

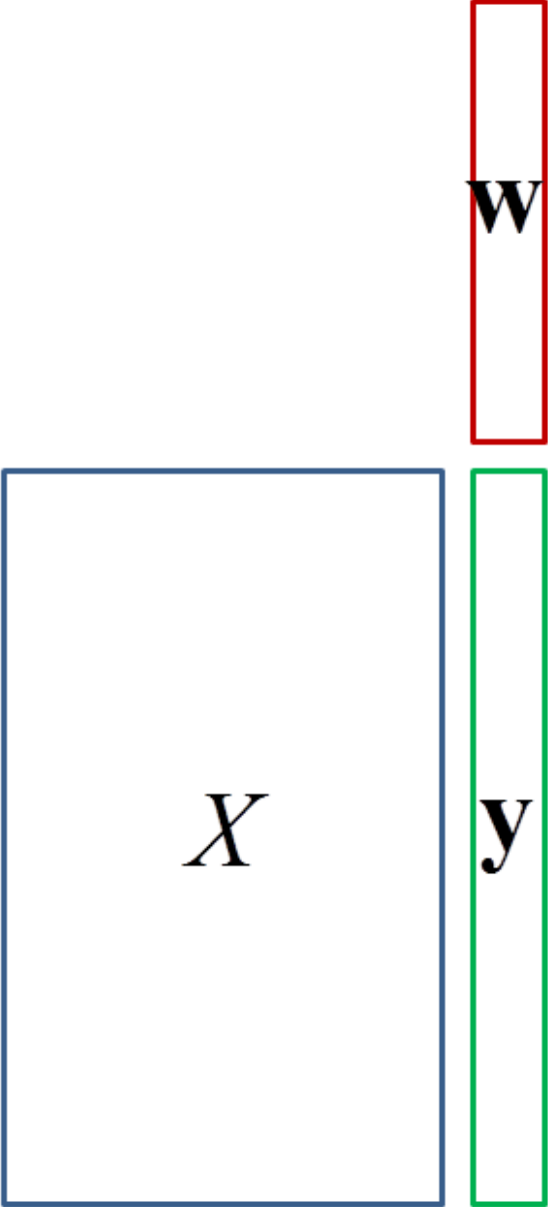
# Factorization, Principal Component Analysis and Singular Value Decomposition

Volker Tresp  
Summer 2016

## Recall: Multiple Linear Regression

- Many inputs and one output

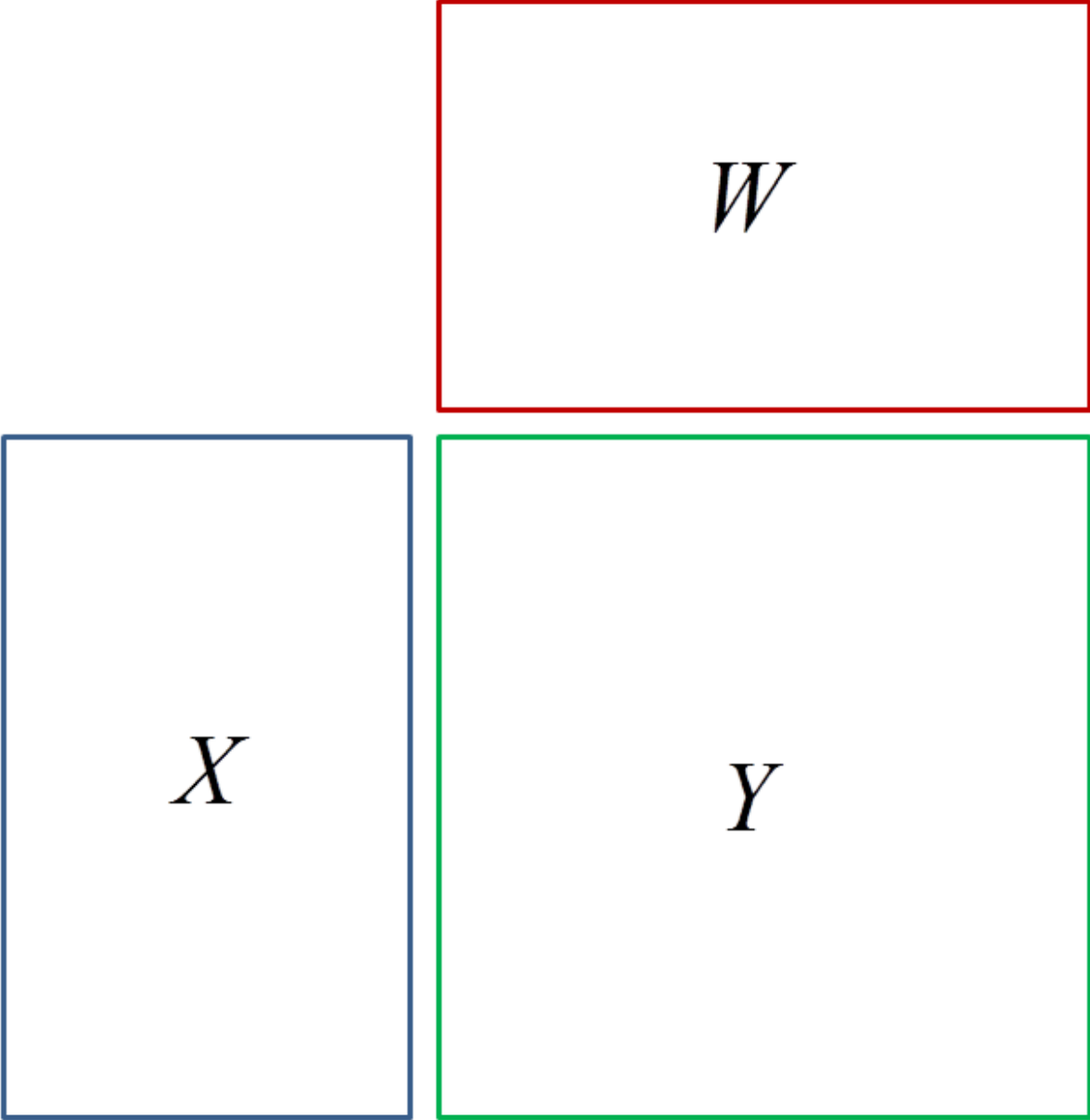
$$\mathbf{y} \approx \mathbf{X}\mathbf{w}$$



## Multivariate Linear Regression: Linear Regression with Several Outputs

- Many inputs and many outputs

$$Y \approx XW$$



## Unknown Inputs

- Now we assume that the inputs  $X$  are also unknown
- We change the notation and write  $A = X$  and  $B = W^T$  and get

$$Y = AB^T$$

- Example: each row of  $Y$  corresponds to a user, each column of  $Y$  corresponds to a movie and  $y_{i,j}$  is the rating of user  $i$  for movie  $j$
- Thus the  $i$ -th row of  $A$  describes the latent attributes or **latent factors of the user** associated with the  $i$ -th row and the  $j$ -th row of  $B$  describes the latent attributes or **latent factors of the movie** associated with the  $j$ -th column

$B^T$

$A$

$Y$

## Cost Function

- A least-squares cost function becomes

$$\sum_{(i,j) \in \mathcal{R}} \left( y_{i,j} - \sum_{k=1}^r a_{i,k} b_{j,k} \right)^2 + \lambda \sum_{i=1}^N \sum_{k=1}^r a_{i,k}^2 + \lambda \sum_{j=1}^M \sum_{k=1}^r b_{j,k}^2$$

Here  $\mathcal{R}$  is the set of existing ratings,  $r$  (rank) is the number of latent factors, and  $\lambda$  is a regularization parameter

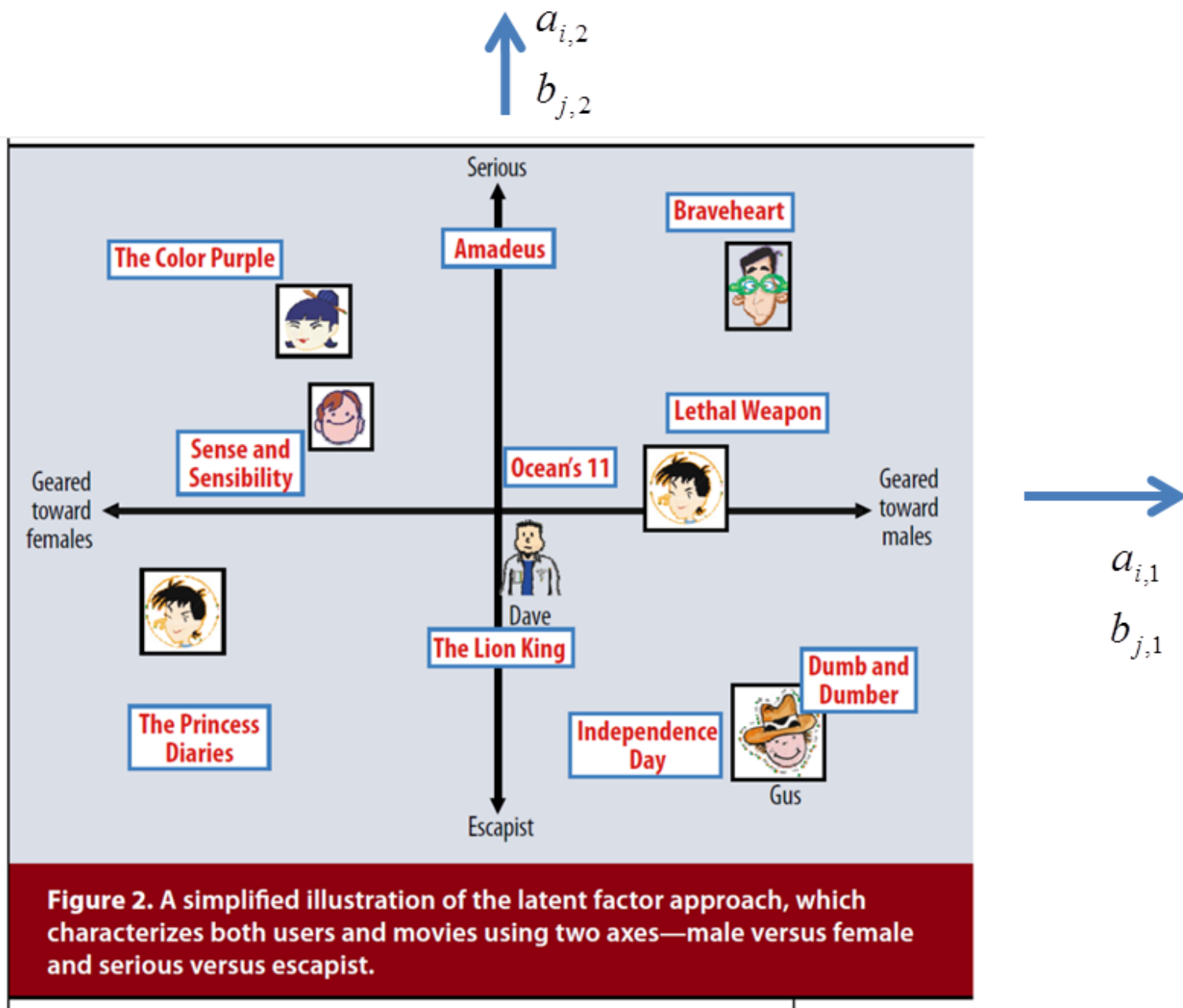
- Note, that the cost function ignores movies which have not been rated yet and treats them as missing
- $A$  and  $B$  are found via stochastic gradient descent
- After convergence, we can predict for any user and any movie

$$\hat{y}_{i,j} = \sum_{k=1}^r a_{i,k} b_{j,k}$$



## Symmetry of the Factorization

- Matrix factorization was the most important component in the winning entries in the Netflix competition: rows are users and columns are movies and  $y_{i,j}$  is the rating user  $i$  gave for movie  $j$
- Note that the  $i$ -th row of  $A$  contains the latent factor of user  $i$  and the  $j$ -th row of  $B$  contains the latent factors of movie  $j$  (symmetry of the decomposition!)



have rated only a small percentage of possible items.

One strength of matrix factorization is that it allows incorporation of additional information. When explicit feedback is not available, recommender systems can infer user preferences using *implicit feedback*, which indirectly reflects opinion by observing user behavior including purchase history, browsing history, search patterns, or even mouse movements. Implicit feedback usually denotes the presence or absence of an event, so it is typically represented by a densely filled matrix.

### A BASIC MATRIX FACTORIZATION MODEL

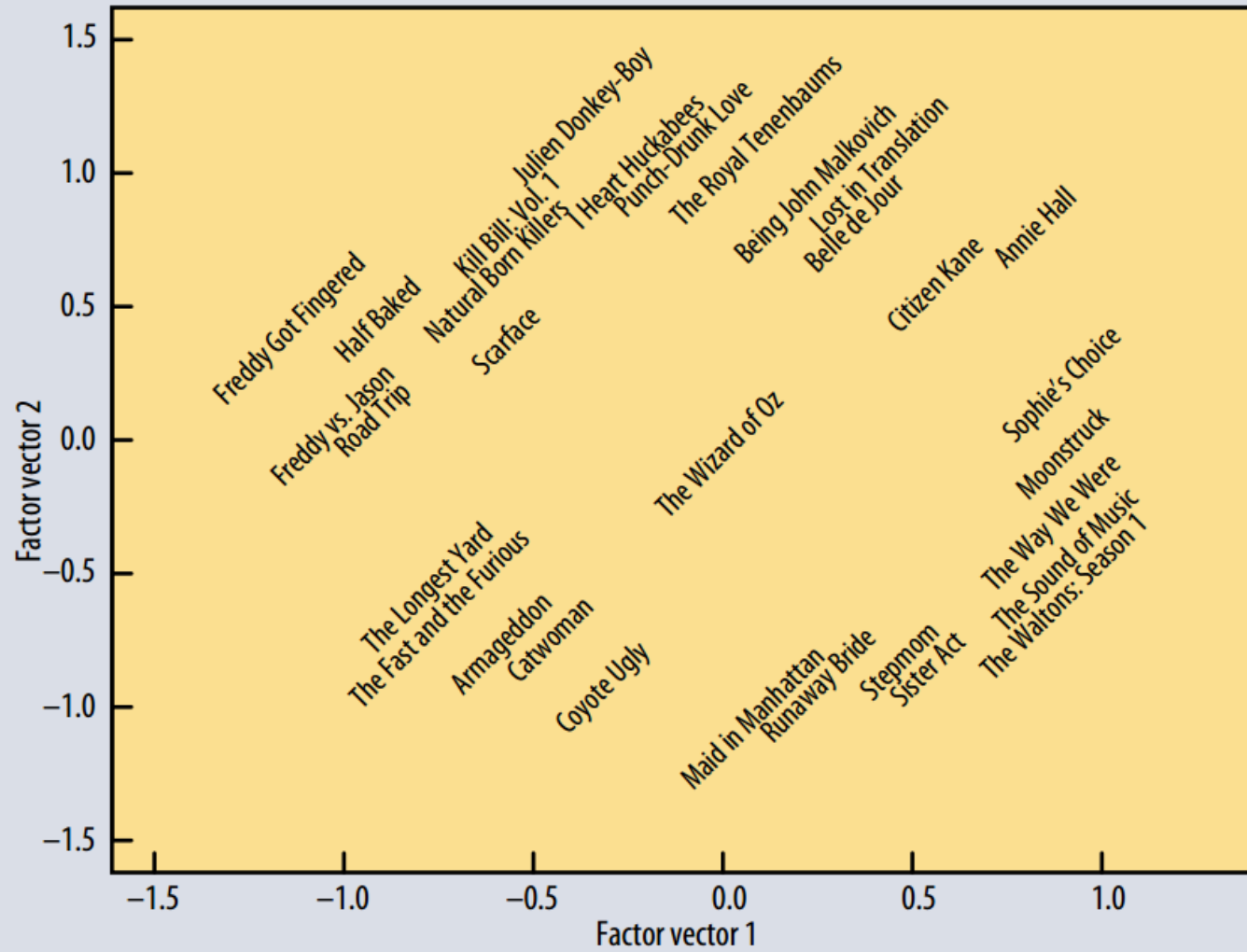
Matrix factorization models map both users and items to a joint latent factor space of dimensionality  $f$ , such that user-item interactions are modeled as inner products in that space. Accordingly, each item  $i$  is associated with a

works - suggested modeling directly the observed ratings only, while avoiding overfitting through a regularized model. To learn the factor vectors ( $p_u$  and  $q_i$ ), the system minimizes the regularized squared error on the set of known ratings:

$$\min_{q^*, p^*} \sum_{(u,i) \in \kappa} (r_{ui} - q_i^T p_u)^2 + \lambda (\|q_i\|^2 + \|p_u\|^2) \quad (2)$$

Here,  $\kappa$  is the set of the  $(u,i)$  pairs for which  $r_{ui}$  is known (the training set).

The system learns the model by fitting the previously observed ratings. However, the goal is to generalize those previous ratings in a way that predicts future, unknown ratings. Thus, the system should avoid overfitting the observed data by regularizing the learned parameters, whose magnitudes are penalized. The constant  $\lambda$  controls



**Figure 3.** The first two vectors from a matrix decomposition of the Netflix Prize data. Selected movies are placed at the appropriate spot based on their factor vectors in two dimensions. The plot reveals distinct genres, including clusters of movies with strong female leads, fraternity humor, and quirky independent films.

## Factorization of the Design Matrix

- So far we started with  $Y \approx XW$ , i.e., we factorized the output matrix
- In other applications it makes sense to factorize the design matrix  $X$  as

$$X \approx AB^T$$

- This is a form of dimensional reduction, if  $r < M$
- As we will see later, a classifier with  $A$  as design matrix can give better results than a classifier with  $X$  as design matrix

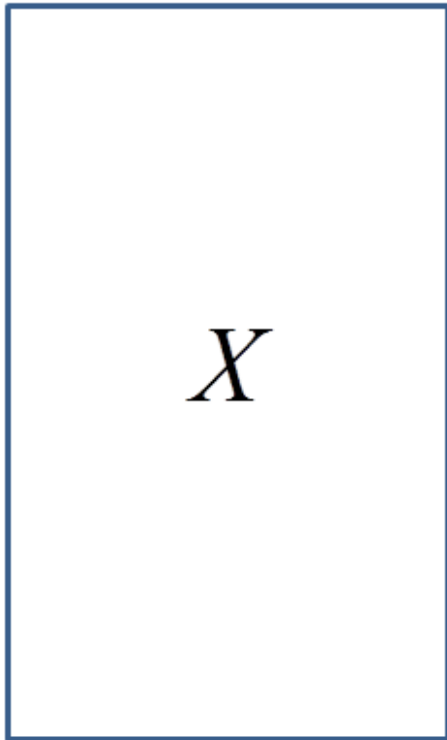
$B^T$

$A$

$X$

Predictions  
with  
original  
attributes

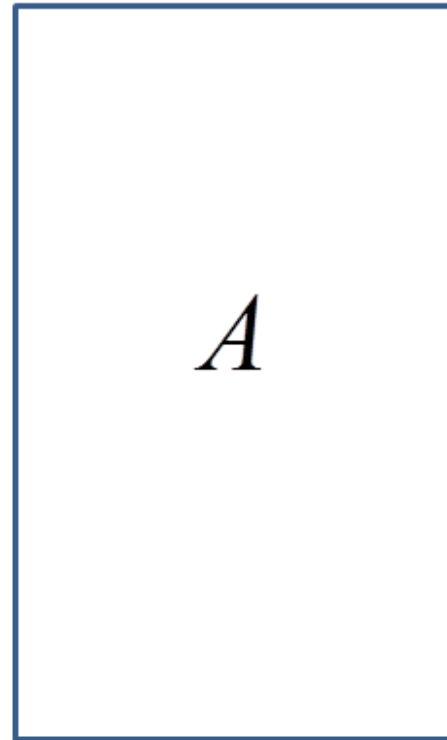
$\mathbf{W}$



$\mathbf{y}$

Predictions  
with latent  
factors

$\tilde{\mathbf{W}}$



$\mathbf{y}$

## As an Autoencoder

- The optimal  $\mathbf{a}_i$  can be written as a function of all attributes of  $i$ , i.e.,  $x_i$ :
- In matrix form

$$A = XV$$

- Then

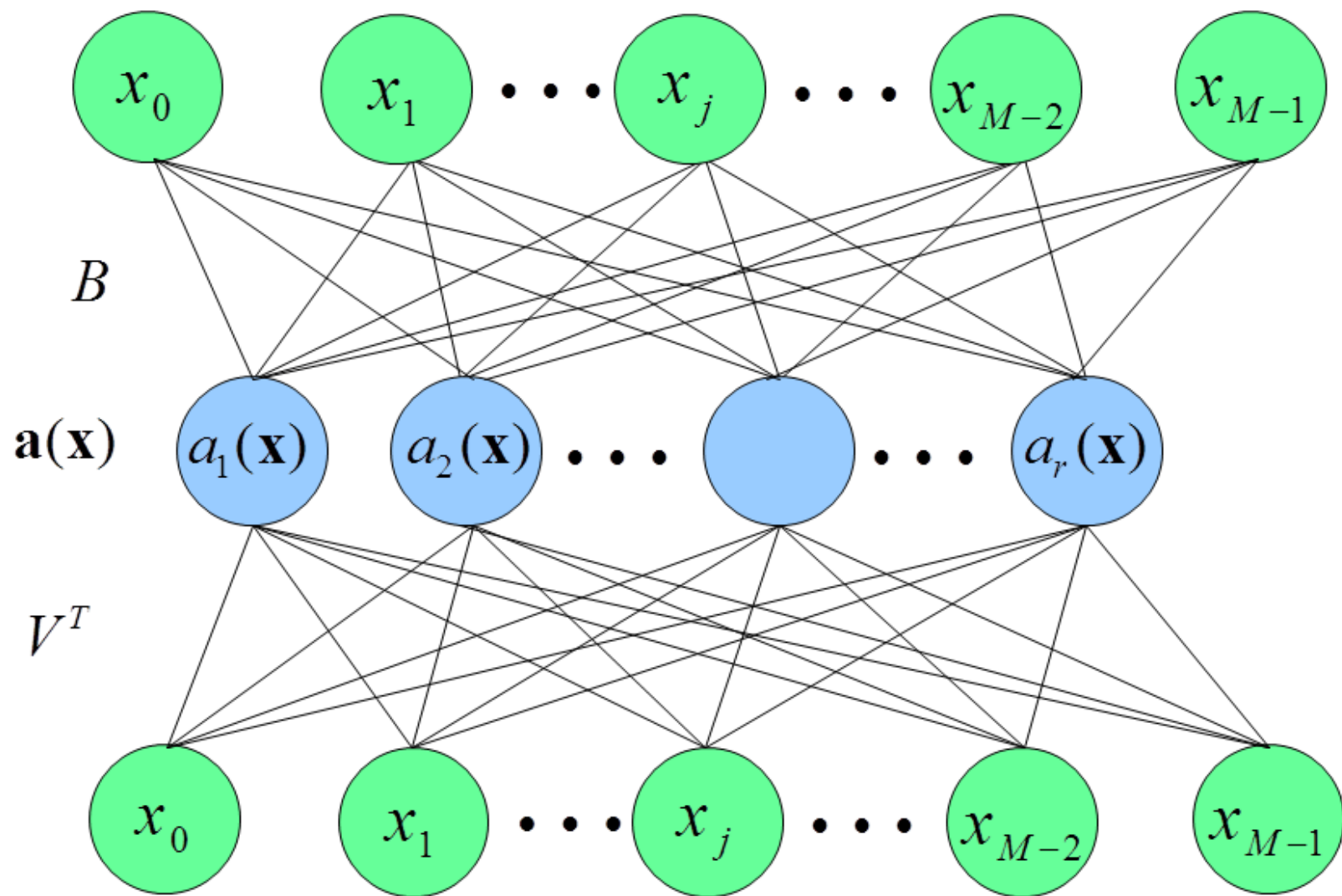
$$X \approx XV B^T$$

or

$$\mathbf{x}_i \approx B V^T \mathbf{x}_i$$

- Thus if  $X$  is complete, we can learn the factorization via an autoencoder





# PCA

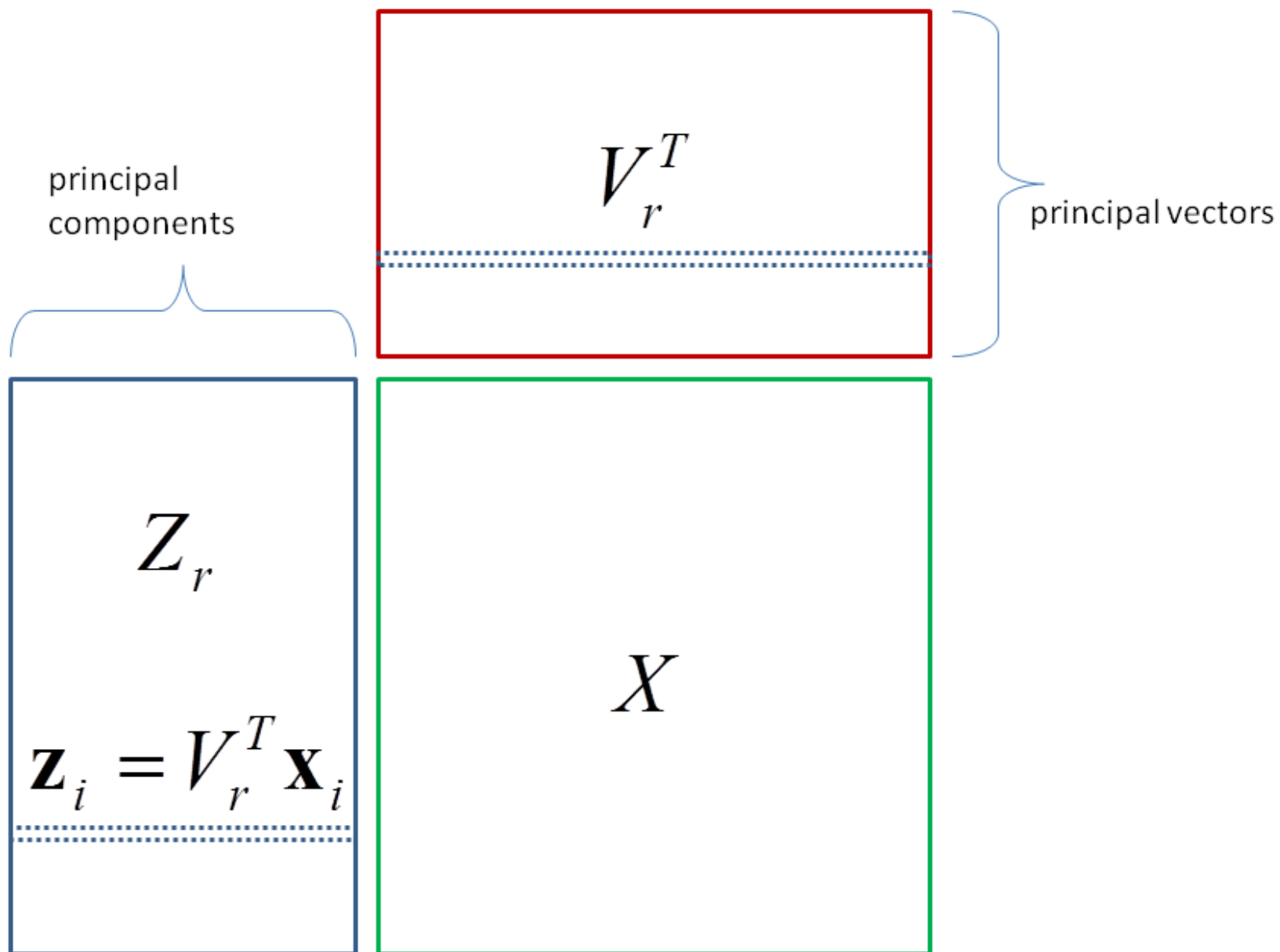
- The factorization approach as described is not unique and it has only been recently used in machine learning
- More traditional is the factorization via a principal component analysis (PCA)
- With  $A \rightarrow Z$  and  $B \rightarrow V$  we get

$$X \approx Z_r V_r^T$$

- The  $i$ -th row of  $A$  contains the  $r$  principal *principal components* of  $i$  (new name for the latent factors). With  $r = \min(M, N)$  the factorization is without error. With  $r < \min(M, N)$  this is an approximation
- The columns of  $V$  are orthonormal
- The decomposition is unique and is optimal for any  $r$  with respect to the cost function

$$\sum_{i,j} \left( x_{i,j} - \sum_{k=1}^r z_{i,k} v_{j,k} \right)^2$$

- We will now derive the solution



## Dimensionality Reconstruction

- We want to compress the  $M$ -dimensional  $\mathbf{x}$  to an  $r$ -dimensional  $\mathbf{z}$  using a linear transformation
- We want that  $\mathbf{x}$  can be reconstructed from  $\mathbf{z}$  as well as possible in the mean squared error sense for all data points  $\mathbf{x}_i$

$$\sum_i (\mathbf{x}_i - V_r \mathbf{z}_i)^T (\mathbf{x}_i - V_r \mathbf{z}_i)$$

where  $V_r$  is an  $M \times r$  matrix.

## First Component

- Let's first look at  $r = 1$  and we want to find the vector  $\mathbf{v}$
- Without loss of generality, we assume that  $\|\mathbf{v}\| = 1$
- The reconstruction error for a particular  $\mathbf{x}_i$  is given by

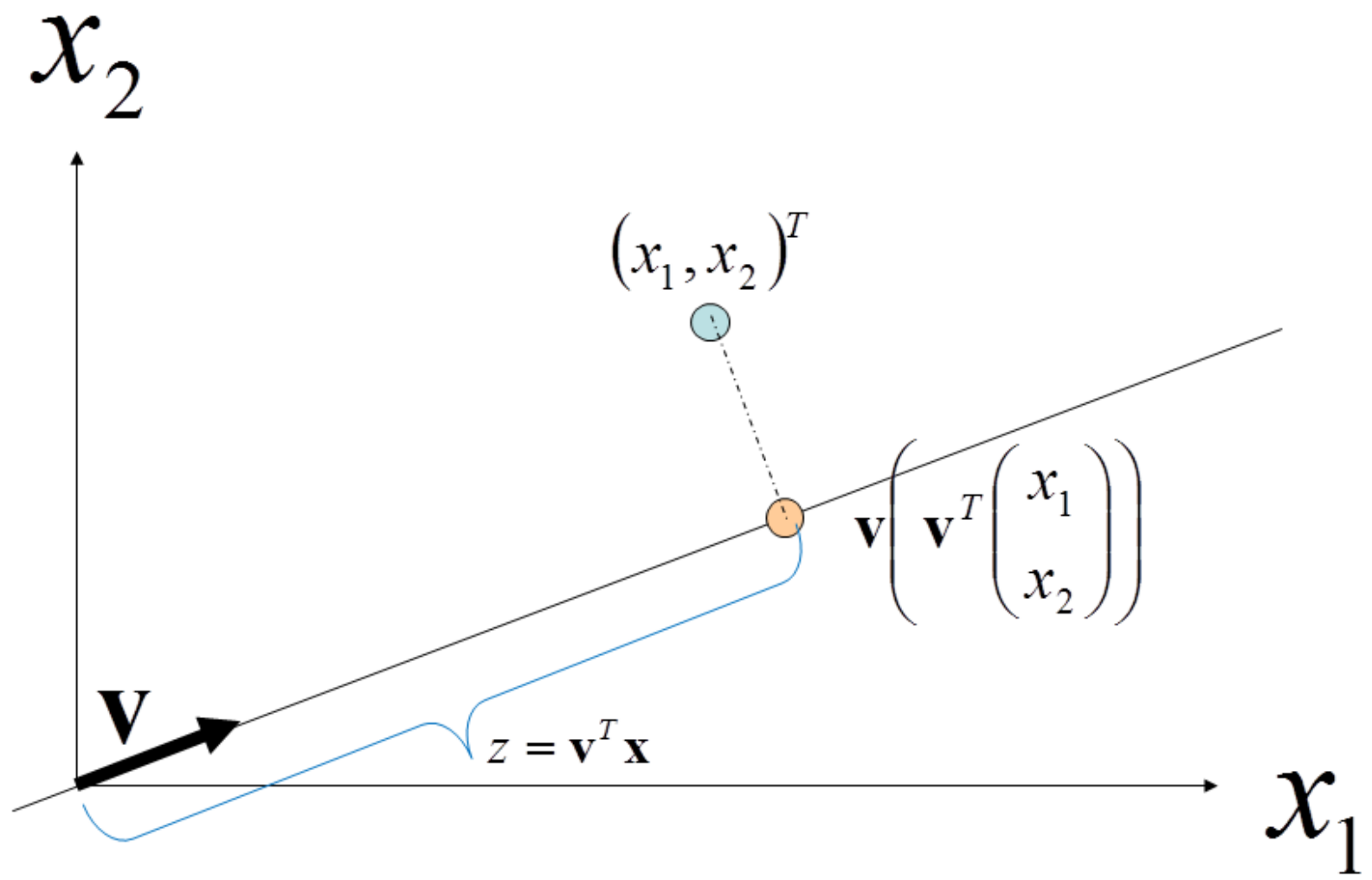
$$(\mathbf{x}_i - \hat{\mathbf{x}}_i)^T (\mathbf{x}_i - \hat{\mathbf{x}}_i) = (\mathbf{x}_i - \mathbf{v}z_i)^T (\mathbf{x}_i - \mathbf{v}z_i).$$

The optimal  $z_i$  is then (see figure)

$$z_i = \mathbf{v}^T \mathbf{x}_i$$

Thus we get

$$\hat{\mathbf{x}}_i = \mathbf{v}\mathbf{v}^T \mathbf{x}_i$$



## Computing the First Principal Vector

- So what is  $\mathbf{v}$ ? We are looking for a  $\mathbf{v}$  that minimized the reconstruction error over all data points. We use the Lagrange parameter  $\lambda$  to guarantee length 1

$$\begin{aligned} L &= \sum_{i=1}^N (\mathbf{v}\mathbf{v}^T \mathbf{x}_i - \mathbf{x}_i)^T (\mathbf{v}\mathbf{v}^T \mathbf{x}_i - \mathbf{x}_i) + \lambda(\mathbf{v}^T \mathbf{v} - 1) \\ &= \sum_{i=1}^N \mathbf{x}_i^T \mathbf{v}\mathbf{v}^T \mathbf{v}\mathbf{v}^T \mathbf{x}_i + \mathbf{x}_i^T \mathbf{x}_i - \mathbf{x}_i^T \mathbf{v}\mathbf{v}^T \mathbf{x}_i - \mathbf{x}_i^T \mathbf{v}\mathbf{v}^T \mathbf{x}_i + \lambda(\mathbf{v}^T \mathbf{v} - 1) \\ &= \sum_{i=1}^N \mathbf{x}_i^T \mathbf{x}_i - \mathbf{x}_i^T \mathbf{v}\mathbf{v}^T \mathbf{x}_i + \lambda(\mathbf{v}^T \mathbf{v} - 1) \end{aligned}$$



## Computing the First Principal Vector

- The first term does not depend on  $\mathbf{v}$ . We take the derivative with respect to  $\mathbf{v}$  and obtain for the second term

$$\frac{\partial}{\partial \mathbf{v}} \mathbf{x}_i^T \mathbf{v} \mathbf{v}^T \mathbf{x}_i$$

$$= \frac{\partial}{\partial \mathbf{v}} (\mathbf{v}^T \mathbf{x}_i)^T (\mathbf{v}^T \mathbf{x}_i) = 2 \left( \frac{\partial}{\partial \mathbf{v}} \mathbf{v}^T \mathbf{x}_i \right) (\mathbf{v}^T \mathbf{x}_i)$$

$$= 2 \mathbf{x}_i (\mathbf{v}^T \mathbf{x}_i) = 2 \mathbf{x}_i (\mathbf{x}_i^T \mathbf{v}) = 2 (\mathbf{x}_i \mathbf{x}_i^T) \mathbf{v}$$

and for the last term

$$\lambda \frac{\partial}{\partial \mathbf{v}} \mathbf{v}^T \mathbf{v} = 2 \lambda \mathbf{v}$$

- We set the derivative to zero and get

$$\sum_{i=1}^N \mathbf{x}_i \mathbf{x}_i^T \mathbf{v} = \lambda \mathbf{v}$$

or in matrix form

$$\Sigma \mathbf{v} = \lambda \mathbf{v}$$

where  $\Sigma = X^T X$

- Recall that the Lagrangian is maximized with respect to  $\lambda$
- Thus the first principal vector  $\mathbf{v}$  is the first eigenvector of  $\Sigma$  (with the largest eigenvalue)
- $z_i = \mathbf{v}^T \mathbf{x}_i$  is called the first principal component of  $\mathbf{x}_i$

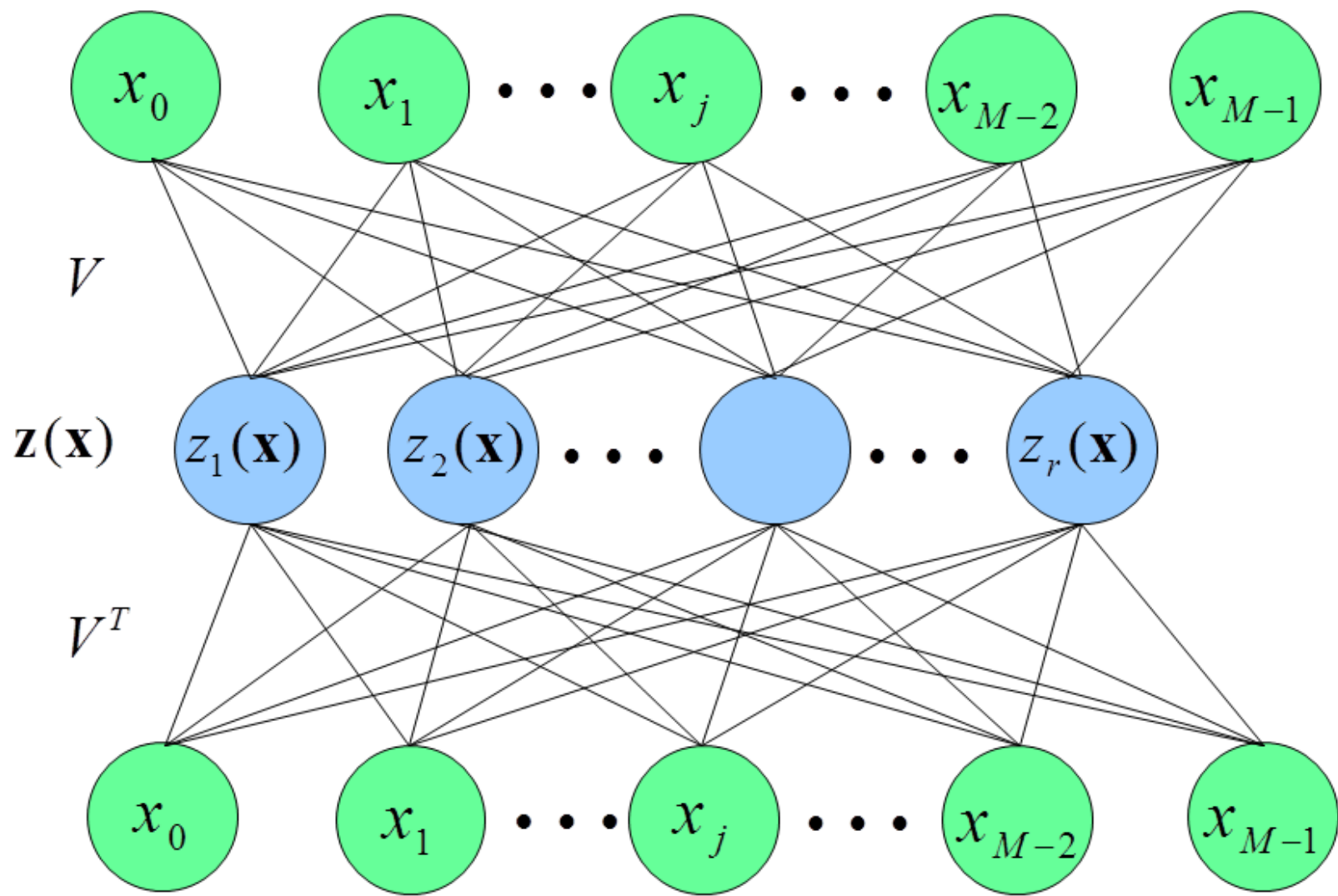
## Computing all Principal Vectors

- The second principal vector is given by the second eigenvector of  $\Sigma$  and so on
- For a rank  $r$  approximation we get

$$\mathbf{z}_i = V_r^T \mathbf{x}_i$$

- Here, the columns of  $V_r$  are all orthonormal and correspond to the  $r$  eigenvectors of  $\Sigma$  with the largest eigenvalues
- The optimal reconstruction is

$$\hat{\mathbf{x}}_i = V_r \mathbf{z}_i$$

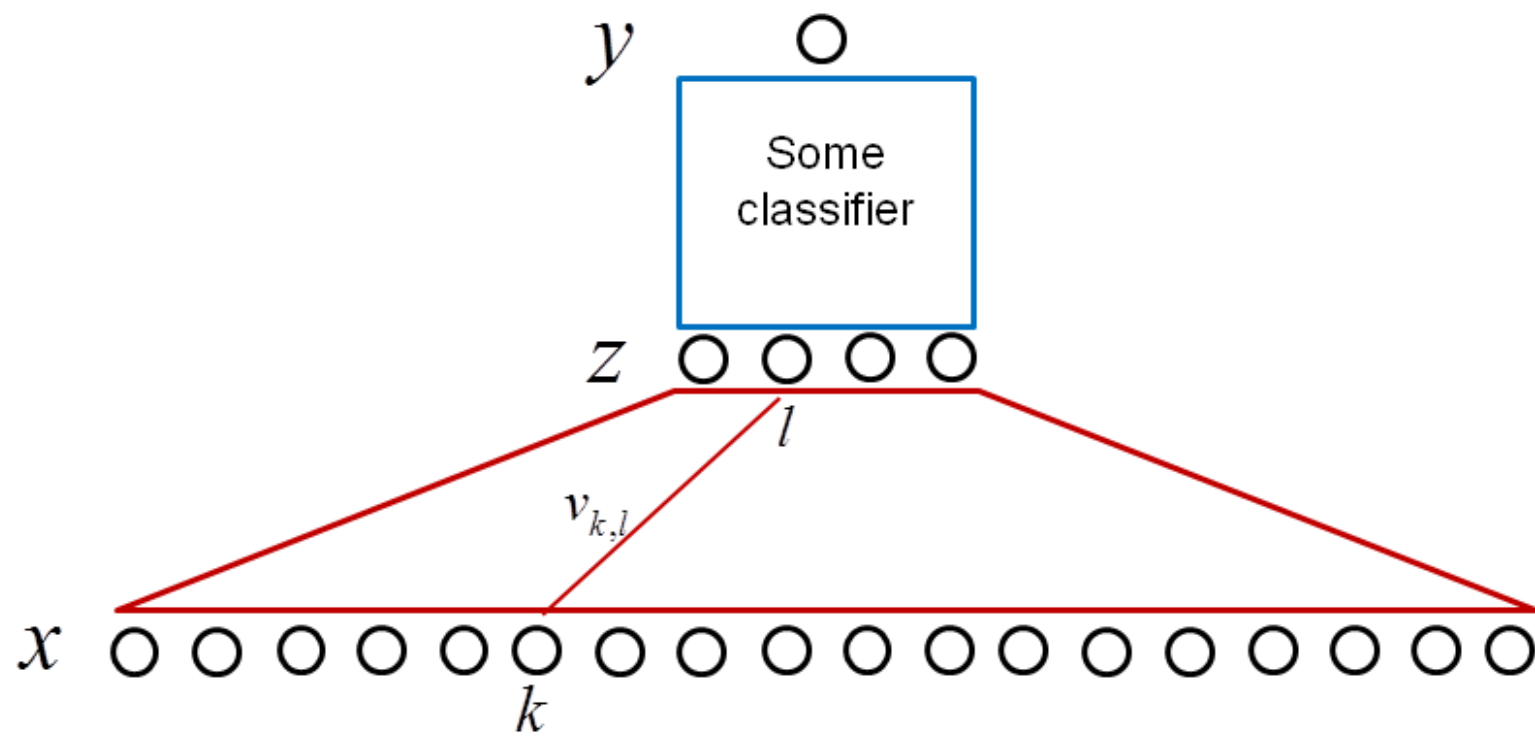


# PCA Applications

## Classification and Regression

- First perform an PCA of  $X$  and then use as input to the classifier  $\mathbf{z}_i$  instead of  $\mathbf{x}_i$ , where

$$\mathbf{z}_i = V_r^T \mathbf{x}_i$$



## Similarity and Novelty

- A distance measure (Euclidian distance) based on the principal components is often more meaningful than a distance measure calculated in the original space
- Novelty detection / outlier detection: We calculate the reconstruction of a new vector  $\mathbf{x}$  and calculate

$$\|\mathbf{x} - V_r V_r^T \mathbf{x}\| = \|V_{-r}^T \mathbf{x}\|$$

If this distance is large, then the new input is unusual, i.e. might be an outlier

- Here  $V_{-r}$  contains the  $M - r$  eigenvectors  $\mathbf{v}_{r+1}, \dots, \mathbf{v}_M$  of  $\Sigma$



# PCA Example: Handwritten Digits

## Data Set

- 130 handwritten digits “ 3 ” (in total: 658): significant difference in style
- The images have  $16 \times 16$  grey valued pixels. Each input vector  $\mathbf{x}$  consists of the becomes a 256 grey values of the pixels: applying a linear classifier to the original pixels gives bad results



## Visualisation

- We see the first two principal vectors  $\mathbf{v}_1$ ,  $\mathbf{v}_2$
- $\mathbf{v}_1$  prolongs the lower portion of the “3”
- $\mathbf{v}_2$  modulates thickness

$$\hat{\mathbf{x}}_i =$$

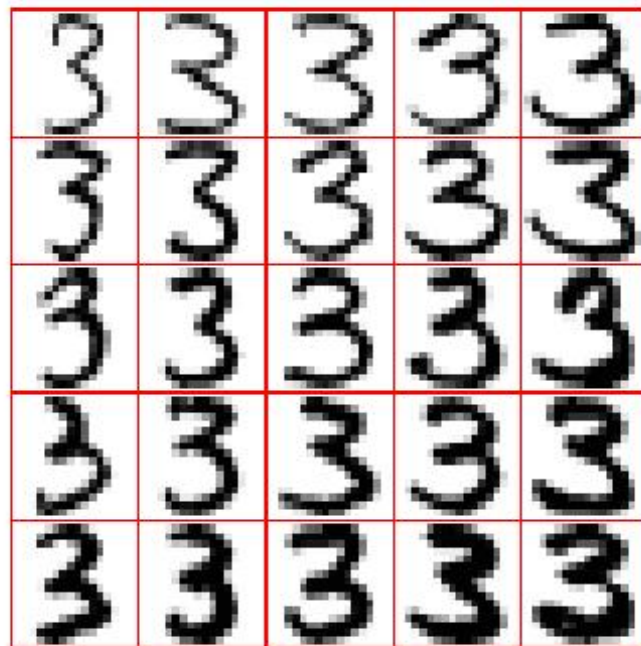
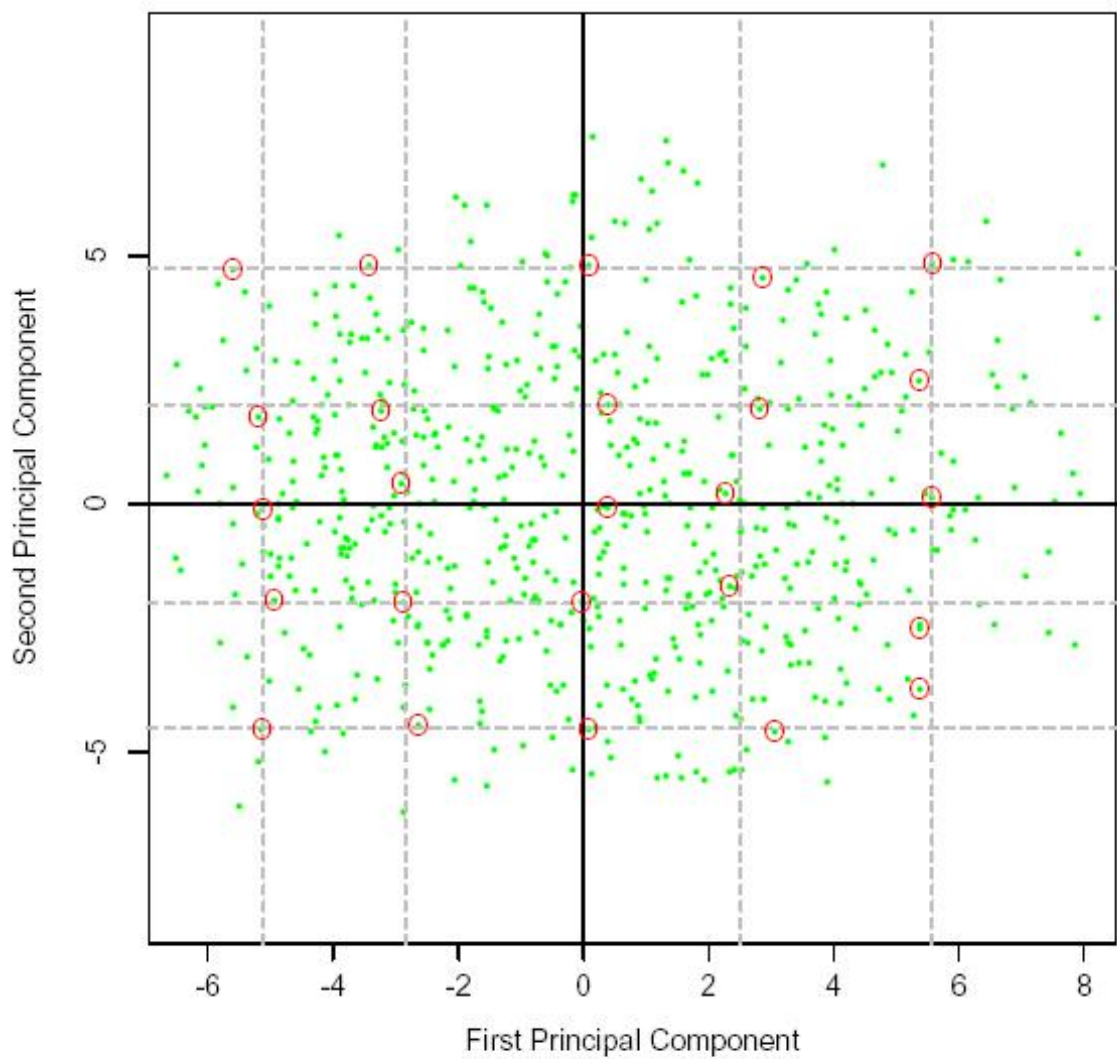
$$\begin{array}{c} \boxed{\text{3}} \\ \mathbf{m} \end{array} + z_{i,1} \cdot \begin{array}{c} \boxed{\text{3}} \\ \mathbf{v}_1 \end{array} + z_{i,2} \cdot \begin{array}{c} \boxed{\text{3}} \\ \mathbf{v}_2 \end{array} .$$

## Visualisation: Reconstruction

- For different values of the principal components  $z_1$  and  $z_2$  the reconstructed image is shown

$$\hat{\mathbf{x}} = \mathbf{m} + z_1 \mathbf{v}_1 + z_2 \mathbf{v}_2$$

- $\mathbf{m}$  is a mean vector that was subtracted before the PCA was performed and is now added again.  $\mathbf{m}$  represents 256 mean pixel values averaged over all samples



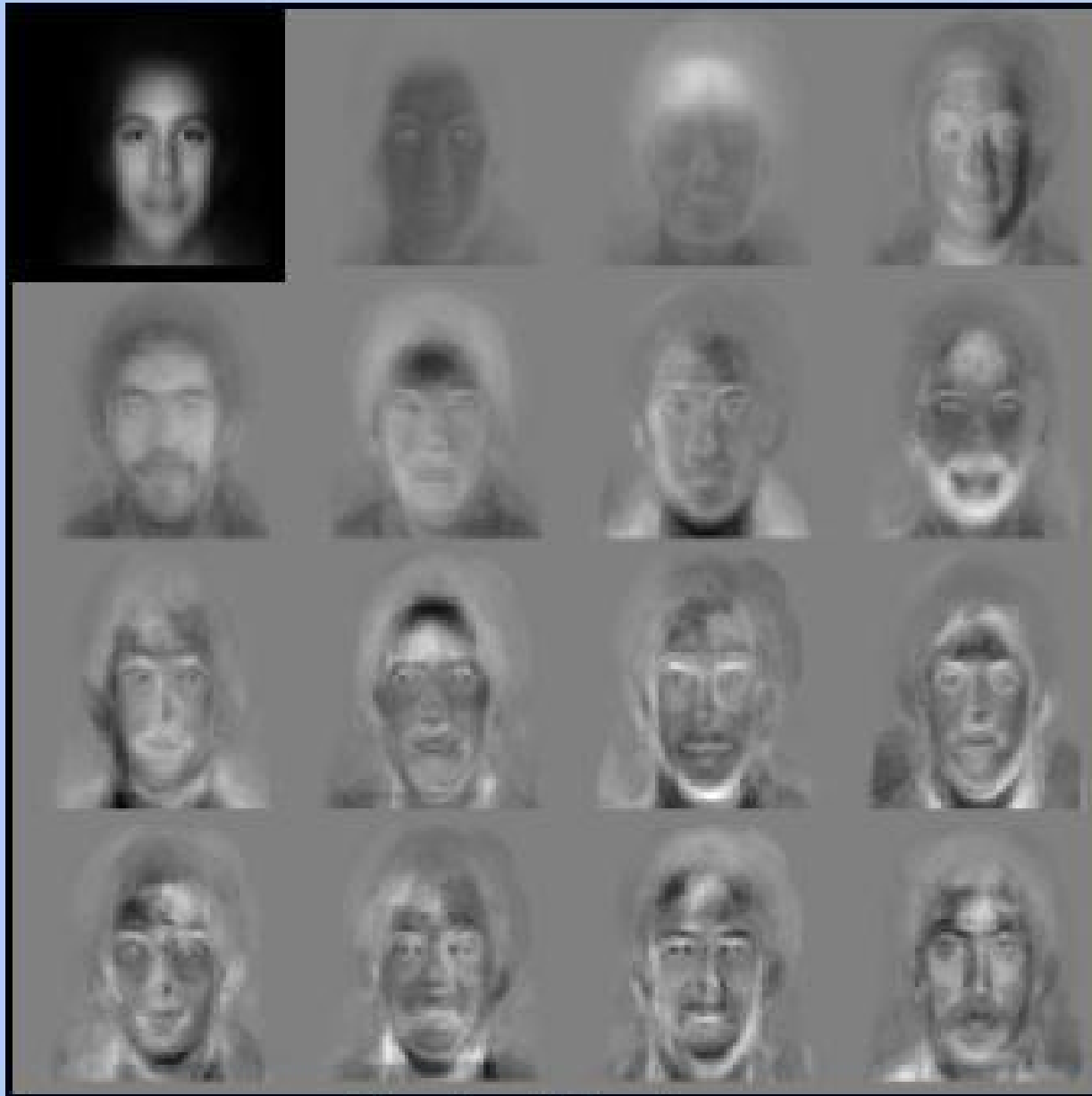
# Eigenfaces



# Eigenfaces

## Data Set

- PCA for face recognition
- <http://vismod.media.mit.edu/vismod/demos/facerec/basic.html>
- 7562 images from 3000 persons
- $\mathbf{x}_i$  contains the pixel values of the  $i$ -th image. Obviously it does not make sense to build a classifier directly on the  $256 \times 256 = 65536$  pixel values
- Eigenfaces were calculated based on 128 images (eigenfaces might sound cooler than principal vectors!) (training set)
- For recognition on test images, the first  $r = 20$  principal components are used
- Almost each person had at least 2 images; many persons had images with varying facial expression, differen hair style, differen beards, ...



Standard Eigenfaces

## Similarity Search based on Principal Components

- The upper left image is the test image. Based on the Euclidian distance in PCA-space the other 15 images were classified as nearest neighbors. All 15 images came from the correct person, although the data base contained more than 7562 images!
- Thus, distance is evaluated following

$$\|\mathbf{z} - \mathbf{z}_i\|$$

Database:

Display mode:

Search metric:

Working Set: 7561

Left button to select  
Middle button to search  
Right button for info

8455 8468 8486 8454

8485 8465 8466 8469

8501 8481 8479 8491

8498 8459 6141 8487

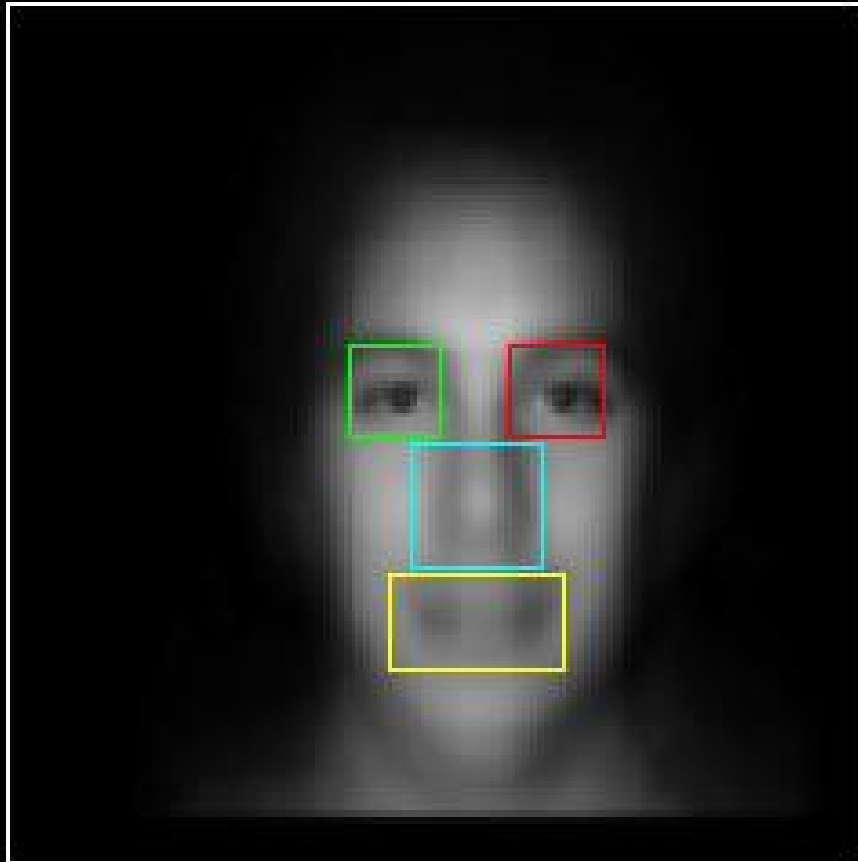
## Recognition Rate

- 200 pictures were selected randomly from the test set. In 96% of all cases the nearest neighbor was the correct person

## Modular Eigenspaces

- The method can also be applied to facial features as eigeneyes, eigen noses, eigenmouths.
- Analysis of human eye movements also showed that humans concentrate on these local features as well

# Facial Feature Domains





## Automatically Finding the Facial Features

- The modular methods require an automatic way of finding the facial features (eyes, nose, mouth)
- One defines rectangular windows that are indexed by the central pixel in the window
- One computes the anomaly of the image window for all locations, where the detector was trained on a feature class (e.g., left eyes) by using a rank 10 PCA. When the anomaly is minimum the feature (eye) is detected.

$$AN_{\text{left eye}}(\mathbf{z}_{pos_k}) = \|\mathbf{z}_{pos_k} - \hat{\mathbf{z}}_{pos_k}\|^2$$

- In the following images, brightness is anomaly

## Input Image



# Distances

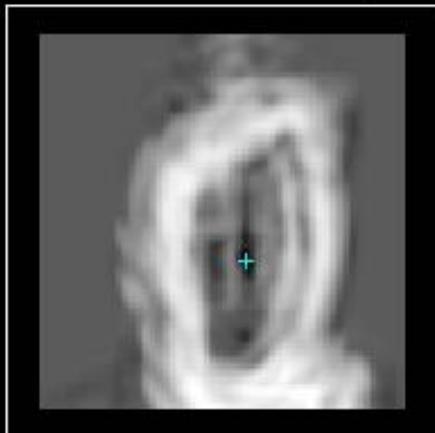
Distance-from-LEye-Space



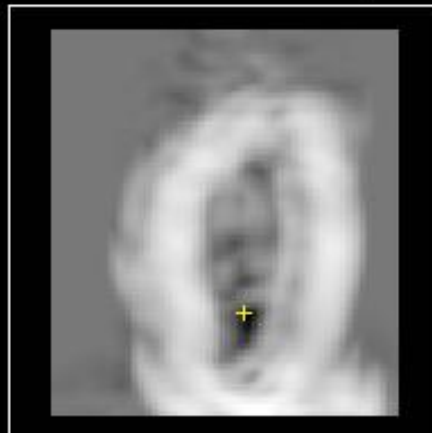
Distance-from-REye-Space



Distance-from-Nose-Space

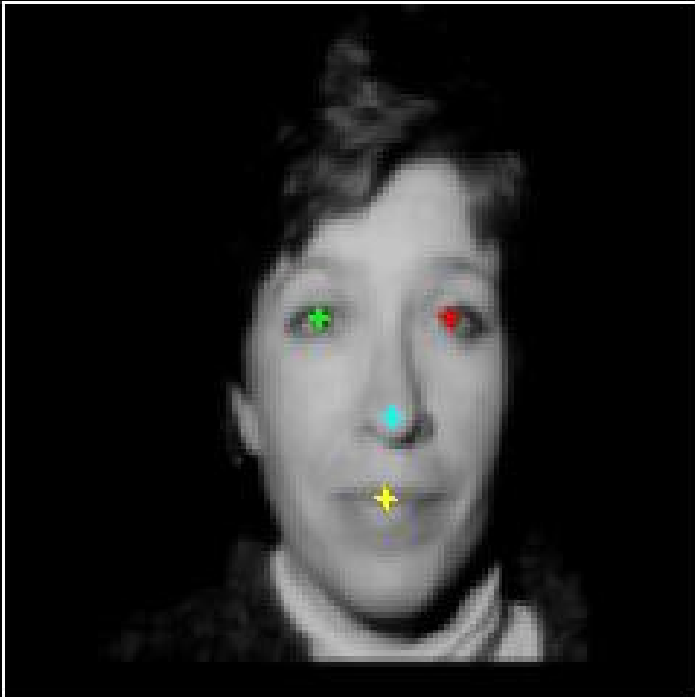


Distance-from-Mouth-Space

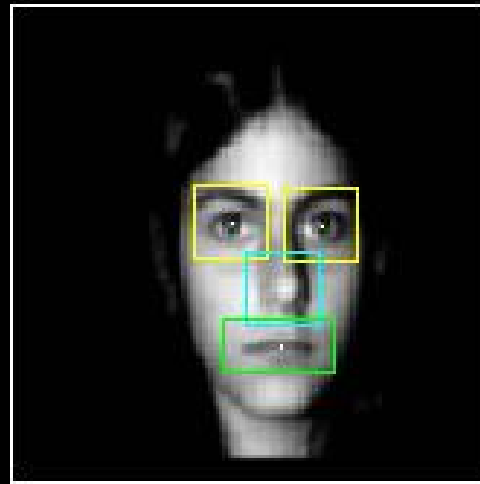
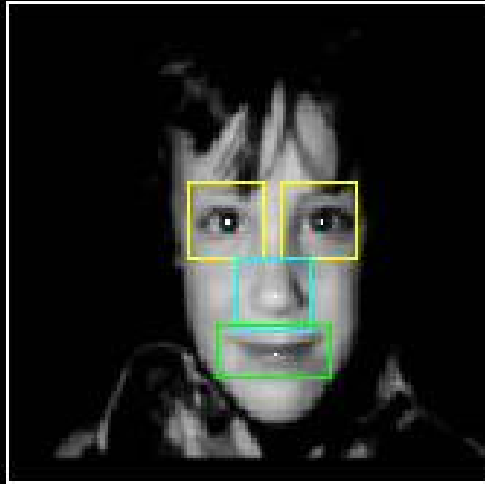


## Detection

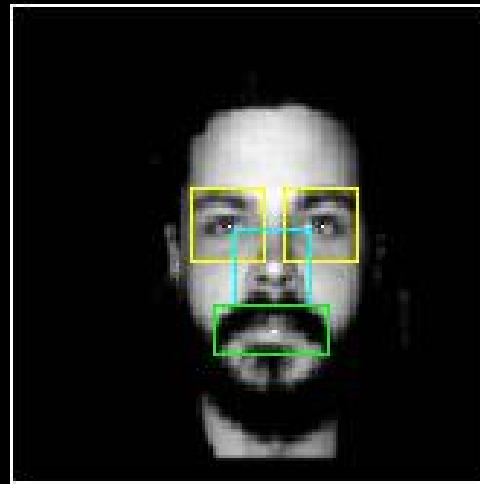
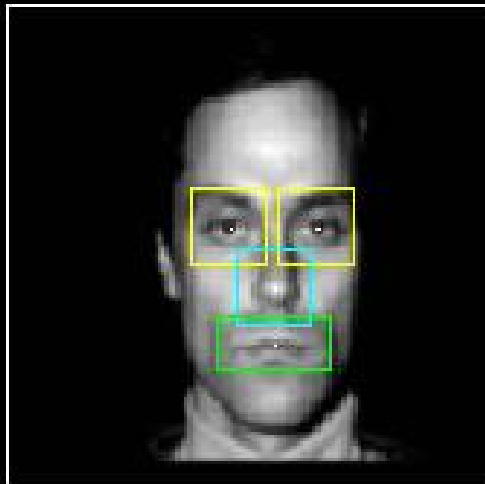
### Feature Detections



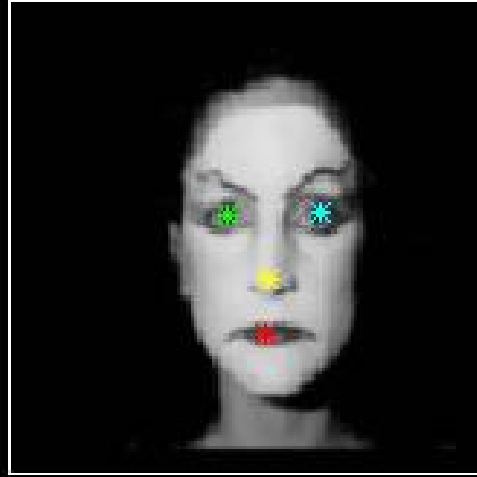
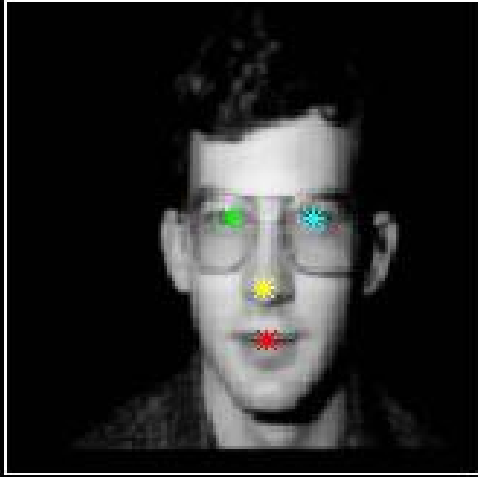
# Training Templates



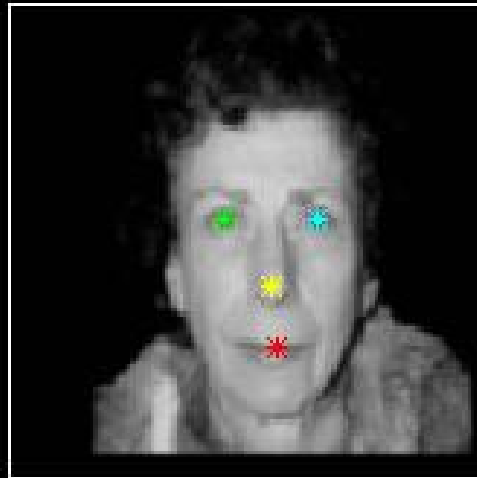
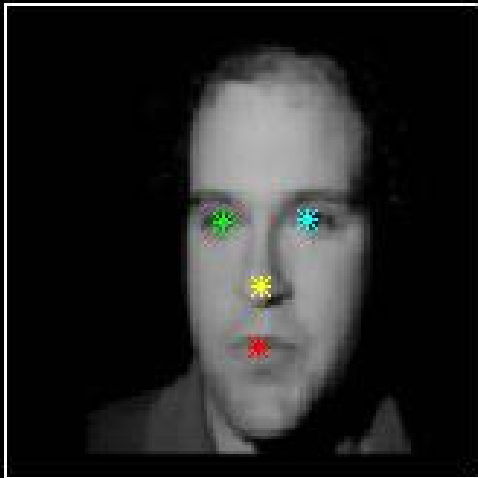
Training Templates



## Typical Detections



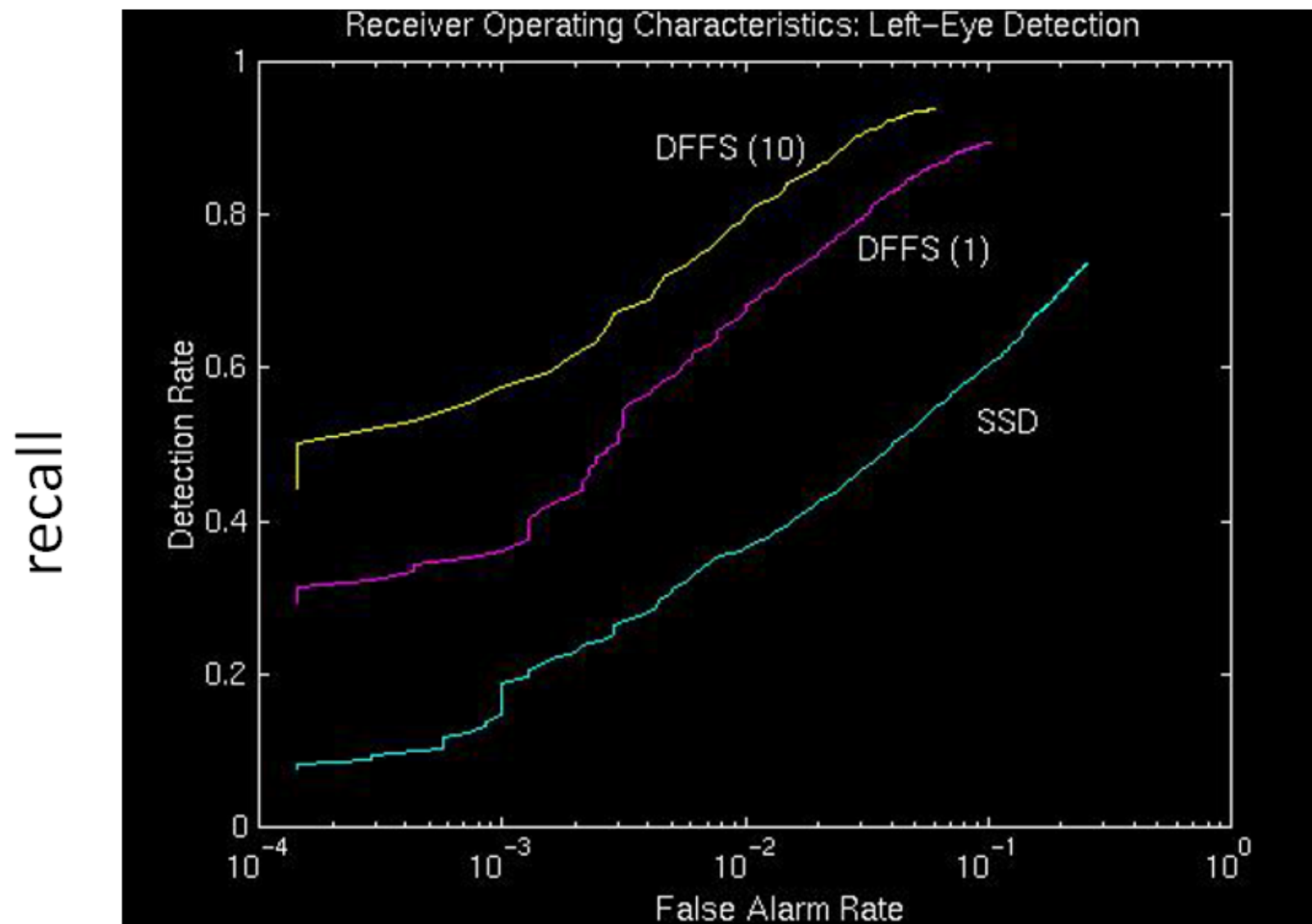
Typical Detections





## Detection Rate

- The next plot shows the performance of the left-eye-detector based on  $AN_{\text{linkes}} \text{ Auge}(z_{\text{pos}_k})$  (labelled as DFFS) with rank one and with rank 10. Also shown are the results for simple template matching (distance to the mean left eye image (SSD)).
- **Definition of Detection:** The global optimum is below a threshold value  $\alpha$  and is within 5 pixels of the correct location. Detection rate = recall =  $P(\text{pred} = 1 | y = 1)$
- **Definition of False Alarm:** The global optimum is below a threshold value  $\alpha$  and is outside of 5 pixels of the correct location. Specificity =  $P(\text{pred} = 0 | y = 0)$
- In the curves,  $\alpha$  is varied. DFFS(10) reaches a correct detection of 94% at a false alarm rate of 6%. this means that in 94% of all cases, where a left eye has been detected in the image, it was detected at the right location and in 6% of all cases, where a left eye has been detected in the image, it was detected at the wrong location



1-specificity

## Robustness

- A potential advantage of the eigenfeature layer is the ability to overcome the shortcomings of the standard eigenface method. A pure eigenface recognition system can be fooled by gross variations in the input image (hats, beards, etc.).
- The first row of the figure above shows additional testing views of 3 individuals in the above dataset of 45. These test images are indicative of the type of variations which can lead to false matches: a hand near the face, a painted face, and a beard.
- The second row in the figure above shows the nearest matches found based on a standard eigenface classification. Neither of the 3 matches correspond to the correct individual.
- On the other hand, the third row shows the nearest matches based on the eyes and nose features, and results in correct identification in each case. This simple example illustrates the advantage of a modular representation in disambiguating false eigenface matches.

### Novel Test Views



### Eigenface-based Matches



### Eigenfeature-based Matches



## PCA with Centered Data

- Sometimes the mean is subtracted first

$$\tilde{x}_{i,j} = x_{i,j} - m_j$$

where

$$m_j = \frac{1}{N} \sum_{i=1}^N x_{j,i}$$

- $\tilde{X}$  now contains the centered data
- Centering is recommended when data are approximately Gaussian distributed

## PCA with Centered Data (cont'd)

- Let

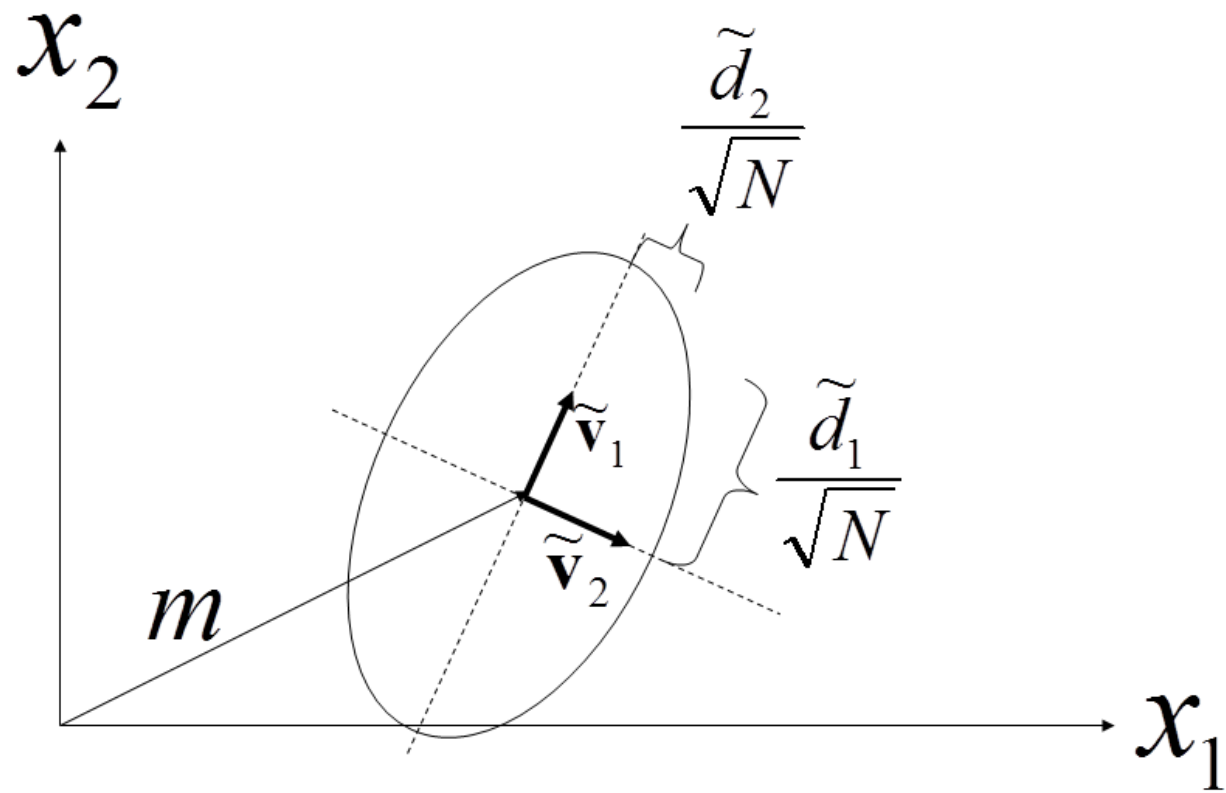
$$\hat{X} = \tilde{V}_r \tilde{V}_r^T X$$

then

$$\hat{\mathbf{x}}_i = \mathbf{m} + \sum_{l=1}^r \tilde{\mathbf{v}}_l \tilde{z}_{i,l}$$

with  $\mathbf{m} = (m_1, \dots, m_M)^T$

$$\tilde{z}_{i,l} = \tilde{\mathbf{v}}_l^T \hat{\mathbf{x}}_i$$



# PCA and Singular Value Decomposition



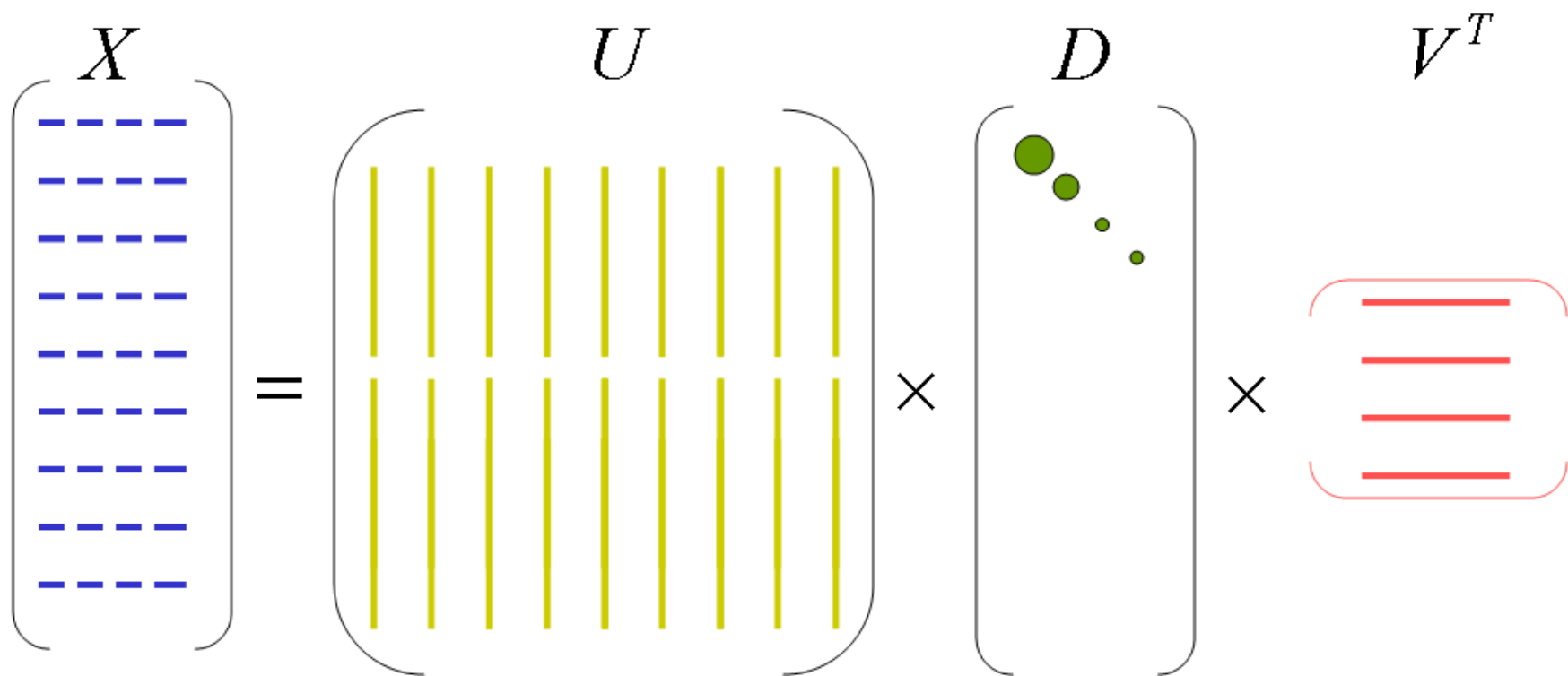
## Singular Value Decomposition (SVD)

- Any  $N \times M$  matrix  $X$  can be factored as

$$X = UDV^T$$

where  $U$  and  $V$  are both **orthonormal** matrices.  $U$  is an  $N \times N$  Matrix and  $V$  is an  $M \times M$  Matrix.

- $D$  is an  $N \times M$  **diagonal matrix** with diagonal entries (singular values)  $d_i \geq 0, i = 1, \dots, \tilde{r}$ , with  $\tilde{r} = \min(M, N)$
- The  $\mathbf{u}_j$  (columns of  $U$ ) are the left singular vectors
- The  $\mathbf{v}_j$  are the right singular vectors
- The  $d_j$  are the singular values

$$X = U D V^T$$


The diagram illustrates the Singular Value Decomposition (SVD) of a matrix  $X$ . On the left, matrix  $X$  is represented by a vertical column of ten horizontal blue dashed lines. This is followed by an equals sign. To the right of the equals sign is matrix  $U$ , shown as a vertical column of ten vertical yellow solid lines. This is followed by a multiplication sign  $\times$ . Next is matrix  $D$ , represented by a vertical column of four green circles of decreasing size, indicating singular values. This is followed by another multiplication sign  $\times$ . Finally, matrix  $V^T$  is shown as a vertical column of four horizontal red solid lines.

## Covariance Matrix and Kernel Matrix

- We get for the empirical covariance matrix

$$\Sigma = \frac{1}{N}X^T X = \frac{1}{N}VD^T U^T UDV^T = \frac{1}{N}VD^T DV^T = \frac{1}{N}VD_V V^T$$

- And for the empirical kernel matrix

$$K = \frac{1}{M}XX^T = \frac{1}{M}UDV^T VD^T U^T = \frac{1}{M}UDD^T U^T = \frac{1}{M}UD_U U^T$$

- With

$$\Sigma V = \frac{1}{N}VD_V \quad KU = \frac{1}{M}UD_U$$

one sees that the columns of  $V$  are the eigenvectors of  $\Sigma$  and the columns of  $U$  are the eigenvectors of  $K$ : The eigenvalues are the diagonal entries of  $D_V$ , respectively  $D_U$ .

- Apparent by now: The columns of  $V$  are both the principal vectors and the eigenvectors!

## More Expressions

- The SVD is

$$X = UDV^T$$

from which we get

$$X = UU^T X$$

$$X = XVV^T$$

## Reduced Rank

- In the SVD, the  $d_i$  are ordered:  $d_1 \geq d_2 \geq d_3 \dots \geq d_{\tilde{r}}$ . In many cases one can neglect  $d_i, i > r$  and one obtains a rank- $r$  Approximation. Let  $D_r$  be a diagonal matrix with the corresponding entries. Then we get the approximation

$$\hat{X} = U_r D_r V_r^T$$

$$\hat{X} = U_r U_r^T X$$

$$\hat{X} = X V_r V_r^T$$

where  $U_r$  contains the first  $r$  columns of  $U$ . Correspondingly,  $V_r$

## Best Approximation

- The approximation above is the best rank- $r$  approximation with respect to the squared error (Frobenius Norm). The approximation error is

$$\sum_{i=1}^N \sum_{j=1}^M (x_{j,i} - \hat{x}_{j,i})^2 = \sum_{j=r+1}^{\tilde{r}} d_j^2$$

## Factors for Rows and Columns

- Recall that in the netflix example on matrix factorization with  $X \approx AB^T$ , the rows of  $A$  contained the factors for the users and the rows of  $B$  contained the factors for the movies
- In the PCA, factors for entities associated with the columns are the rows of

$$T_r = X^T U_r$$

- With this definition,

$$\hat{X} = Z_r D_r^{-1} T_r^T$$

since

$$Z_r D_r^{-1} T_r^T = X V_r D_r^{-1} U_r^T X = U_r D V_r^T V_r D_r^{-1} U_r^T U_r D_r V_r^T = U_r D_r V_r^T$$



# LSA: Similarities Between Documents

## Feature Vectors for Documents

- Given a collection of  $N$  documents and  $M$  keywords
- $X$  is the *term-frequency* (tf) matrix;  $x_{i,j}$  indicates how often word  $j$  occurred in document  $i$ .
- Some classifiers use this representation as inputs
- On the other hand, two documents might discuss similar topics (are “semantically similar”) without using the same key words
- By doing a PCA we can find document representations as rows of  $Z_r = XV$  and term representations as rows of  $T = X^T U$
- This is known as *Latent Semantic Analysis* (LSA)

## Simple Example

- In total 9 sentences (documents):
  - 5 documents on human-computer interaction) (c1 - c5)
  - 4 texts on mathematical graph theory (m1 - m4)
- The 12 key words are in italic letters

Example of text data: Titles of Some Technical Memos

- c1: *Human machine interface for ABC computer applications*
- c2: *A survey of user opinion of computer system response time*
- c3: *The EPS user interface management system*
- c4: *System and human system engineering testing of EPS*
- c5: *Relation of user perceived response time to error measurement*
  
- m1: *The generation of random, binary, ordered trees*
- m2: *The intersection graph of paths in trees*
- m3: *Graph minors IV: Widths of trees and well-quasi-ordering*
- m4: *Graph minors: A survey*

## tf-Matrix and Word Correlations

- The tf-Matrix  $X$
- Based on the original data, the Pearson correlation between *human* and *user* is negative, although one would assume a large semantic correlation

$X^T$ 

	<b>c1</b>	<b>c2</b>	<b>c3</b>	<b>c4</b>	<b>c5</b>	<b>m1</b>	<b>m2</b>	<b>m3</b>	<b>m4</b>
<b>human</b>	1	0	0	1	0	0	0	0	0
<b>interface</b>	1	0	1	0	0	0	0	0	0
<b>computer</b>	1	1	0	0	0	0	0	0	0
<b>user</b>	0	1	1	0	1	0	0	0	0
<b>system</b>	0	1	1	2	0	0	0	0	0
<b>response</b>	0	1	0	0	1	0	0	0	0
<b>time</b>	0	1	0	0	1	0	0	0	0
<b>EPS</b>	0	0	1	1	0	0	0	0	0
<b>survey</b>	0	1	0	0	0	0	0	0	1
<b>trees</b>	0	0	0	0	0	1	1	1	0
<b>graph</b>	0	0	0	0	0	0	1	1	1
<b>minors</b>	0	0	0	0	0	0	0	1	1

$r(\text{human.user}) = -.38$       Pearson correlation between the words *human* and *user*

$r(\text{human.minors}) = -.29$       Pearson correlation between the words *human* and *minor*

## Singular Value Decomposition

- Decomposition  $X = UDV^T$

$$V =$$

0.22	-0.11	0.29	-0.41	-0.11	-0.34	0.52	-0.06	-0.41
0.20	-0.07	0.14	-0.55	0.28	0.50	-0.07	-0.01	-0.11
0.24	0.04	-0.16	-0.59	-0.11	-0.25	-0.30	0.06	0.49
0.40	0.06	-0.34	0.10	0.33	0.38	0.00	0.00	0.01
0.64	-0.17	0.36	0.33	-0.16	-0.21	-0.17	0.03	0.27
0.27	0.11	-0.43	0.07	0.08	-0.17	0.28	-0.02	-0.05
0.27	0.11	-0.43	0.07	0.08	-0.17	0.28	-0.02	-0.05
0.30	-0.14	0.33	0.19	0.11	0.27	0.03	-0.02	-0.17
0.21	0.27	-0.18	-0.03	-0.54	0.08	-0.47	-0.04	-0.58
0.01	0.49	0.23	0.03	0.59	-0.39	-0.29	0.25	-0.23
0.04	0.62	0.22	0.00	-0.07	0.11	0.16	-0.68	0.23
0.03	0.45	0.14	-0.01	-0.30	0.28	0.34	0.68	0.18

$$D =$$

3.34								
	2.54							
		2.35						
			1.64					
				1.50				
					1.31			
						0.85		
							0.56	
								0.36

$$X = UDV^T$$

$$U =$$

0.20	0.61	0.46	0.54	0.28	0.00	0.01	0.02	0.08
-0.06	0.17	-0.13	-0.23	0.11	0.19	0.44	0.62	0.53
0.11	-0.50	0.21	0.57	-0.51	0.10	0.19	0.25	0.08
-0.95	-0.03	0.04	0.27	0.15	0.02	0.02	0.01	-0.03
0.05	-0.21	0.38	-0.21	0.33	0.39	0.35	0.15	-0.60
-0.08	-0.26	0.72	-0.37	0.03	-0.30	-0.21	0.00	0.36
0.18	-0.43	-0.24	0.26	0.67	-0.34	-0.15	0.25	0.04
-0.01	0.05	0.01	-0.02	-0.06	0.45	-0.76	0.45	-0.07
-0.06	0.24	0.02	-0.08	-0.26	-0.62	0.02	0.52	-0.45



## Approximation with $r = 2$ and Word Correlations

- Reconstruction  $\hat{X}$  with  $r = 2$
- Shown is  $\hat{X}^T$
- Based on  $\hat{X}$  the correlation between *human* and *user* is almost one! The similarity between *human* and *minors* is strongly negative (as it should be)
- In document *m4*: “*Graph minors: a survey*” the word *survey* which is in the original document gets a smaller value than the term *trees*, which was not in the document originally

$\hat{X}^T$ 

	c1	c2	c3	c4	c5	m1	m2	m3	m4
human	0.16	0.40	0.38	0.47	0.18	-0.05	-0.12	-0.16	-0.09
interface	0.14	0.37	0.33	0.40	0.16	-0.03	-0.07	-0.10	-0.04
computer	0.15	0.51	0.36	0.41	0.24	0.02	0.06	0.09	0.12
user	0.26	0.84	0.61	0.70	0.39	0.03	0.08	0.12	0.19
system	0.45	1.23	1.05	1.27	0.56	-0.07	-0.15	-0.21	-0.05
response	0.16	0.58	0.38	0.42	0.28	0.06	0.13	0.19	0.22
time	0.16	0.58	0.38	0.42	0.28	0.06	0.13	0.19	0.22
EPS	0.22	0.55	0.51	0.63	0.24	-0.07	-0.14	-0.20	-0.11
survey	0.10	0.53	0.23	0.21	0.27	0.14	0.31	0.44	0.42
trees	-0.06	0.23	-0.14	-0.27	0.14	0.24	0.55	0.77	0.66
graph	-0.06	0.34	-0.15	-0.30	0.20	0.31	0.69	0.98	0.85
minors	-0.04	0.25	-0.10	-0.21	0.15	0.22	0.50	0.71	0.62

$r(\text{human.user}) = .94$

Pearson correlation between the words *human* and *user*

$r(\text{human.minors}) = -.83$

Pearson correlation between the words *human* and *minor*

## Document Correlations in the Original and the Reconstructed Data

- Top: document correlation in the original data  $X$ : The average correlation between documents in the  $c$ -class is almost zero
- Bottom: in  $\hat{X}$  there is a strong correlation between documents in the same class and strong negative correlation across document classes

Correlations between titles in raw data:

	c1	c2	c3	c4	c5	m1	m2	m3
c2	-0.19							
c3	0.00	0.00						
c4	0.00	0.00	0.47					
c5	-0.33	0.58	0.00	-0.31				
m1	-0.17	-0.30	-0.21	-0.16	-0.17			
m2	-0.26	-0.45	-0.32	-0.24	-0.26	0.67		
m3	-0.33	-0.58	-0.41	-0.31	-0.33	0.52	0.77	
m4	-0.33	-0.19	-0.41	-0.31	-0.33	-0.17	0.26	0.56

0.02  
-0.30 0.44

Average Pearson correlation in the three document blocks in the raw data

Correlations in two dimensional space:

c2	0.91							
c3	1.00	0.91						
c4	1.00	0.88	1.00					
c5	0.85	0.99	0.85	0.81				
m1	-0.85	-0.56	-0.85	-0.88	-0.45			
m2	-0.85	-0.56	-0.85	-0.88	-0.44	1.00		
m3	-0.85	-0.56	-0.85	-0.88	-0.44	1.00	1.00	
m4	-0.81	-0.50	-0.81	-0.84	-0.37	1.00	1.00	1.00

0.92  
-0.72 1.00

Average Pearson correlation in the three document blocks in the reconstructed data

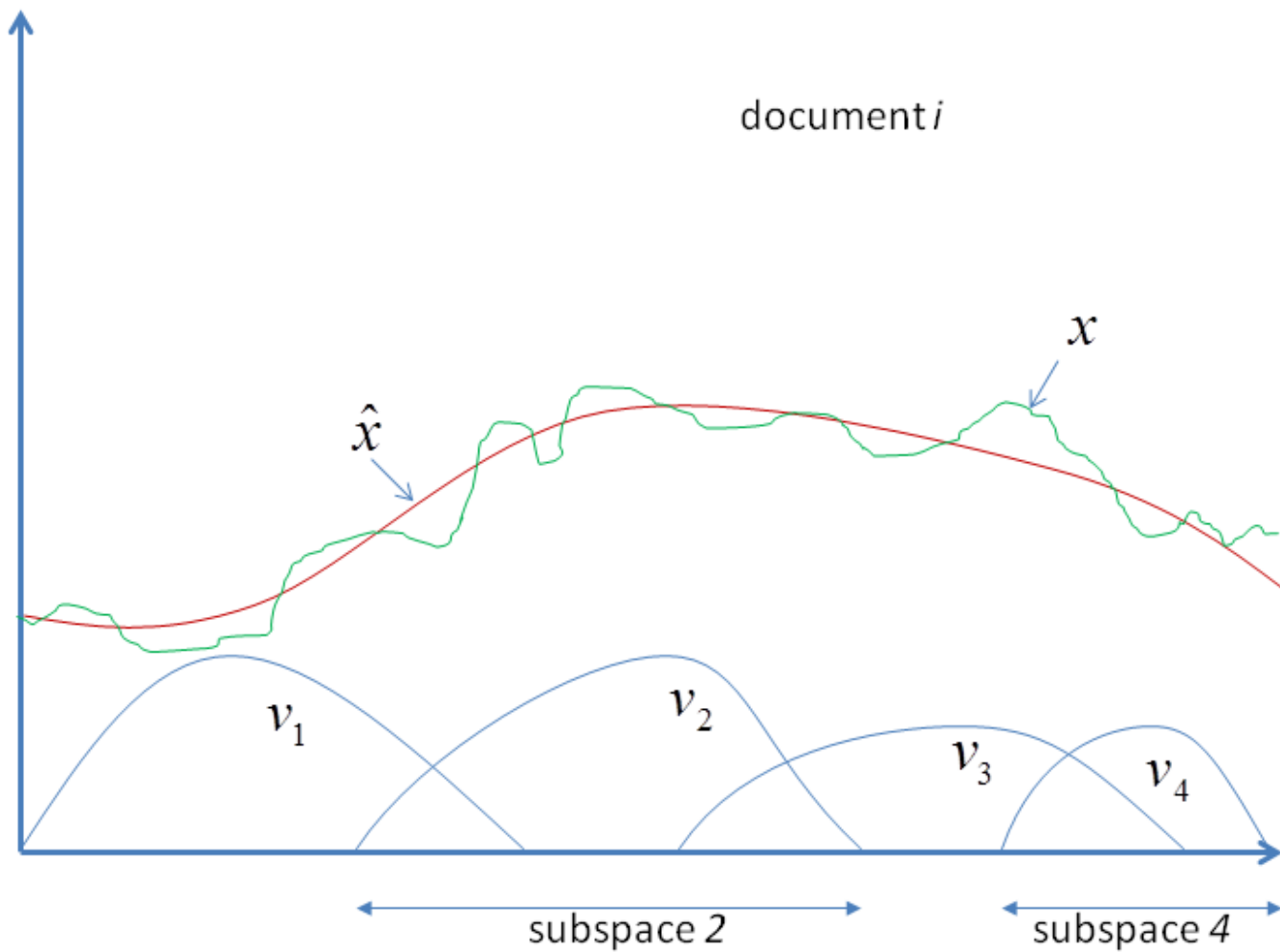
## Applications of LSA

- LSA-similarity often corresponds to the human perception of document or word similarity
- There are commercial applications in the evaluation of term papers
- There are indications that search engine providers like Google and Yahoo, use LSA for the ranking of pages and to filter out Spam (spam is unusual, novel)

## Illustration

- The next slides illustrate LSA, where the horizontal axis stands for the word index and the vertical axis stands for the word count
- If we consider word counts as functions of the index (functions as infinite-dimensional vectors) then the LSA (and the PCA) does function smoothing
- The columns of  $V$  would then define the basis functions (note that in the LSI the columns would be orthonormal, in contrast to the situation displayed in the plot)
- The columns of  $V$  define patterns
- If, as shown, the columns of  $V$  have limited support, they define different subspaces

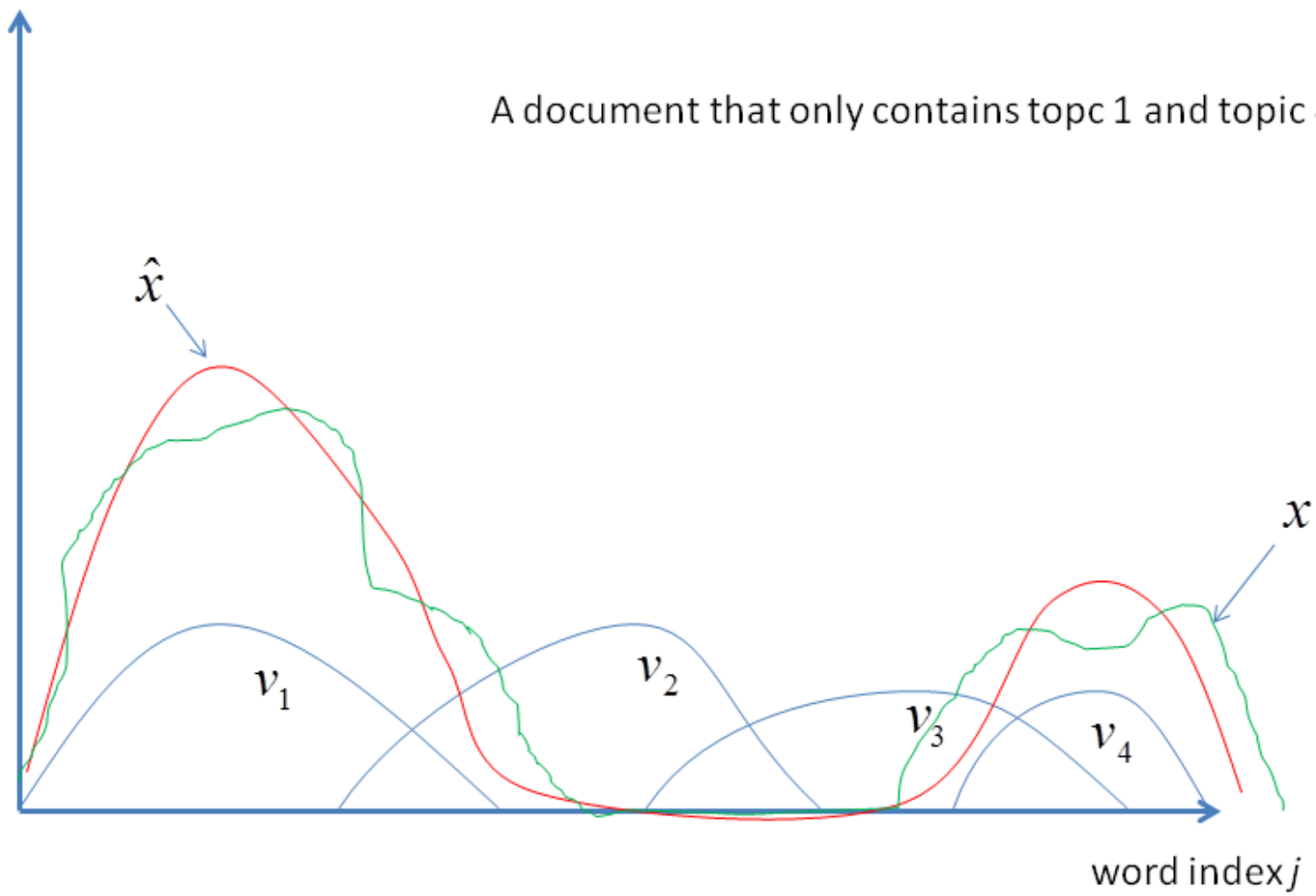
word counts  $x$



word index  $j$

word counts  $x$

A document that only contains topic 1 and topic 4





## Extensions

- Factorization approaches are part of many machine learning solutions
- An autoencoder, as used in deep learning, is closely related
- Factorization can be generalized to more dimensions:
- For example a 3-way array (tensor)  $\underline{X}$  with dimensions subject, predicate, object. The tensor has a one where the triple is known to exist and zero otherwise. Then we can approximate (PARAFAC)

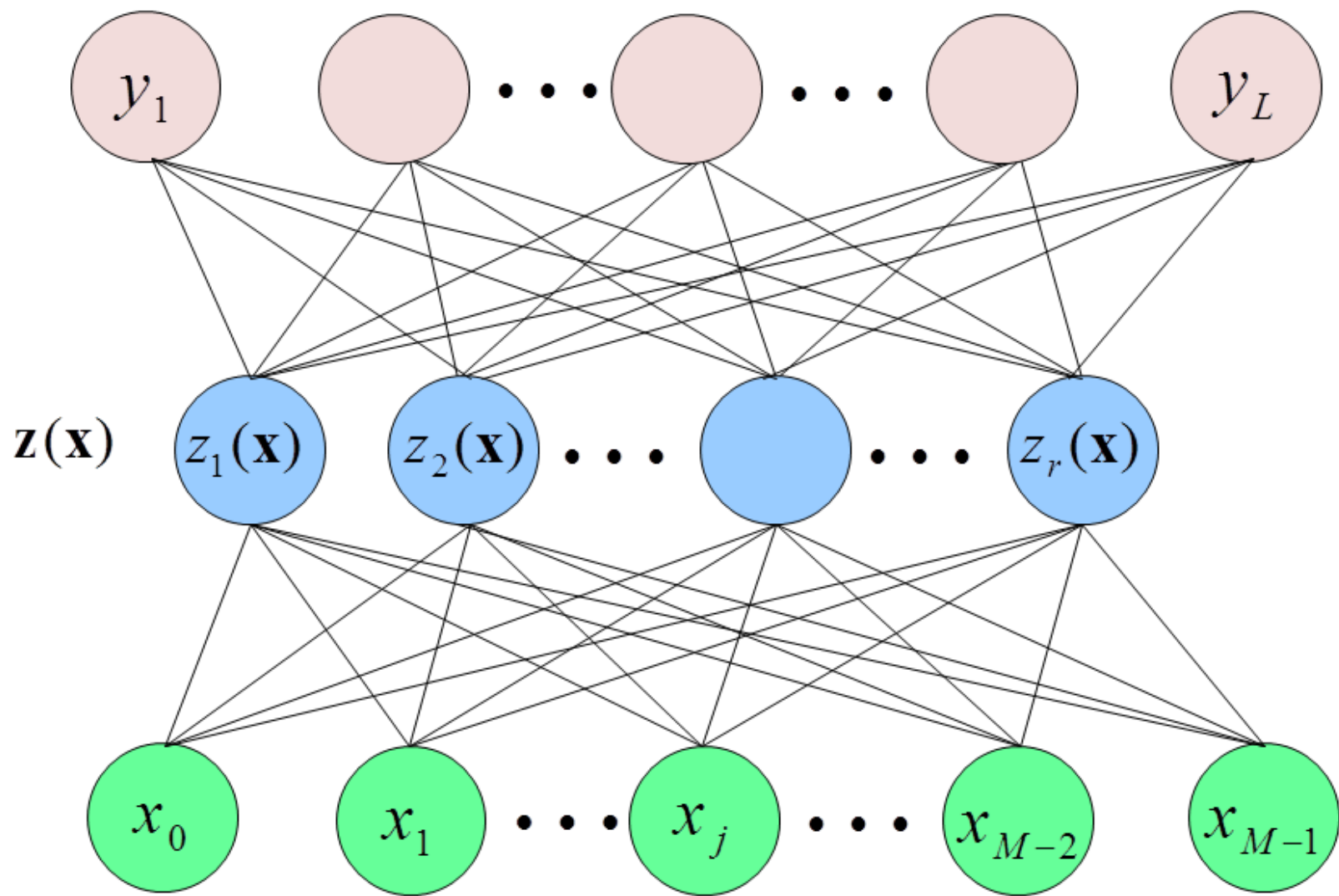
$$\hat{x}_{i,j,l} = \sum_{k=1}^r a_{i,k} b_{j,k} c_{l,k}$$

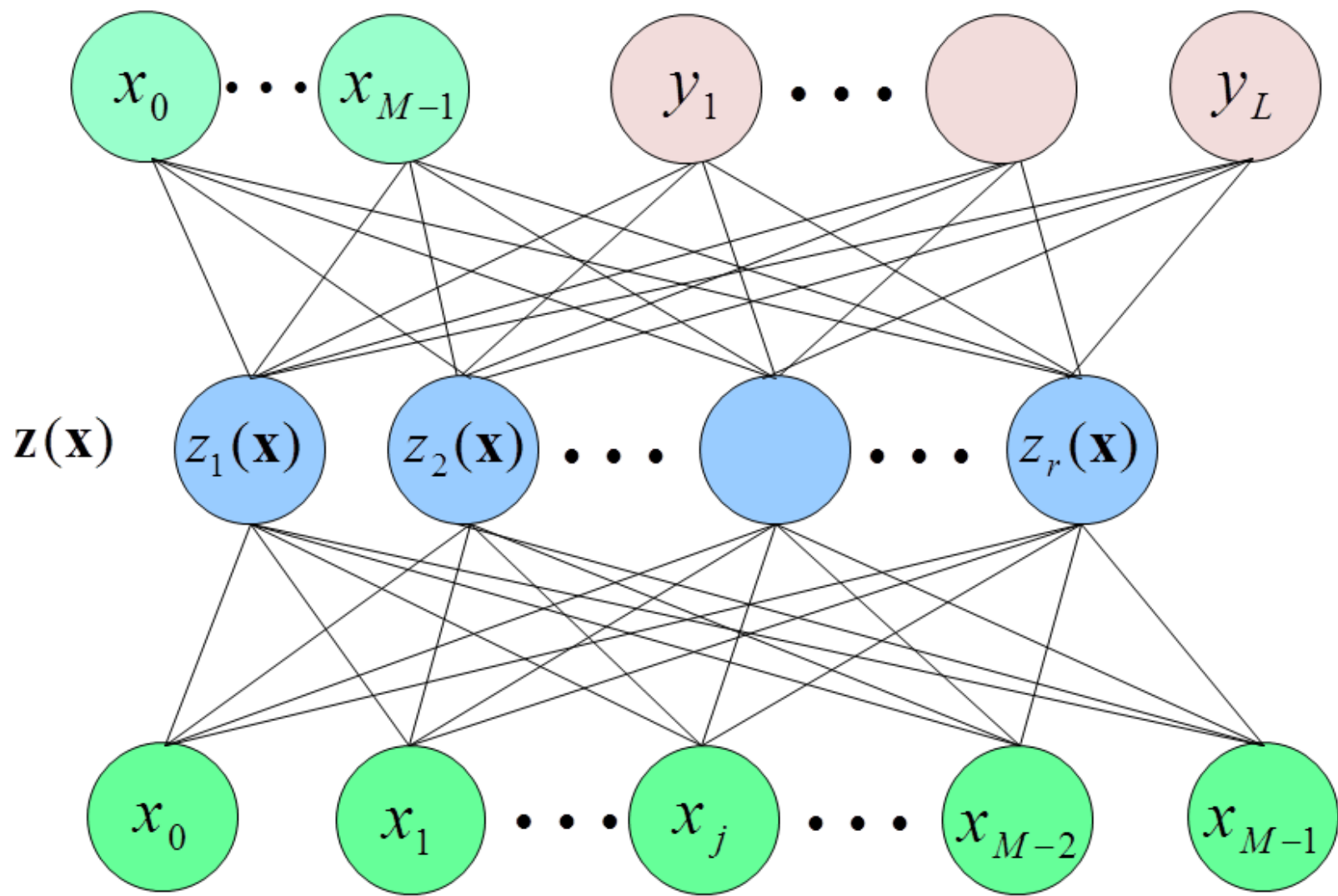
Here  $A$  contains the latent factors of the subject,  $B$  of the object, and  $C$  of the predicate

- If the entries of  $X$  are nonnegative (for example represent counts) it sometimes improves interpretability of the latent factors by enforcing that the factor matrices are nonnegative as well (nonnegative matrix factorization (NMF), probabilistic LSA (pLSA), latent Dirichlet allocation (LDA))

## Extensions: Improving Multivariate Linear Regression

- Consider that we have several input dimensions and several output dimensions
- It makes sense to maintain that the latent factors should be calculated from just the input representation but that this mapping itself should be derived by also including the training outputs
- The next two slides show some possible architectures
- In classical analysis this is done via partial least squares (pLS) or via a canonical correlation analysis (CCA)



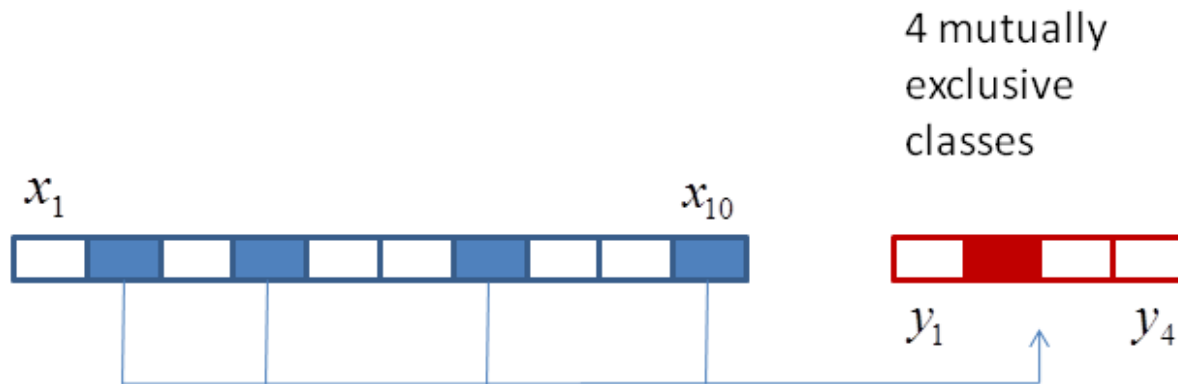


## Relationships to Clustering and Classification

- In **multiclass classification** an object is assigned to one out of several classes. In the ground truth the object belongs to exactly one class. The classifier might only look at a subset of the inputs
- Clustering is identical to classification, only that the class labels are unknown in the training data
- In **multi-label classification** an object can be assigned to several classes. This means that also in the ground truth the object can belong to more than one class. Each class might only look at an individual subset of the inputs. Let  $\mathcal{I}_k$  be the set of inputs affiliated with class  $k$
- Factor analysis and topic models are related to multi-label classification where the class labels (latent factors) are unknown in the training set (this interpretation works best with non-negative approaches like NMF, pLSI, LDA)
- This also leads to interpretable similarity. Consider a term-document matrix

- Two documents  $i$  and  $i'$  are semantically similar if their topic profiles are similar, i.e.  $\mathbf{z}_i \approx \mathbf{z}_{i'}$
- Two terms  $j$  and  $j'$  are semantically similar if they appear in the same sets  $\mathcal{I}_k$ , i.e., if their input set profiles are similar (since  $T_r = X^T U_r = V_r D_r$ ) (again, this interpretation works best with non-negative approaches like NMF, pLSI, LDA)
- Related in data mining: subspace clustering and frequent item set mining (the input set profiles  $\mathcal{I}_k$  are the frequent item sets)

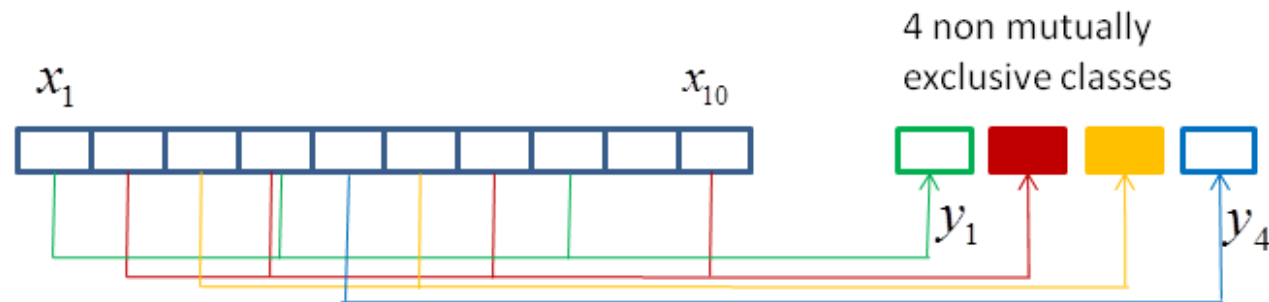
# Multiclass classification / Clustering



Only the four dark blue inputs are found to be important for the classification decision

- Classification: targets ( $y$ ) are known during training
- Clustering: targets ( $y$ ) are unknown during training

## Multi-label (multi-output) Classification / Factor Analysis



- In a factor analysis the  $y$  are the factors and the relevant inputs are the one where the principal vectors are not close to zero
- Thus, each class  $k$  might be sensitive to other input sets  $I_k$
- Examples:
  - Each data point is a document, each factor represents a topic (sports, politics, ...), a document might cover several topics and the topic-specific inputs  $I_k$  are keywords relevant for classifying a topic
  - Each data point is a customer, each factor represents a buying pattern (party, baby at home, single, ...), a customer might cover several buying patterns and the buying-pattern specific inputs  $I_k$  are items relevant for classifying a buying pattern (beer, pretzels) , (diapers, baby food)
- Multi-label classification: targets ( $y$ ) are known during training
- Factor analysis: targets ( $y$ ) are unknown during training



