Pattern Recognition Lecture
Feature Generation: Data Transformation and Dimensionality Reduction

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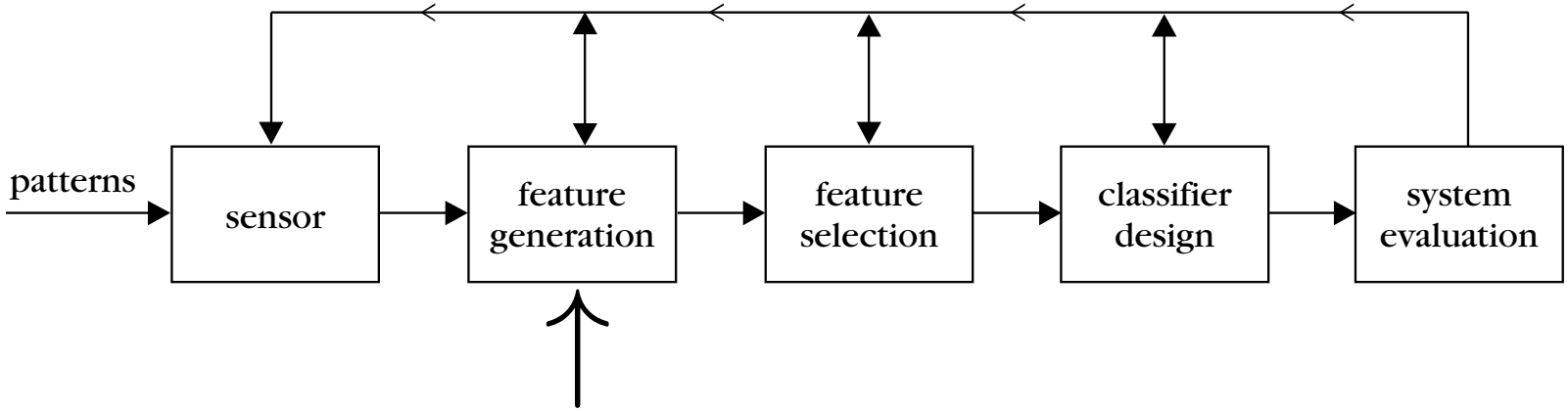
Pattern Recognition Chain

Introduction
KLT
SVD



Overview

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1 Introduction

2 The Karhunen-Loeve Transform

3 The Singular Value Decomposition

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3 The Singular Value Decomposition

Introduction (1)

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- Given a set of measurements, the goal is to discover compact and informative representations of the obtained data - features.
- The representations are generated after processing a large amount of sensory data.
- Measurements are transformed to a new set of features.
- In good features, the classification-related information is "squeezed" in a relatively small number of features.

Introduction (2)

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- Appropriately chosen feature transform can exploit and remove information redundancies.
- E. g., using image pixels as features would be highly inefficient as pixels have a large degree of correlation.
- However, the Fourier transform turns out to be much more efficient for feature extraction. Why?
- Fourier transform is just one of the tools from a palette of possible transforms.

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Introduction

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- The Karhunen-Loeve transform known also as Principal Component Analysis (PCA) is one of the most popular methods for feature generation and dimensionality reduction in pattern recognition.
- The computation of the transformation matrix exploits the statistical information describing the data.
- The labels of the training samples are not used (unsupervised mode).

The Karhunen-Loeve Transform (1)

- Let $\mathbf{x}$ be vectors representing samples. In order to simplify the presentation, the data samples are assumed to have zero mean. If this is not the case, we can always subtract the mean value.

- Let $\mathbf{y} = \mathbf{A}^{\mathsf{T}}\mathbf{x}$

- From the definition of the correlation matrix we have

$$\mathbf{R}_y \equiv E[\mathbf{y}\mathbf{y}^{\mathsf{T}}] = E[\mathbf{A}^{\mathsf{T}}\mathbf{x}\mathbf{x}^{\mathsf{T}}\mathbf{A}] = \mathbf{A}^{\mathsf{T}}\mathbf{R}_x\mathbf{A}$$

The Karhunen-Loeve Transform (2)

- In practice, $\mathbf{R}_x$ is estimated as an average over the given set of training vectors

$$\mathbf{R}_x = \frac{1}{n} \sum_{k=1}^{n} \mathbf{x}_k \mathbf{x}_k{}^{\mathsf{T}}$$

- Note that $\mathbf{R}_x$ is a symmetric matrix and hence its eigenvectors are mutually orthogonal.

The Karhunen-Loeve Transform (3)

- Thus, if matrix $\mathbf{A}$ is chosen so that its columns are the orthonormal eigenvectors $\mathbf{a}_{i=0,\ldots,N-1}$, then

$$\mathbf{R}_y = \mathbf{A}^{\mathsf{T}} \mathbf{R}_x \mathbf{A} = \boldsymbol{\Lambda}$$

  where $\boldsymbol{\Lambda}$ is a diagonal matrix having as elements the respective eigenvalues $\lambda_{i=0,\ldots,N-1}$ of $\mathbf{R}_x$.

- The resulting transform is known as the Karhunen-Loeve (KL) transform.

- The KL transform generates mutually uncorrelated features.

Example (1)

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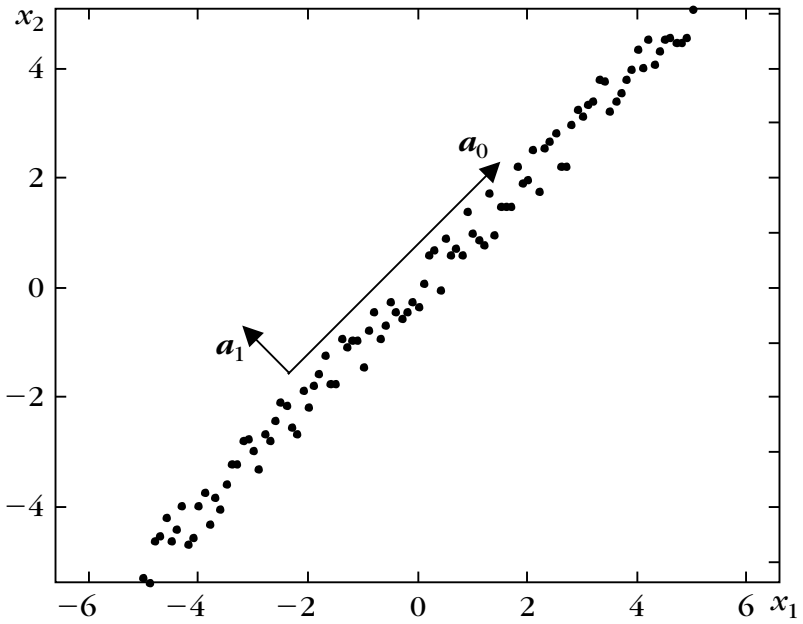
- In the figure below, we see 100 points in the two-dimensional space spread around the $x_1 = x_2$ line generated by the model $x_2 = x_1 + \epsilon$, where ϵ is a noise source following the uniform distribution in $[-0.5, 0.5]$.



Example (2)

- We first compute the covariance matrix and perform an eigen decomposition. The resulting eigenvectors are

$$\mathbf{a}_0 = [0.7045, 07097]^{\mathsf{T}} \quad \text{and} \quad \mathbf{a}_1 = [-0.7097, 0.7045]^{\mathsf{T}}$$

- The corresponding eigenvalues are

$$\lambda_0 = 17.26 \quad \text{and} \quad \lambda_1 = 0.04 \quad \text{thus} \quad \lambda_0 \gg \lambda_1$$

- Projecting along the direction of maximum variability ($\mathbf{a}_0$) retains most of the variance.

- The number of dimensions of the feature space can be reduced to 1.

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SVD Statement (1)

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- Given a $I \times n$ matrix $\mathbf{X}$ of rank r ($r \leq \min\{I, n\}$) there exist unitary matrices $\mathbf{U}$ and $\mathbf{V}$ of dimensions $I \times I$ and $n \times n$, respectively, so that

$$\mathbf{X} = \mathbf{U} \begin{bmatrix} \boldsymbol{\Lambda}^{\frac{1}{2}} & O \\ O & 0 \end{bmatrix} \mathbf{V}^H \Rightarrow \mathbf{Y} \equiv \begin{bmatrix} \boldsymbol{\Lambda}^{\frac{1}{2}} & O \\ O & 0 \end{bmatrix} = \mathbf{U}^H \mathbf{X} \mathbf{V}$$

- $\boldsymbol{\Lambda}^{\frac{1}{2}}$ is the $r \times r$ diagonal matrix with elements $\sqrt{\lambda_i}$ and λ_i are the r nonzero eigenvalues of the associated matrix $\mathbf{X}^H \mathbf{X}$. O denotes a zero element matrix.

- In other words, there exist unitary matrices $\mathbf{U}$ and $\mathbf{V}$ that transform $\mathbf{X}$ into the special diagonal structure of $\mathbf{Y}$.

SVD Statement (2)

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- If $\mathbf{u}_i$ and $\mathbf{v}_i$ denote the column vectors of matrices $\mathbf{U}$ and $\mathbf{V}$, respectively, then the SVD can be written as

$$\mathbf{X} = [\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_{r-1}] \begin{bmatrix} \sqrt{\lambda_0} & 0 & \ldots & 0 \\ 0 & \sqrt{\lambda_1} & \ldots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \ldots & \sqrt{\lambda_{r-1}} \end{bmatrix} \begin{bmatrix} \mathbf{v}_0^H \\ \mathbf{v}_1^H \\ \vdots \\ \mathbf{v}_{r-1}^H \end{bmatrix}$$

$$\Downarrow$$

$$\mathbf{X} = \sum_{i=0}^{r-1} \sqrt{\lambda_i} \mathbf{u}_i \mathbf{v}_i^H$$

SVD Statement (3)

- Sometimes, the above is also written as

$$\mathbf{X} \equiv \mathbf{U}_r \boldsymbol{\Lambda}^{\frac{1}{2}} \mathbf{V}_r^H$$

- $\mathbf{U}_r$ denotes the $l \times r$ matrix that consists of the first r columns of $\mathbf{U}$ and $\mathbf{V}_r$ the $r \times n$ matrix formed by using the first r columns of $\mathbf{V}$.

- More precisely, $\mathbf{u}_i$ and $\mathbf{v}_i$ are the eigenvectors corresponding to the nonzero eigenvalues of the matrices $\mathbf{X}\mathbf{X}^H$ and $\mathbf{X}^H\mathbf{X}$, respectively.

- The eigenvalues λ_i are known as singular values of $\mathbf{X}$ and the expansion as the singular value decomposition of $\mathbf{X}$ or the spectral representation of $\mathbf{X}$.

Low Rank Approximation via SVD (1)

- The SVD proposes an exact representation of matrix $\mathbf{X}$

$$\mathbf{X} = \sum_{i=0}^{r-1} \sqrt{\lambda_i} \mathbf{u}_i \mathbf{v}_i^H$$

- A very interesting implication occurs, if one uses less than r (the rank of $\mathbf{X}$) terms in the summation.

- Let $\mathbf{X}$ be approximated by

$$\mathbf{X} \approx \widehat{\mathbf{X}} = \sum_{i=0}^{k-1} \sqrt{\lambda_i} \mathbf{u}_i \mathbf{v}_i^H, \qquad k \leq r$$

- Matrix $\widehat{\mathbf{X}}$ being a sum of $k \leq r$ rank-one independent $l \times n$ matrices is of rank k.

Low Rank Approximation via SVD (2)

- If the k largest eigenvalues are involved, it can be shown that the squared error

$$\epsilon^2 = \sum_{i=0}^{l-1} \sum_{j=0}^{n-1} |X(i,j) - \widehat{X}(i,j)|^2$$

  is the minimum one with respect to all $l \times n$ matrices of rank k.

- The square root of the right-hand side is also known as the Frobenius norm $\|\mathbf{X} - \widehat{\mathbf{X}}\|_{\mathrm{F}}$ of the difference $\mathbf{X} - \widehat{\mathbf{X}}$.

Low Rank Approximation via SVD (3)

- The error in the approximation turns out to be

$$\epsilon^2 = \sum_{i=k}^{r-1} \lambda_i$$

- Hence, if we order the eigenvalues in descending order $\lambda_0 \geq \lambda_1 \geq \ldots \geq \lambda_{r-1}$, then for a given number of k terms in the expansion, the SVD leads to the minimum square error.

- Thus, $\widehat{\mathbf{X}}$ is the best rank-k approximation of $\mathbf{X}$ with respect to the Frobenius norm.

KL Transform vs. SVD

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- The statement of the previous slide reminds us of the Karhunen-Loeve expansion.
- However, while KL is optimal with respect to the mean square error, SVD is optimal in accordance with the Frobenius norm.

Dimensionality Reduction via SVD (1)

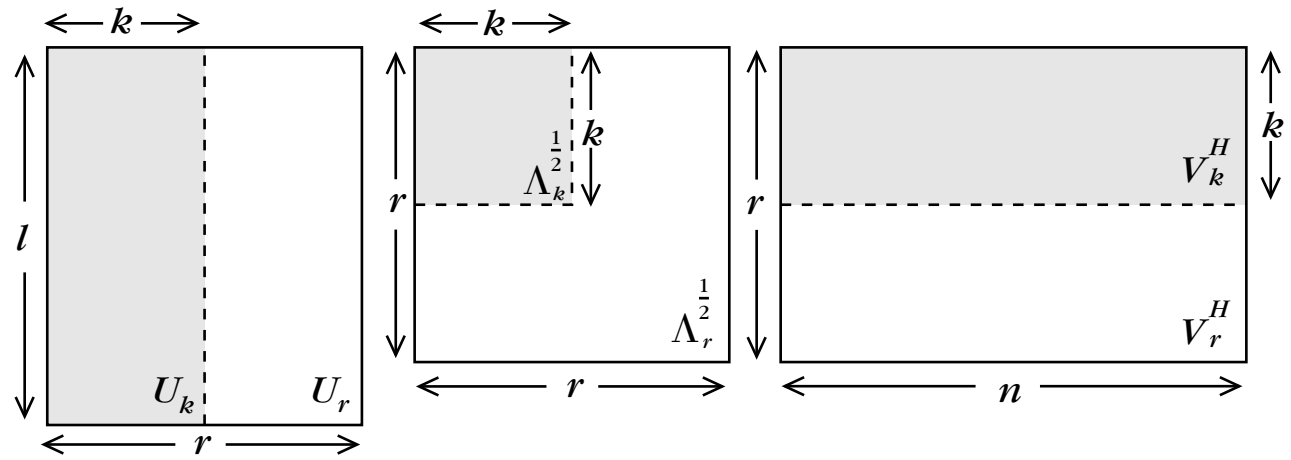
- SVD is used for dimensionality reduction in pattern recognition and information retrieval.
- Using the equations before, we can see that

$$\mathbf{X} \approx \widehat{\mathbf{X}} = [\mathbf{u}_0, \ldots, \mathbf{u}_{k-1}] \begin{bmatrix} \mathbf{v}_0^H \sqrt{\lambda_o} \\ \vdots \\ \mathbf{v}_{k-1}^H \sqrt{\lambda_{k-1}} \end{bmatrix} = \mathbf{U}_k [\mathbf{a}_0, \ldots, \mathbf{a}_{n-1}]$$

where $\mathbf{U}_k$ consists of the first k columns of $\mathbf{U}$ and the k-dimensional vectors $\mathbf{a}_{i=0,\ldots,n-1}$ are the column vectors of the $k \times n$ product matrix $\boldsymbol{\Lambda}_k^{\frac{1}{2}} \mathbf{V}_k^H$.

Dimensionality Reduction via SVD (2)

- The figure below gives a diagrammatic interpretation of the matrix products involved in the SVD



- In the approximation of $\mathbf{X}$ by $\widehat{\mathbf{X}}$, the first k columns of $\mathbf{U}_r$ and the first k rows of $\mathbf{V}_r^H$ are involved.

Dimensionality Reduction via SVD (3)

- Each l-dimensional column vector $\mathbf{x}_i$ of $\mathbf{X}$ is approximated by the k-dimensional vector $\mathbf{a}_i$ lying in the subspace spanned by $\mathbf{u}_{i=0,\ldots,k-1}$ ($\mathbf{a}_i$ is the projection of $\mathbf{x}_i$ on this subspace)

$$\mathbf{x}_i \approx \mathbf{U}_k \mathbf{a}_i = \sum_{m=0}^{k-1} \mathbf{u}_m a_i(m), \quad i = 0, \ldots, n-1$$

- Due to the orthonormality of the columns $\mathbf{u}_{i=0,ldots,k-1}$ can be seen that

$$\|\mathbf{x}_i - \mathbf{x}_j\| \approx \|\mathbf{U}_k(\mathbf{a}_i - \mathbf{a}_j)\| = \|\sum_{m=0}^{k-1} \mathbf{u}_m(a_i(m) - a_j(m))\| =$$

$$= \|\mathbf{a}_i - \mathbf{a}_j\|, \qquad i = 0, \ldots, n-1$$

SVD Conclusions

- The SVD has excellent information packing properties. E, g., an image array can be represented efficiently by a few of its singular values. Thus, SVD is a natural candidate as a tool for feature generation/selection in classification.

- Since SVD approximately keeps the Euclidean distance (see previous slide), it is suitable for information retrieval tasks.