Machine Intelligence II

Kernel PCA

Tutorial

Neural Information Processing Group (Prof. Dr. Klaus Obermayer)

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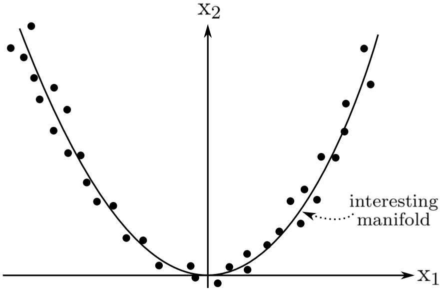
Projection Methods

- Principal Component Analysis (PCA)
- Online-PCA $\Rightarrow$ Hebbian Learning
- Nonlinear Structure $\Rightarrow$ Kernel PCA
- Source Separation
  - Model based $\Rightarrow$ Independent Component Analysis (ICA)
  - Cost Function Based $\Rightarrow$ Projection Pursuit

Kernel Principal Component Analysis

Goal: finding nonlinear regularities

Kernel Principal Component Analysis: Motivation



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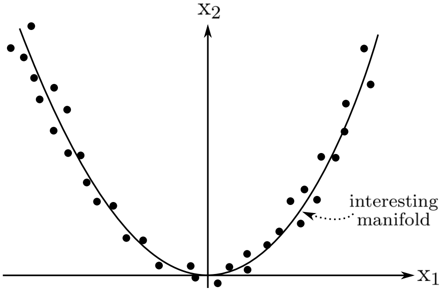

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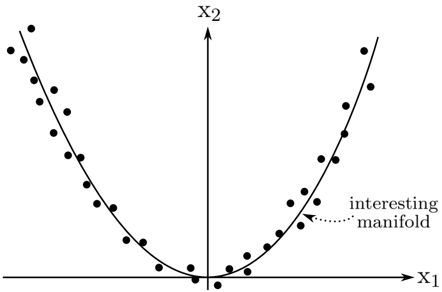

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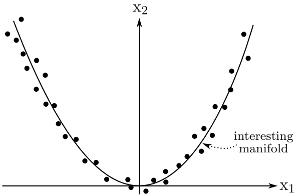
$\Rightarrow$ problem for standard PCA

Kernel Principal Component Analysis: Intuition



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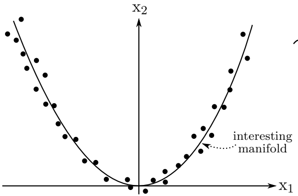

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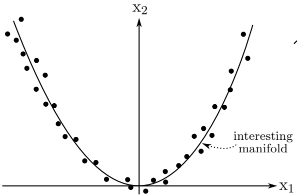

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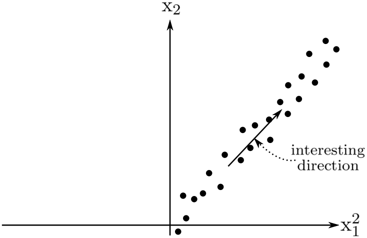

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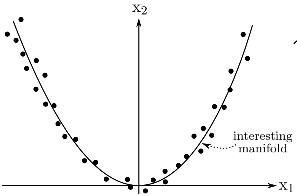

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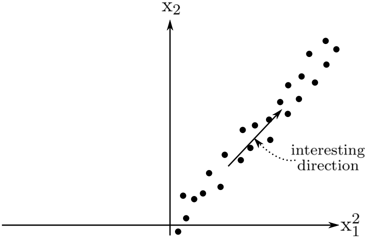

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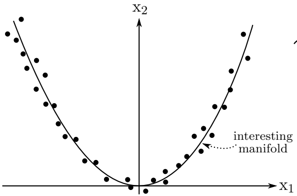

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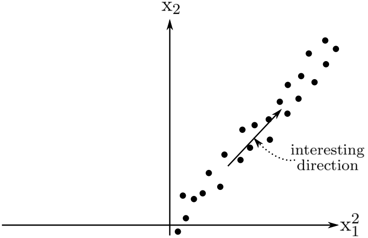

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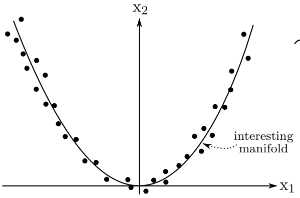

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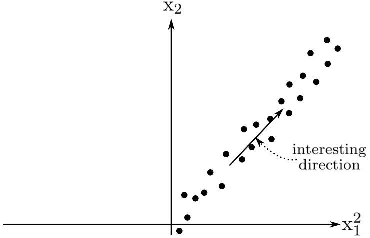

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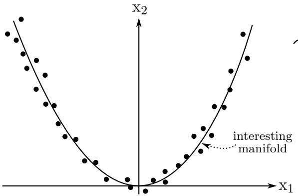

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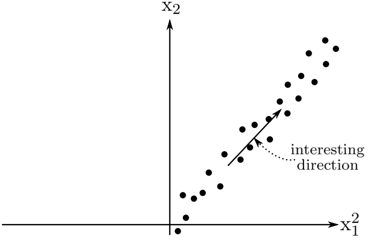

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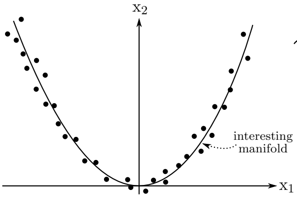

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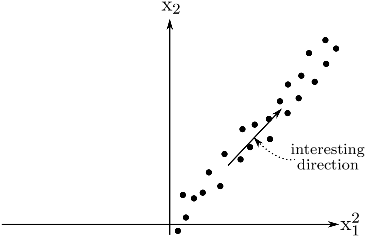

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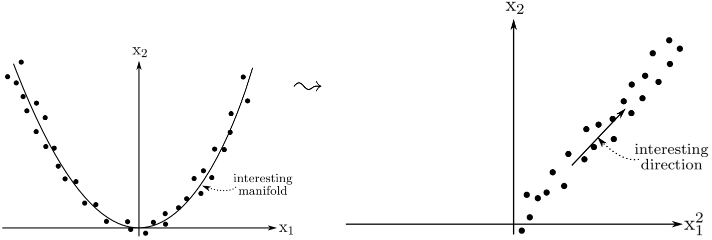

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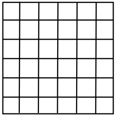
2. apply standard linear methods

Why we need the Kernel Trick

Problem: Some feature spaces may be extremely high-dimensional



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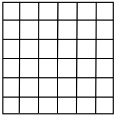

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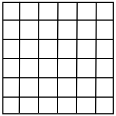

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- suitable feature space: space spanned by all d^{th}-order monomials

$$\text{e.g. } d = 2 : \mathrm{x}_1^2, \mathrm{x}_1\mathrm{x}_2, \mathrm{x}_2^2, \mathrm{x}_1\mathrm{x}_3, \mathrm{x}_2\mathrm{x}_3, \mathrm{x}_3^2, \ldots$$

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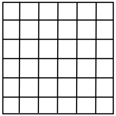

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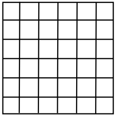

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$\rightsquigarrow$ **kernel trick** allows to avoid this problem

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note: Eigenvectors $\underline{\mathbf{e}}_k \in \mathbb{R}^N$ but coefficients $\underline{\mathbf{a}}_k \in \mathbb{R}^p$

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if an algorithm can be formulated solely in terms of scalar products, a non-linear version can be derived "without actually projecting" into the (highdimensional) feature space

Kernels and Applications

Popular Kernel Functions

$$k_{(\underline{\mathbf{x}},\underline{\mathbf{x}}')} = \left(\underline{\mathbf{x}}^T \underline{\mathbf{x}}' + 1\right)^d$$

polynomial kernel of degree d
image processing (pixel correlation)

$$k_{(\underline{\mathbf{x}},\underline{\mathbf{x}}')} = \exp\left\{ -\frac{\left(\underline{\mathbf{x}}-\underline{\mathbf{x}}'\right)^2}{2\sigma^2} \right\}$$

RBF-kernel with range σ
infinite dimensional feature space

$$k_{(\underline{\mathbf{x}},\underline{\mathbf{x}}')} = \tanh\left\{ K\underline{\mathbf{x}}^T \underline{\mathbf{x}}' + \theta \right\}$$

neural network kernel with parameters K and θ
not necessarily positive definite

Other Kernelizable Methods

- Support Vector Machines (MI I)
- Fisher Discriminant Analysis, Canonical Correlation Analysis
- K-Means Clustering, Self-Organizing Maps (both MI II)

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5. calculate projections of data points $\underline{\mathbf{x}}^{(\alpha)}$ onto eigenvectors $\underline{\mathbf{e}}_k$

$$u_k\left(\underline{\mathbf{x}}^{(\alpha)}\right) = \sum_{\beta=1}^{p} a_k^{(\beta)} K_{\beta\alpha} \quad \leftarrow$$ use centered kernel matrix and normalized eigenvector!

Projections of new points onto PCs in feature space

For data points $\underline{\mathbf{x}}^{(\alpha)}$ we have onto the k-th PC:

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More generally, for arbitrary $\underline{\mathbf{x}}$ the projection is computed as:

$$\begin{aligned} u_k\left(\underline{\mathbf{x}}\right) &= \sum_{\beta=1}^{p} a_k^{(\beta)} \underline{\phi}^T_{\left(\underline{\mathbf{x}}^{(\beta)}\right)} \underline{\phi}_{(\underline{\mathbf{x}})} \qquad \leftarrow \text{centered feature vectors} \\ &= \sum_{\beta=1}^{p} a_k^{(\beta)} \left(k(\underline{\mathbf{x}}^{(\beta)}, \underline{\mathbf{x}}) - \frac{1}{p}\sum_{\delta=1}^{p} \widetilde{K}_{\beta\delta} - \frac{1}{p}\sum_{\gamma=1}^{p} k(\underline{\mathbf{x}}^{(\gamma)}, \underline{\mathbf{x}}) + \frac{1}{p^2}\sum_{\gamma,\delta=1}^{p} \widetilde{K}_{\gamma\delta} \right) \end{aligned}$$

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  - $\rightsquigarrow$ "minimal" mean-squared approximation of data (in feature space)
- #PCs can exceed #dimensions in the original space
- kernel matrices may be very large
  - $\rightsquigarrow$ only first few eigenvectors (largest eigenvalues) are of interest
  - $\rightsquigarrow$ use specialized (iterative) routines (e.g. ARPACK via `eigs`)