Pattern Recognition

(EE5907R)

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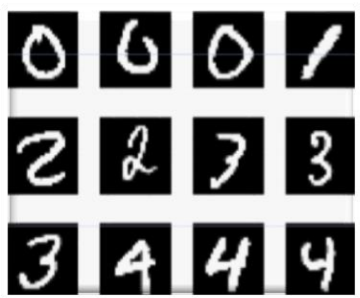
What people think about Pattern Recognition

From “Fantastic Four (2015)” movie

What we are doing with Pattern Recognition



Binary valued data

Color images

Raw Data

⇩

Informative Pattern Representation

⇩

PR Model Design & Learning

⇩

Recognition on New Data

"3" or "8" …

"A man riding a bicycle"

An Example of Pattern Recognition

- What kind of research we can do with facial images?

Image source: http://www.uni-regensburg.de/Fakultaeten/phil_Fak_II/Psychologie/Psy_II/beautycheck/english/durchschnittsgesichter/durchschnittsgesichter.htm

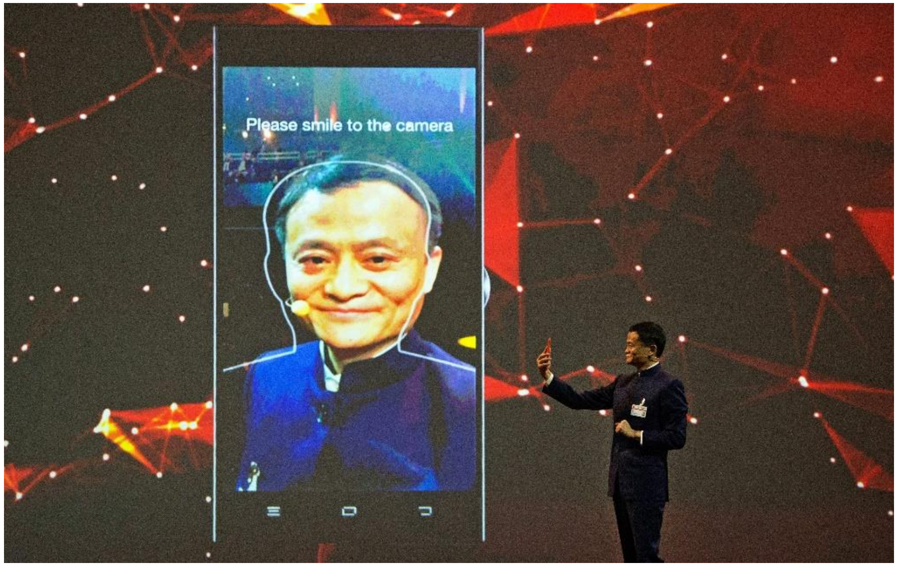
Cross-Age Face Recognition

Kinship or NOT?

Positive (left) and negative (right) examples

Eye? Hair? Mouth?

Face Recognition as Login Password



Textbooks and References

(no fixed textbook)

- Books
  - R. O. Duda, P. E. Hart & D.G. Stork,
    "**Pattern Classification**",
    John Wiley, 2001.
  - K. P. Murphy,
    “**Machine Learning: A Probabilistic Perspective**",
    MIT Press, 2012.
- References
  - Lists of important papers will be provided with some lectures

Outlines

- Representation Learning
  - Unsupervised Feature Learning (PCA, NMF)
  - Supervised Feature Learning (LDA, GE)
  - Clustering and Applications
- Patter Recognition Methods
  - Gaussian Mixture Model and Boosting
  - Support Vector Machines
  - Deep Learning

Outlines

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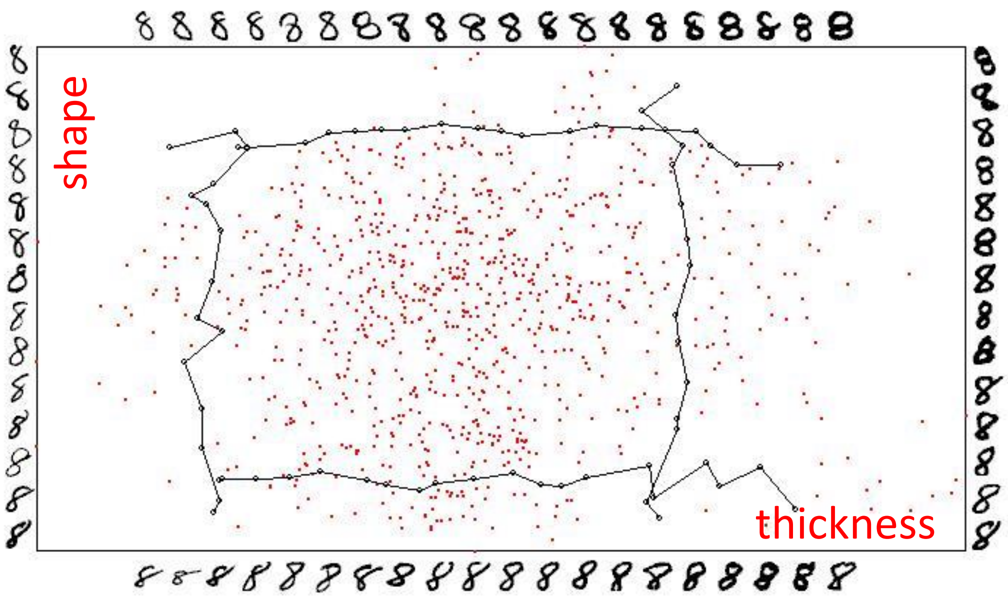
Unsupervised Feature Learning I:

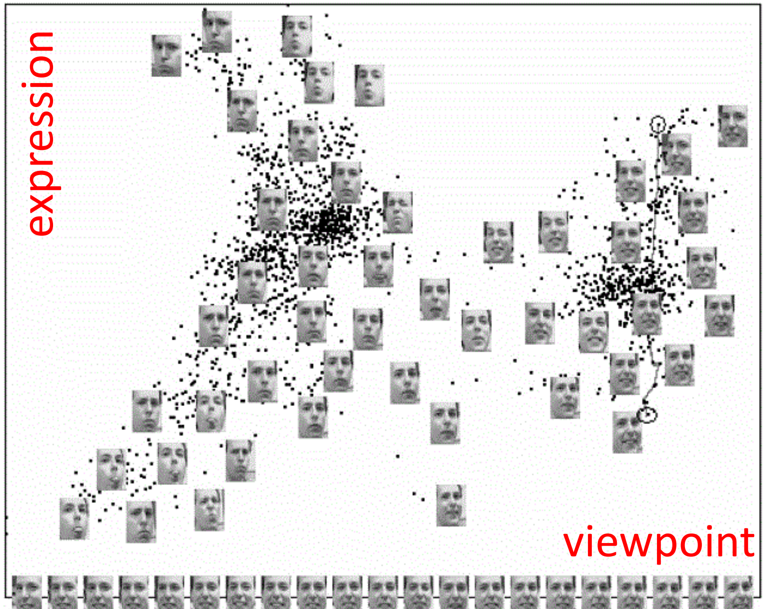
Principal Component Analysis

What is Feature Learning

- Feature learning refers to mapping the raw data into another (possibly lower-dimensional) space.
- Such that, in the new space, one can perform pattern recognition more easily.
- Criterion for feature learning is different in different problem settings.
  - *Unsupervised*: minimize information loss (no class information)
  - *Supervised*: maximize discrimination (with class information)

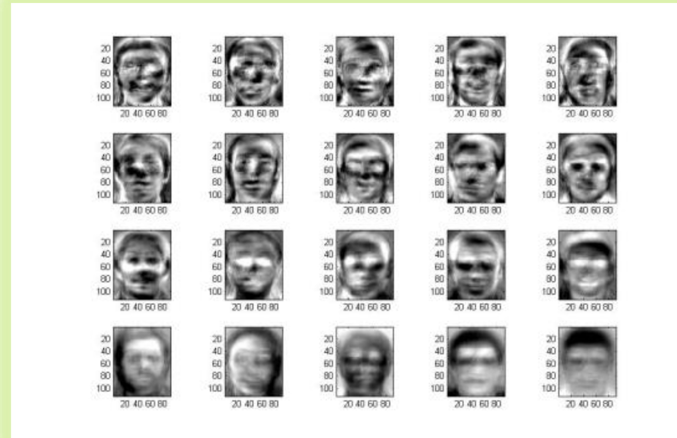
What is Feature Learning

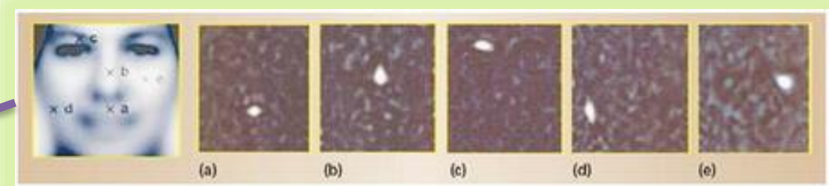




Feature Extraction vs. Feature Selection

- Feature Extraction
  - All original features are used
  - The transformed features are linear combinations of the original features.



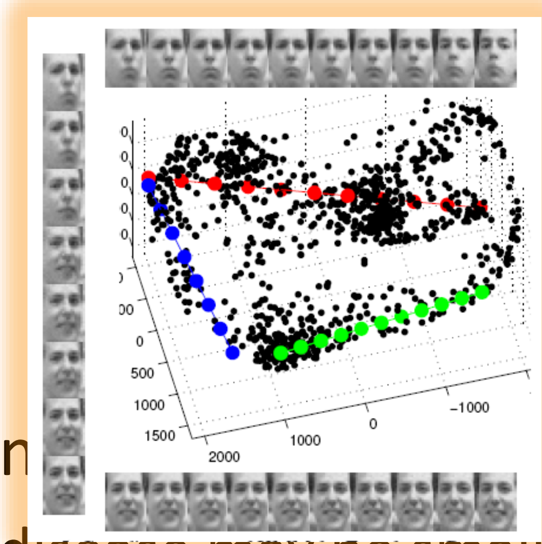


- Feature Selection
  - Only a subset of the original features are used.

Why need feature selection?

Why Feature Extraction?

- Many pattern recognition techniques may not be effective for high-dimensional data
  - Curse of Dimensionality
  - Computational cost increases rapidly along with the dimension increases



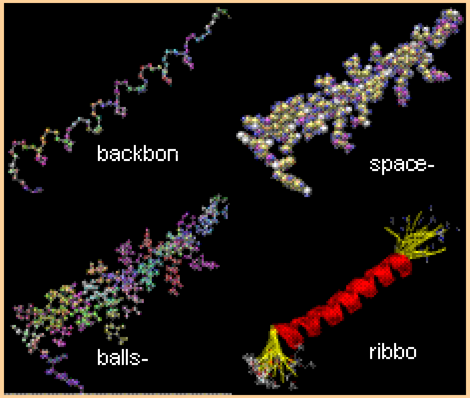
- Patterns may have small intrinsic din
  - E.g., # genes responsible for a certain disease may be small
  - E.g., face images of one person captured with different illumination conditions

Why Feature Extraction?

- Visualization: projecting high-dimensional data onto 2D or 3D planes
- Data compression: efficient storage and retrieval
- Noise removal: positive effect on testing accuracy

Applications of Feature Learning

- Face recognition
- Handwritten digit recog.
- Text mining
- Image retrieval
- Protein classification



Proteins

Face Images

Feature Extraction Algorithms

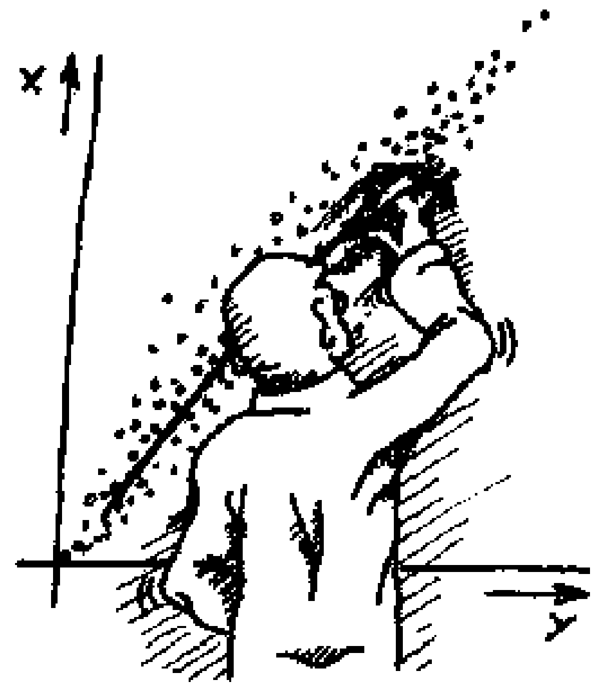
- Unsupervised
  - Principal Component Analysis (PCA)
  - Nonnegative Matrix Factorization (NMF)
  - Independent Component Analysis (ICA) [Reading]

- Supervised
  - Linear Discriminant Analysis (LDA)
  - General Graph Embedding (GE)
  - Canonical Correlation Analysis (CCA) [Reading, encouraged]

- Semi-supervised
  - Research topic [Further study, encouraged]

Principal Component Analysis

- Probably the most widely-used and well-known multivariate analysis method.
- Introduced by Pearson (1901)
- First applied in ecology by Goodall (1954) under the name "factor analysis".



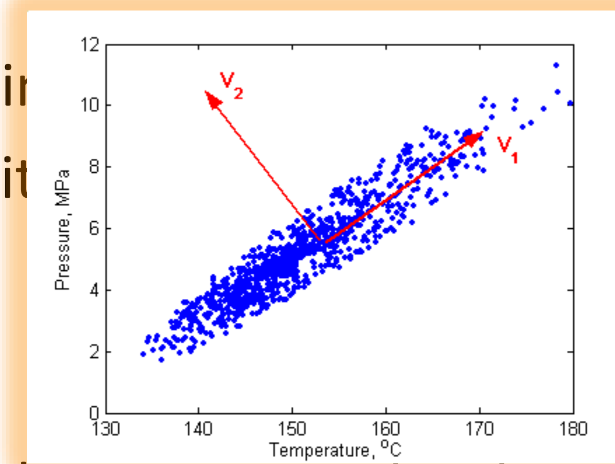
Least Square Fitting to Data

Pearson, K. (1901). "On Lines and Planes of Closest Fit to Systems of Points in Space" Philosophical Magazine **2** (11): 559–572.

What is Principal Component Analysis?

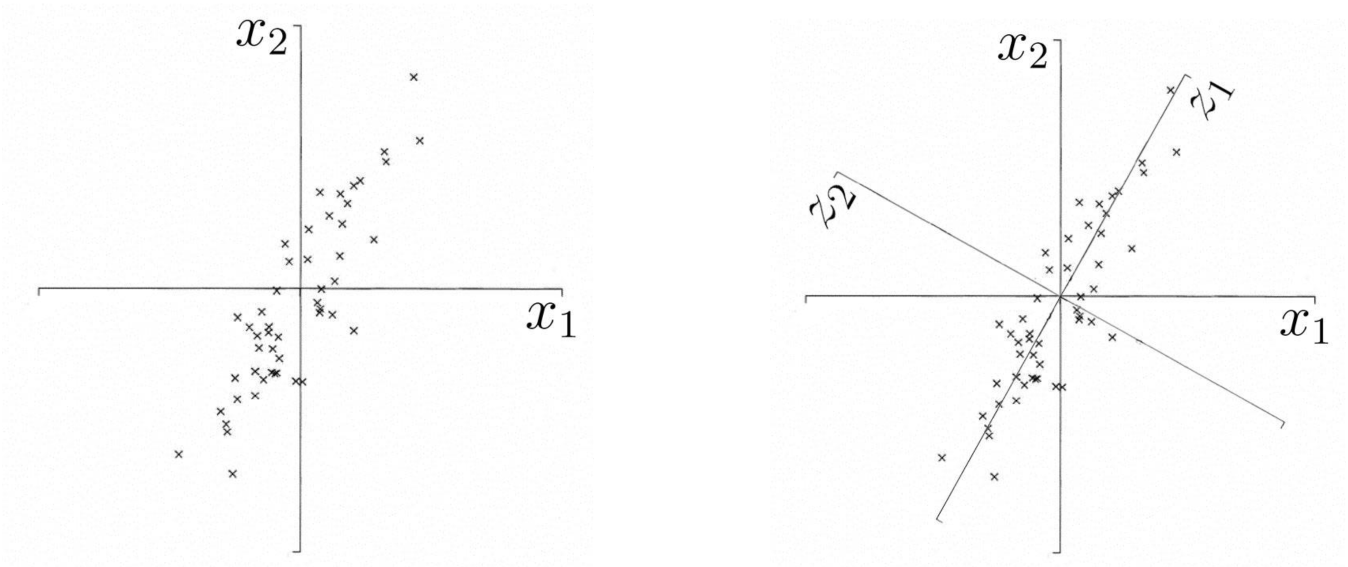
- Principal component analysis (PCA)
  - Reduce the dimensionality of a collection of observations by finding a new set of variables, smaller than the original set of variables
  - Capture big (principal) variability i

    the data and ignore small variabilit



- Variation in samples
  - The new variables, called principal components (PCs), are ordered by variations corresponding to different PCs.

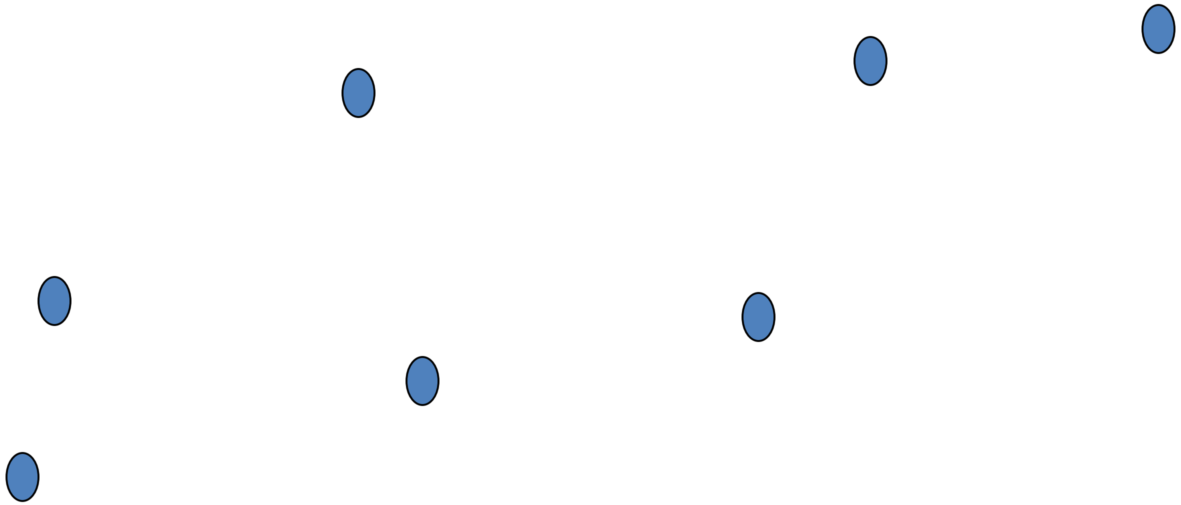
Geometric Picture of Principal Components



- The 1[st] PC Z_1 is a minimum distance fit to a line in X space
- The 2[nd] PC Z_2 is a minimum distance fit to a line in the plane orthogonal to the 1[st] PC

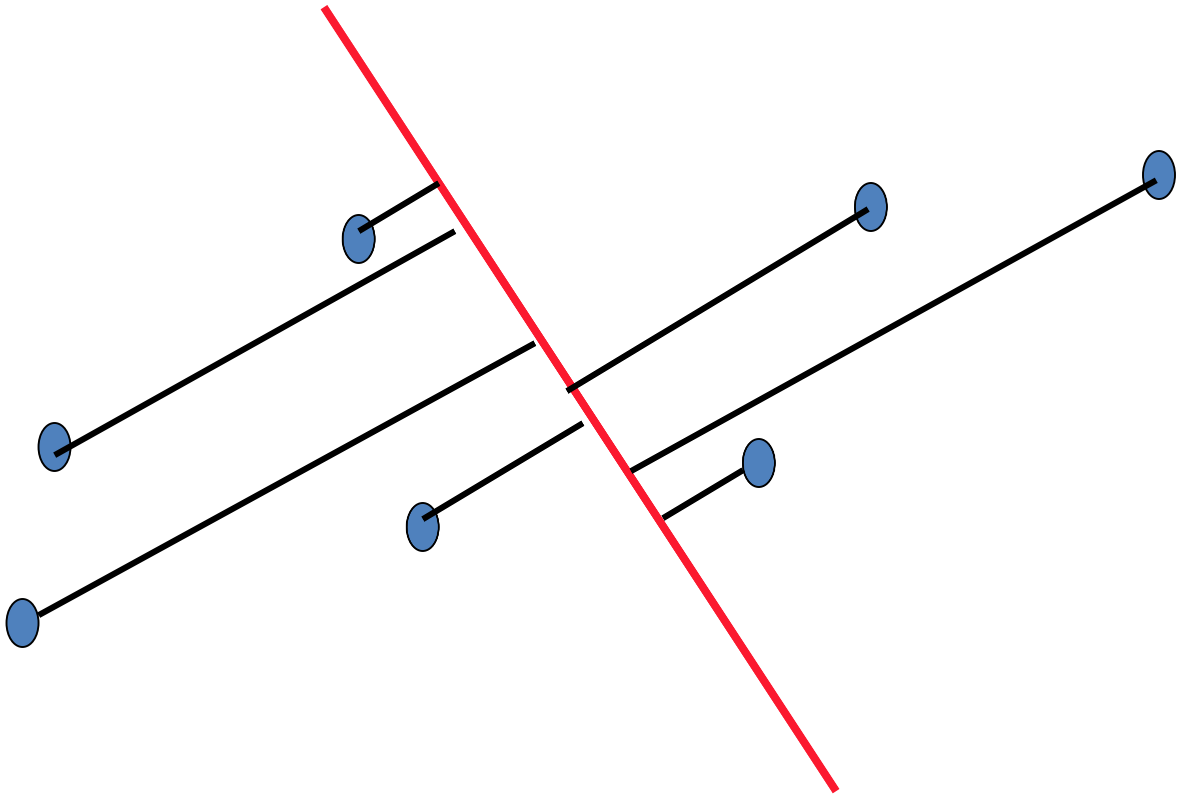
PCs are a series of linear least squares fits to a sample set, each orthogonal to all the previous ones.

Geometric Picture of Principal Components



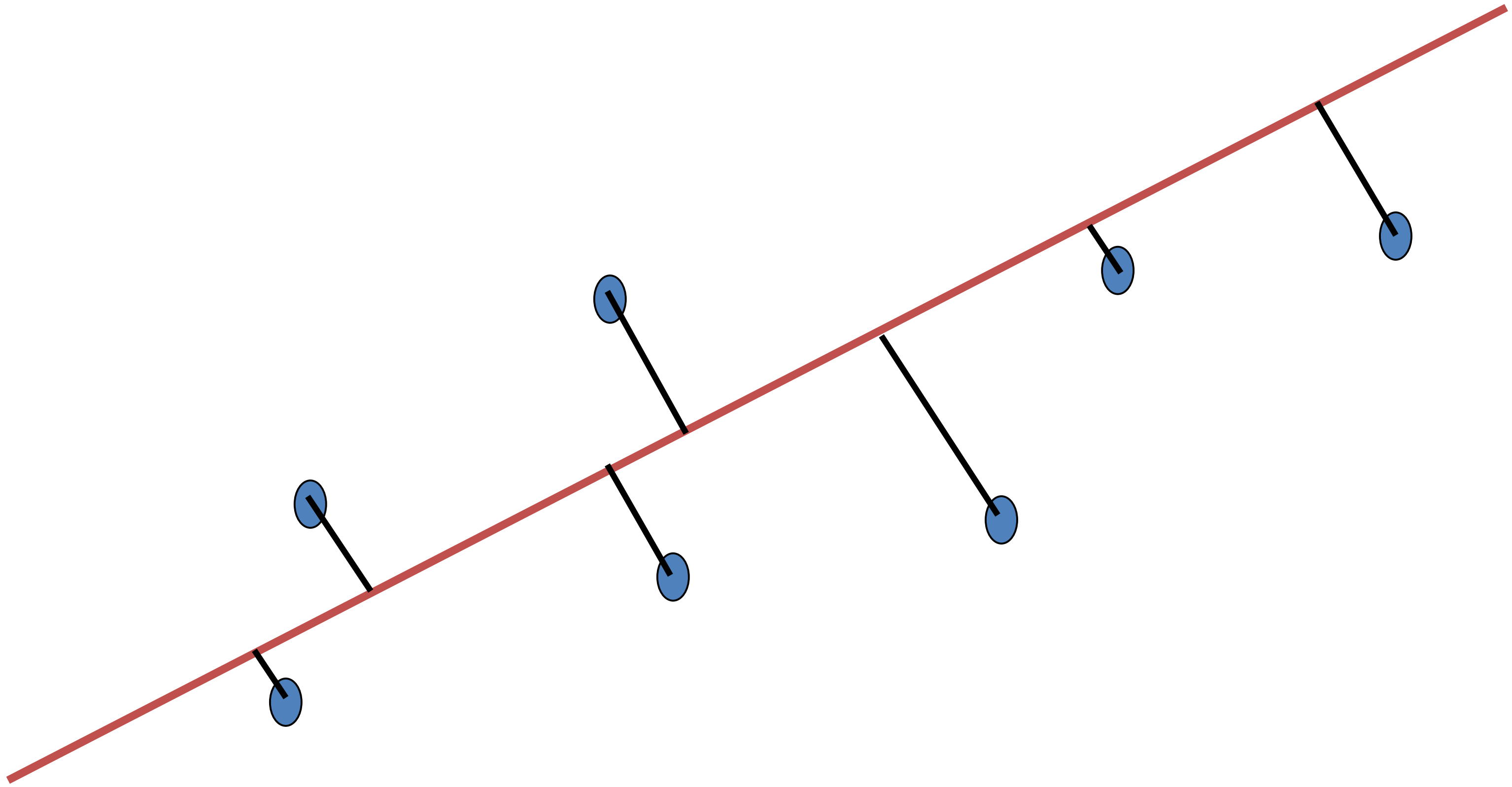
Sample Points

Geometric Picture of Principal Components



linear least squares fit: Large

Geometric Picture of Principal Components



linear least squares fit: Small

Algebraic Definition of PCs

Given a sample set of n observations on a vector of d variables

$$\{x_1, x_2, \cdots, x_n\} \subset \Re^d$$

define the first principal component by the linear projection a_1

$$z_1 = a_1^T x$$

where the vector $a_1 = (a_{11}, a_{21}, \cdots, a_{d1})^T$

is chosen such that $\mathrm{var}[z_1]$ is maximum.

Algebraic Definition of PCs

To find a_1 first note that

$$\text{var}[z_1] = E((z_1 - \bar{z}_1)^2) = \frac{1}{n}\sum_{i=1}^{n}\left(a_1^T x_i - a_1^T \bar{x}\right)^2$$

$$= \frac{1}{n}\sum_{i=1}^{n} a_1^T \left(x_i - \bar{x}\right)\left(x_i - \bar{x}\right)^T a_1 = a_1^T S a_1$$

where $S = \frac{1}{n}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)\left(x_i - \bar{x}\right)^T$

What is S?

is the covariance matrix,

$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ is the mean.

Algebraic Derivation of PCs

To find a_1 that maximizes $\mathrm{var}[z_1]$ subject to $a_1^T a_1 = 1$

Let λ be a Lagrange multiplier

$$L = a_1^T S a_1 - \lambda(a_1^T a_1 - 1)$$

$$\Rightarrow \frac{\partial}{\partial a_1} L = S a_1 - \lambda a_1 = 0$$

$$\Rightarrow (S - \lambda I_d) a_1 = 0$$

therefore a_1 is an eigenvector of S

corresponding to the largest eigenvalue $\lambda = \lambda_1$.

Algebraic Derivation of PCs

Similarly, a_2 is also an eigenvector of S

whose eigenvalue $\lambda = \lambda_2$ is the second largest.

In general

$$\text{var}[z_k] = a_k^T S a_k = \lambda_k$$

- The k^{th} largest eigenvalue of S is the variance of the k^{th} PC.
- The k^{th} PC z_k retains the k^{th} greatest variation in the samples

Algebraic Derivation of PCs

- Main steps for computing PCs
  - Calculate the covariance matrix S.
  - Compute its eigenvectors: $\{a_i\}_{i=1}^{d}$
  - The first p eigenvectors $\{a_i\}_{i=1}^{p}$ form the p PCs.
  - The transformation matrix G consists of the p PCs:

$$G \leftarrow [a_1, a_2, \cdots, a_p]$$

$$y = G^T x$$

Practical Computation of PCA

- In practice, we compute the PCs via singular value decomposition (SVD) on the centered data matrix.

- Form the centered data matrix:

$$X_{d,n} = \left[(x_1 - \bar{x}) \ldots\ldots (x_n - \bar{x}) \right]$$

- Compute its SVD:

$$X = U_{d,d} D_{d,n} (V_{n,n})^T$$

- U and V are orthogonal matrices, D is a diagonal matrix

Practical Computation of PCA

- Note that the scatter/covariance matrix can be written as:

$$S = XX^T = UD^2U^T$$

- So the eigenvectors of S are the columns of U and the eigenvalues are the diagonal elements of D^2

- Take only a few significant eigenvalue-eigenvector pairs p << d. The new reconstructed sample from low-dim space is:

$$\widehat{x}_i = \overline{x} + U_{d,p}(U_{d,p})^T(x_i - \overline{x})$$

PCA and Classification

- Classification with PCA
  - Project both training and testing data into the PCs space
  - For each testing datum, use NN for classification
  - Issue: accuracy is sensitive to the number of PCs

How to determine the number of PCs?

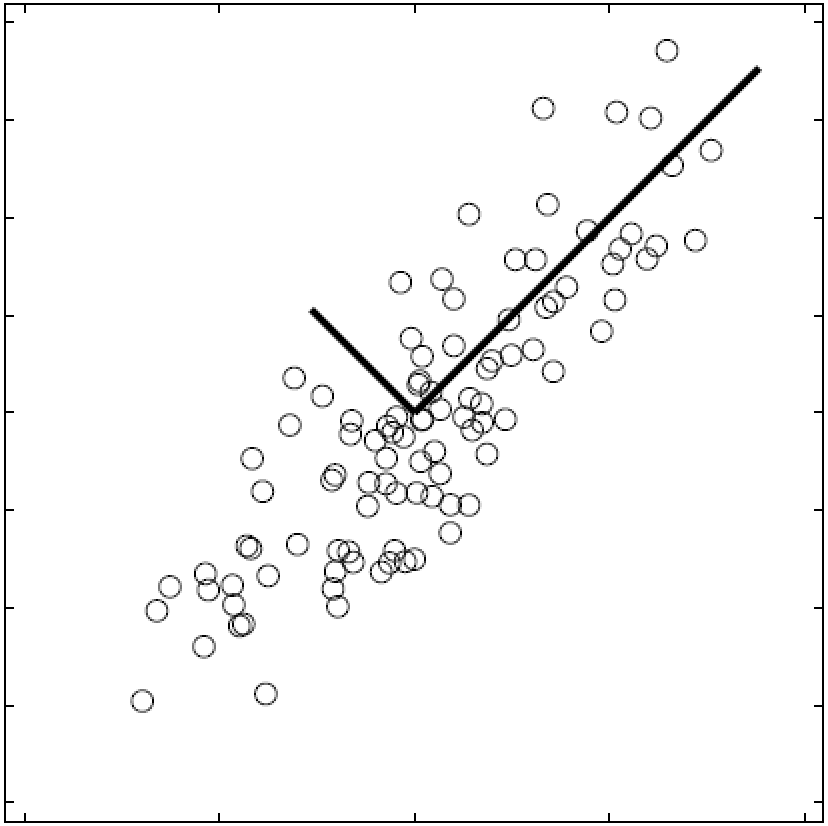
- PCA is not always an optimal feature extraction procedure for classification purpose
  - Suppose there are C classes in the training data
  - PCA is based on the sample covariance which characterizes the scatter of the entire data set, irrespective of class-membership
  - The projection axes chosen by PCA might not provide good discrimination power

How many principal components to keep?

- To choose *p* based on percentage of variation to retain, we can use the following criterion (smallest *p*):

$$\frac{\sum_{i=1}^{p} \lambda_i}{\sum_{i=1}^{d} \lambda_i} \geq Threshold\ (e.g., 0.95)$$

Visualize PCs



Data points are represented in a rotated orthogonal coordinate system: the origin is the mean of the data points and the axes are provided by the eigenvectors.

Visualize PCs

Face images

Eigenfaces, how to plot like this?

Reconstruction with PCs

Adding eigenfaces one at a time

Adding eigenfaces eight at a time

$$\widehat{x}_i = \bar{x} + U_{d,p}(U_{d,p})^T(x_i - \bar{x})$$

What shall happen for Other Objects

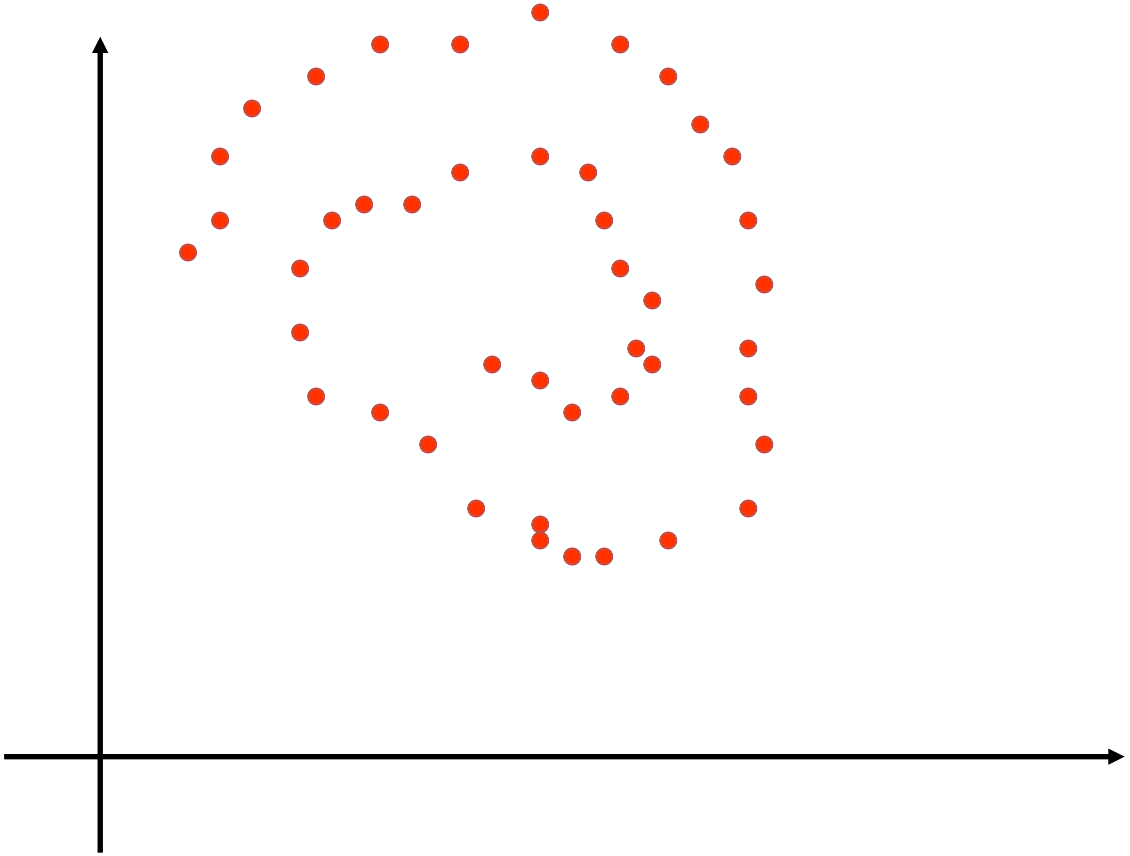
- For faces of person not in training set or non-faces (upper), what shall the reconstruction results (bottom) be?

PCA Remarks

- PCA
  - finds orthonormal basis for data
  - Sorts dimensions in order of “importance”
  - Discard low significance dimensions

- Uses:
  - Get compact description
  - Ignore noise
  - Improve classification (hopefully)

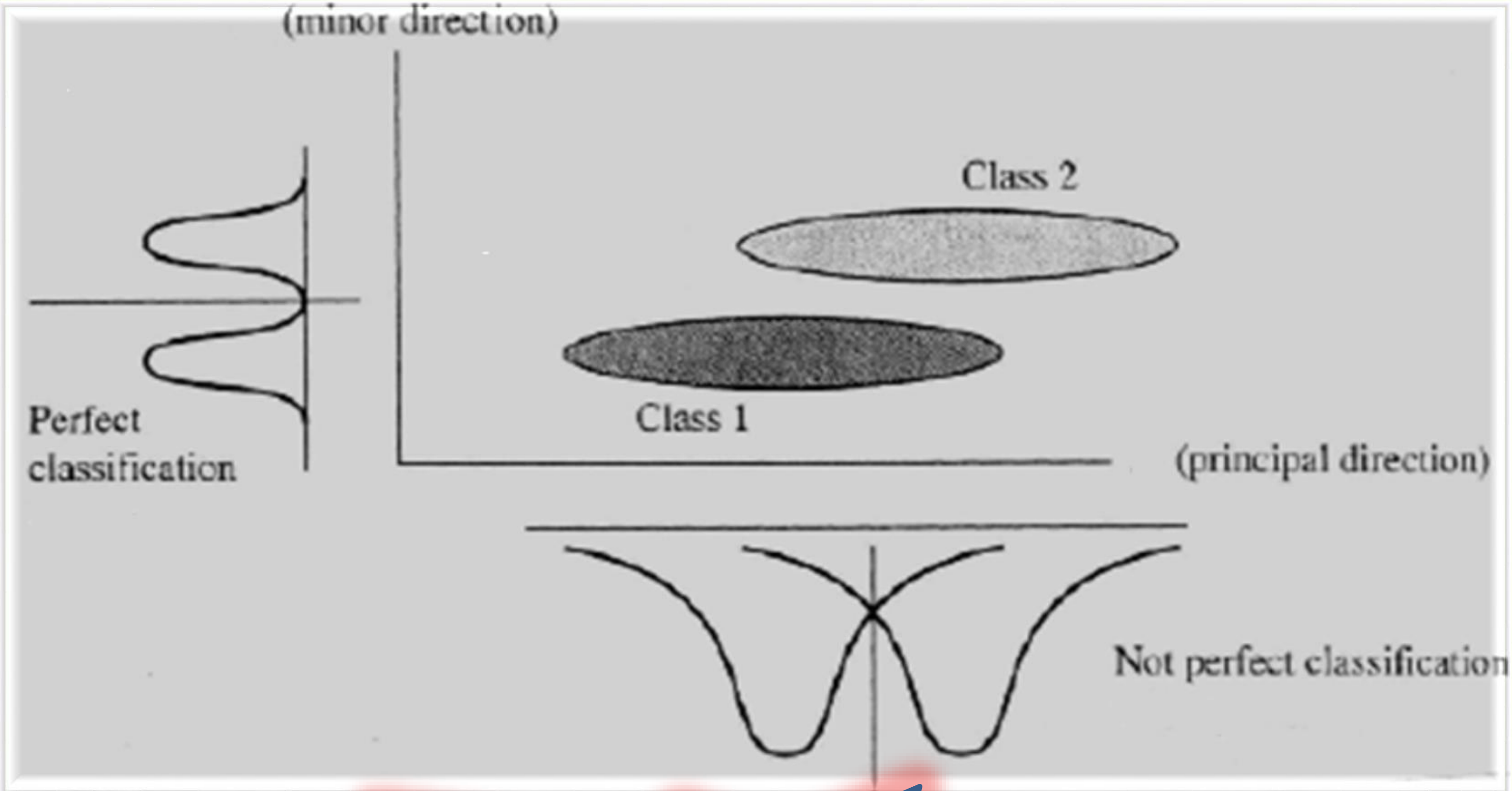
PCA Remarks



PCA cannot capture NON-LINEAR structure!

Note: Curvilinear Component Analysis can solve this case. Study this work if you are interested.

PCA doesn't know class labels



So LDA next week!

Summary of PCA

Algorithm 1 Algorithm for PCA

Input: Samples $\{x_1, x_2, \cdots, x_N\}$.

1. Compute the covariance matrix:
   $S = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$;
2. Perform Eigenvalue Decomposition: $[U] = \mathrm{eig}(S)$;
3. Output PCs matrix $U(:, 1 : p)$.

Discussions

- What can we do with PCA (given that it is generally worse for classification than other supervised algorithms)?

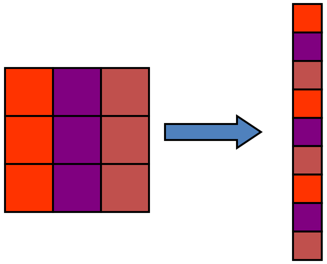
Unsupervised Feature Extraction II: Nonnegative Matrix Factorization

A Quick Review of Linear Algebra

- Every vector can be expressed as the linear combination of basis vectors

$$\begin{bmatrix} 2 \\ 6 \end{bmatrix} = 2 \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 6 \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} \text{ or } \begin{bmatrix} 2 \\ 6 \end{bmatrix} = 2 \cdot \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 0 \cdot \begin{bmatrix} -6 \\ 2 \end{bmatrix}$$

- Can think of images as big vectors

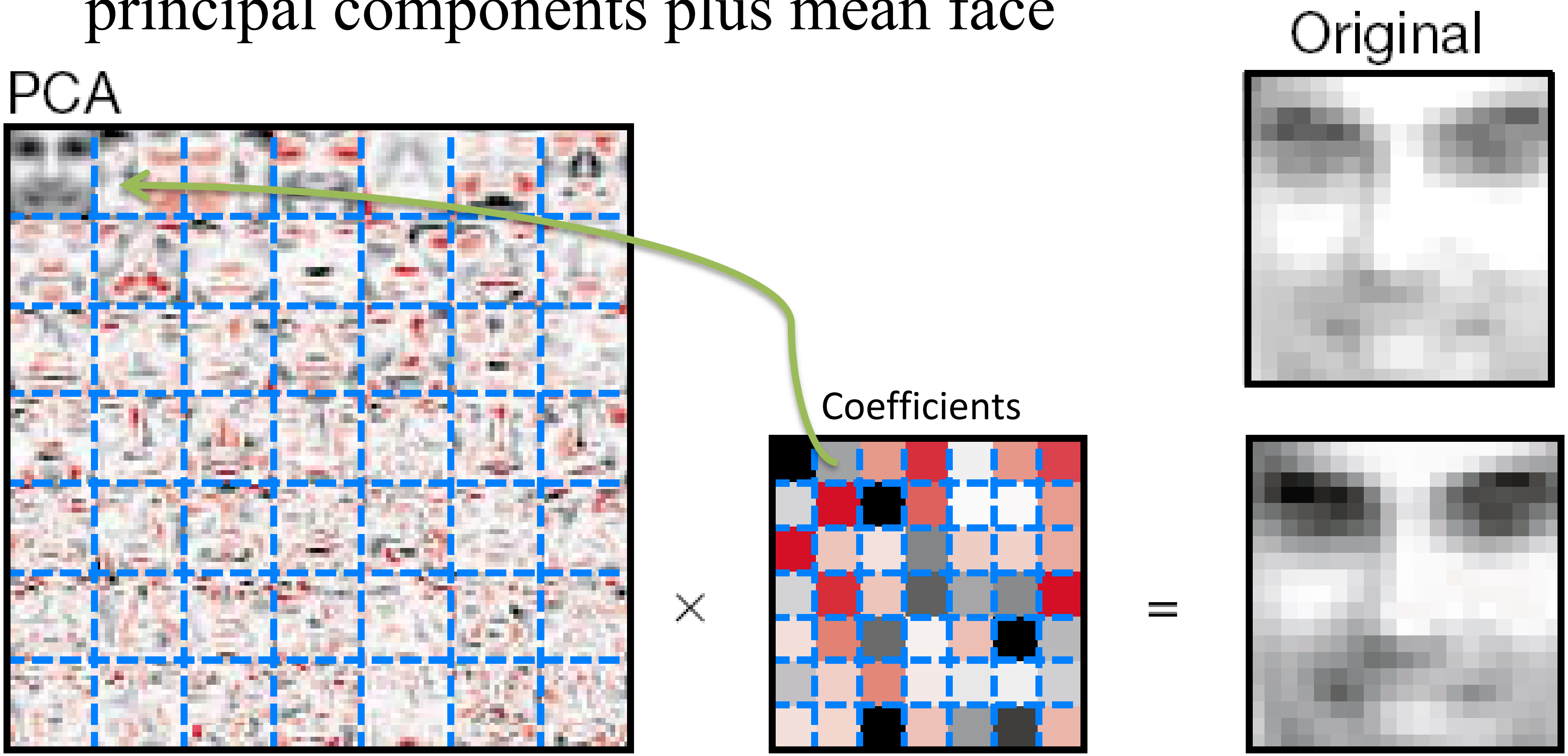


(Raster scan image into vector)

- This means we can express an image as the linear combination of a set of basis images

PCA Review

- Find a set of orthogonal principal components (basis)
- The reconstructed image is a linear combination of the principal components plus mean face

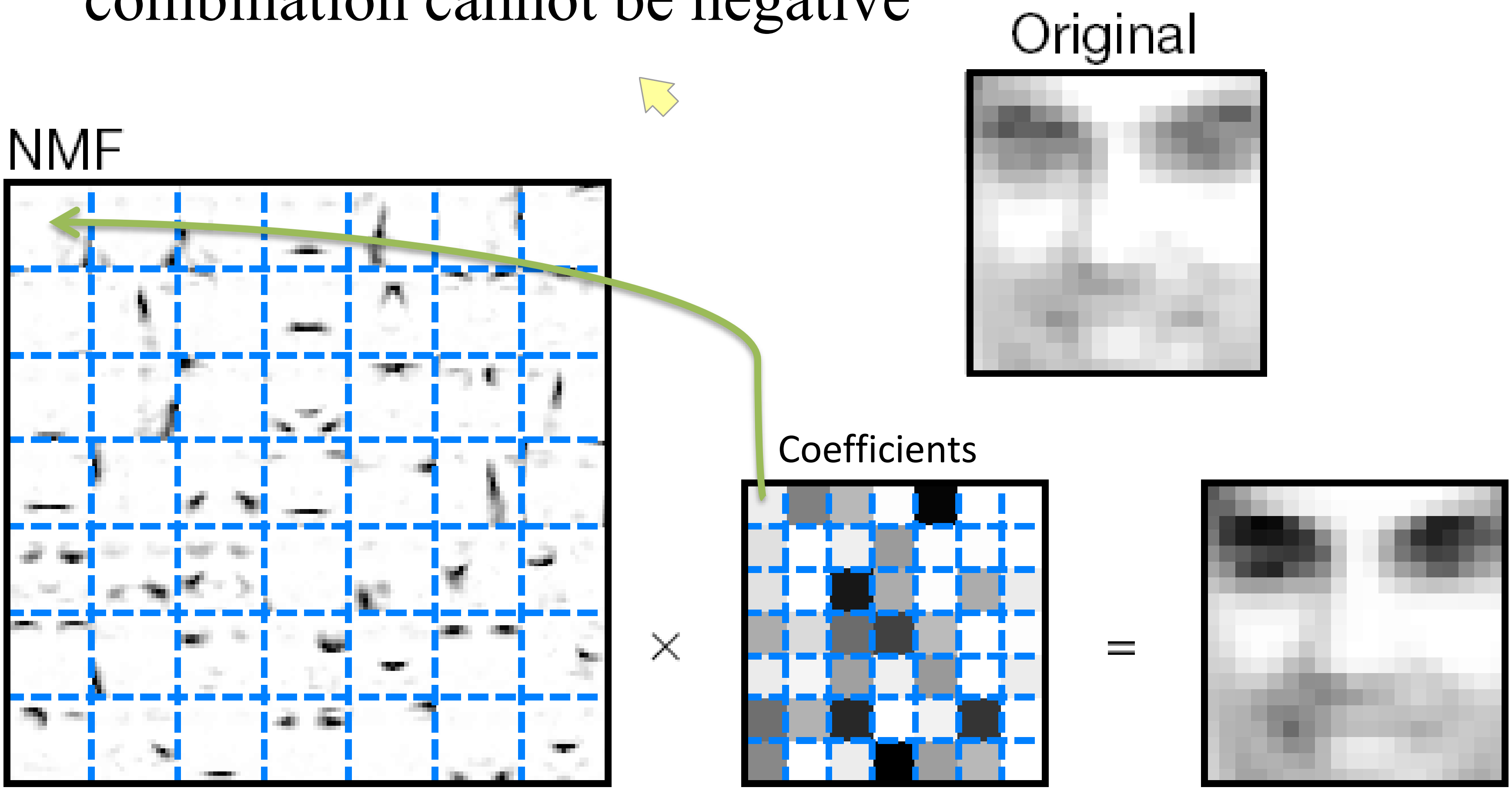


What we do not like about PCA?

- PCA involves adding up some basis vectors then subtracting others
- Basis vectors aren't physically intuitive (negative) for many applications, e.g. documents
- Subtracting doesn't make sense in context of some applications
  - How do you subtract a face?
  - What does subtraction mean in the context of document classification?

Non-negative Matrix Factorization

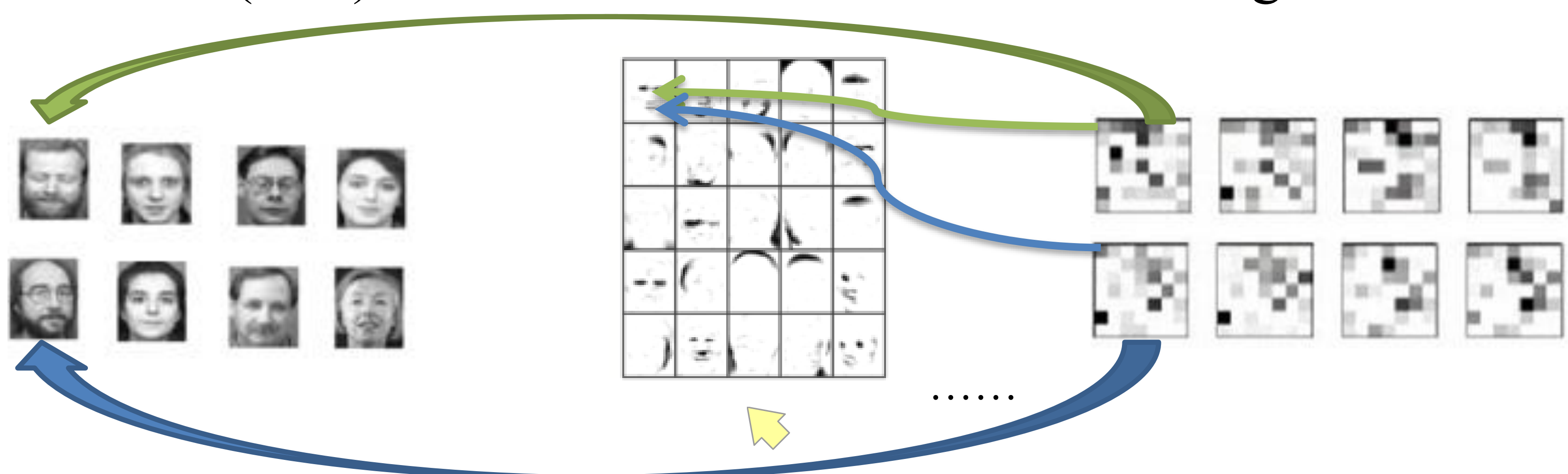
- Like PCA, except that the coefficients in the linear combination cannot be negative



Proposed by D. Lee and H. Seung (NIPS 2000)

Non-negative Matrix Factorization

- Matrix factorization: V≈WH
  - V: n×m matrix. Each column of which contains n nonnegative pixel values of one of the m facial images.
  - W: (n×r): r columns of W are called basis images.
  - H: (r×m): each column of H is called encoding.



V: an image is a column vector

W: a basis image is a column vector

H: a coefficient vector (shown as matrix here) is a column vector

NMF Basis Vectors

- Only allowing adding basis vectors makes intuitive sense
  - Has physical similarity in neurons
- Forcing the reconstruction coefficients to be nonnegative leads to **nice** basis vectors
  - To reconstruct vector (image), all you can do is to add in more basis vectors
  - This leads to basis vectors that represent parts

Objective Function

- Assume V is the sample matrix, the task is to approximate the original data matrix with two nonnegative data matrices:

$$\min_{W,H} \|V - WH\|^2 \quad s.t. \quad W \geq 0, H \geq 0.$$

- Let the value of a pixel in the original input image be $V_{i\mu}$. Let $(WH)_{i\mu}$ be the reconstructed pixel.

$$V_{i\mu} = (WH)_{i\mu} = \sum_{a=1}^{r} W_{ia} H_{a\mu}$$

How do we derive the update rules (H only, W similar)?

- Use gradient descent to find a local minimum

- The gradient descent update rule is:

$$H_{a\mu} \leftarrow H_{a\mu} + \eta_{a\mu} \left[(W^T V)_{a\mu} - (W^T W H)_{a\mu} \right]$$

Try by yourself

Deriving Update Rules (H only, W similar)

- Gradient Descent Rule:

$$H_{a\mu} \leftarrow H_{a\mu} + \eta_{a\mu}\left[(W^TV)_{a\mu} - (W^TWH)_{a\mu}\right]$$

- Set $\eta_{a\mu} = \dfrac{H_{a\mu}}{(W^TWH)_{a\mu}}$

- The update rule becomes

$$H_{a\mu} \leftarrow H_{a\mu}\frac{(W^TV)_{a\mu}}{(W^TWH)_{a\mu}}$$

Try by yourself

What's significant about this?

- This is a multiplicative update
  - If the initial values of W and H are all non-negative, then the W and H can never become negative.
- This lets us produce a non-negative factorization
- See NIPS Paper for full proof that this will converge if you are interested.

http://papers.nips.cc/paper/1861-algorithms-for-non-negative-matrix-factorization.pdf

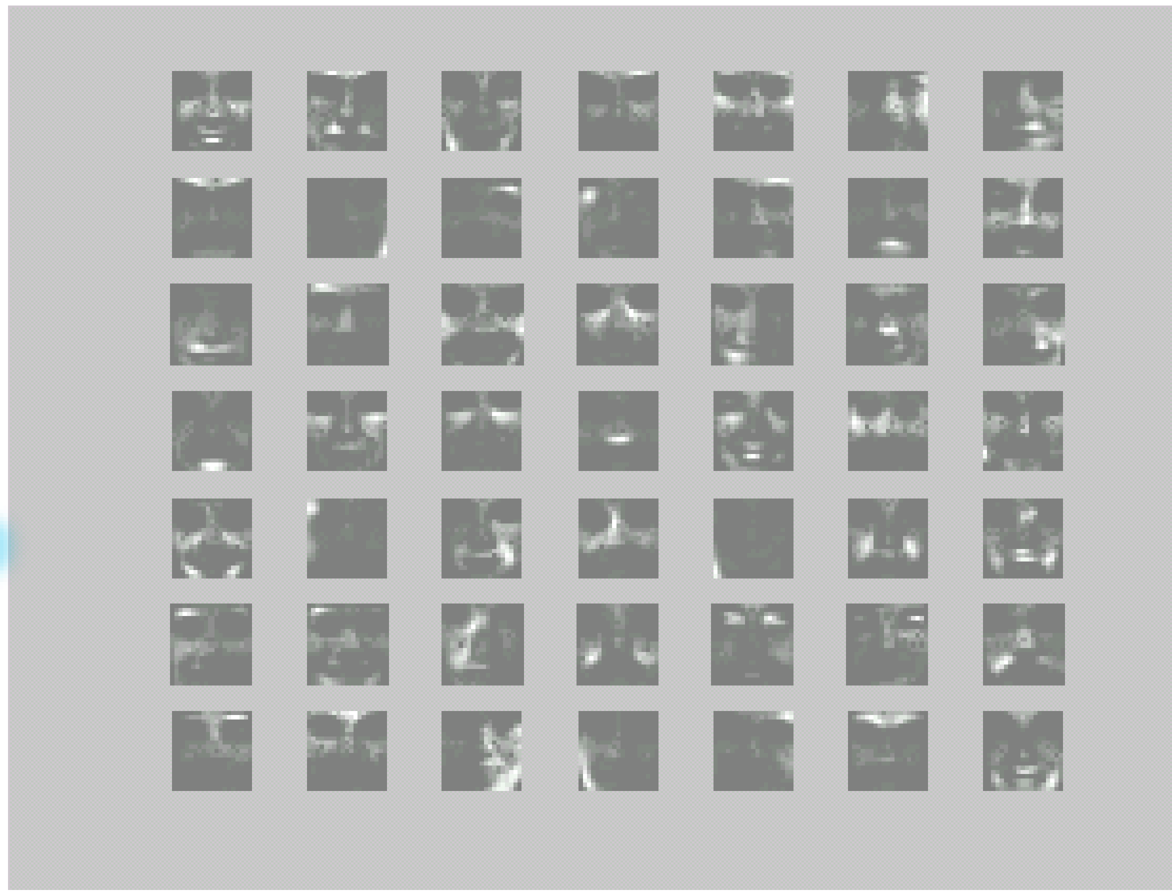
Example: Faces

- Training set: 2429 examples
- First 25 examples shown at right
- Set consists of 19x19 face images

Example: Faces

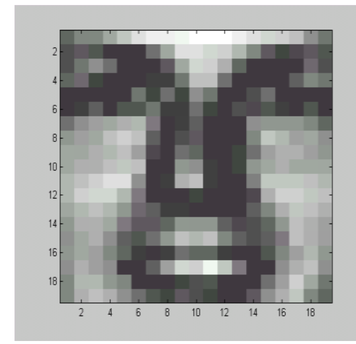
- Basis Images:
  - Basis no.: 49
  - Iterations: 50

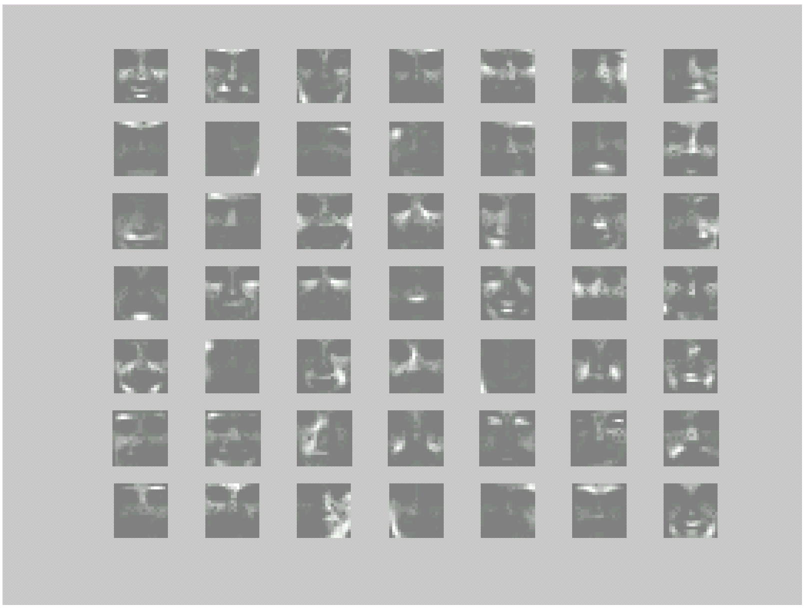
How to draw this figure?



Face Reconstruction from Basis Vectors

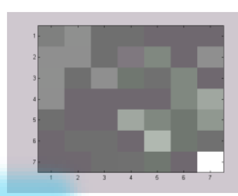
Original





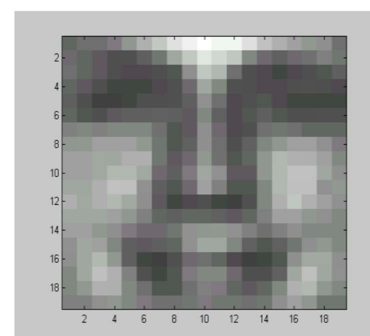
W

x



h

=



W * h

How to get h?

Example: Cars

- Training set: 200 examples
- First 25 examples shown at right
- Set consists of car images taken at various orientations

Example: Cars

- Basis Images
  - Basis no.: 49
  - Iterations: 310

Car Reconstruction from Basis Vectors

Originals (1-25)

Output (1-25)

Car Reconstruction from Basis Vectors

Original image

Reconstructed image

Why fence disappeared?

Discussions

- For new image, how to obtain the reconstruction coefficients?

- How to use NMF for classification, e.g. face recognition?

Summary of NMF

Algorithm 2 Algorithm for NMF

Input: Sample matrix $V = [v_1, v_2, \cdots, v_N]$.
Initialize W^0 and H^0 as arbitrary positive matrices.

for $t = 0 : 1 : T_{max}$ **do**

$$H_{a\mu}^{t+1} = H_{a\mu}^{t} \frac{({W^t}^T V)_{a\mu}}{({W^t}^T W^t H^t)_{a\mu}};$$

$$W_{a\mu}^{t+1} = W_{a\mu}^{t} \frac{(V {H^{t+1}}^T)_{a\mu}}{(W^t H^{t+1} {H^{t+1}}^T)_{a\mu}};$$

If $\|W^t - W^{t+1}\| < \epsilon$ and $\|H^t - H^{t+1}\| < \epsilon$
  return;
end for
3. Output matrices W and H.

Discussions

- What are differences between NMF and PCA?

	NMF	PCA
Representation	Part-based	Holistic
Basis Image	Localized features	Eigenfaces
Constrains on W and H	Allow multiple basis images to represent a face but only additive combinations	Each face is approximated by a linear combination of all eigenfaces

Papers to Read and Self-Study

- D. Lee and H. Seung. Algorithms for Non-negative Matrix Factorization NIPS (2000).
- ICA (Independent Component Analysis): http://en.wikipedia.org/wiki/Independent_component_analysis
- CCA (Canonical Correlation Analysis): http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.101.6359&rep=rep1&type=pdf