf{x}')$$

Fisher Kernels (cont.)

Application: learning from partially labeled data

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- If the data can be modeled with a small number of well separated components (with each component corresponding to a distinct category), little labeled data would suffice to assign a proper label to each of them.

Fisher Kernels (cont.)

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- If the data can be modeled with a small number of well separated components (with each component corresponding to a distinct category), little labeled data would suffice to assign a proper label to each of them.
- A machine learning approach that makes use of only partially labeled data usually achieves much better classification performance than using only the labeled data alone.
- Fisher kernels describe a generative model that can be used in a discriminative approach (e. g. SVM).

Lessons Learned

- Limitations of linear decision boundaries
- Non-linear feature transforms
- Kernel function and kernel matrix
- Kernel trick
- Probabilities and kernels



**Pattern
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Lab**



**FRIEDRICH-ALEXANDER
UNIVERSITÄT
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TECHNISCHE FAKULTÄT

Next Time in

Pattern Recognition



Further Readings

- Bernhard Schölkopf, Alexander J. Smola:
[Learning with Kernels](#),
The MIT Press, Cambridge, 2003.
- Vladimir N. Vapnik:
[The Nature of Statistical Learning Theory](#),
Information Science and Statistics, Springer, Heidelberg, 2000.
- John Shawe-Taylor, Nello Cristianini:
 [Kernel Methods for Pattern Analysis](#),
Cambridge University Press, Cambridge, 2004

Comprehensive Questions

- What are the properties of kernel functions?
- What is the kernel matrix?
- What is the kernel trick?
- How can we use kernels for string comparison?