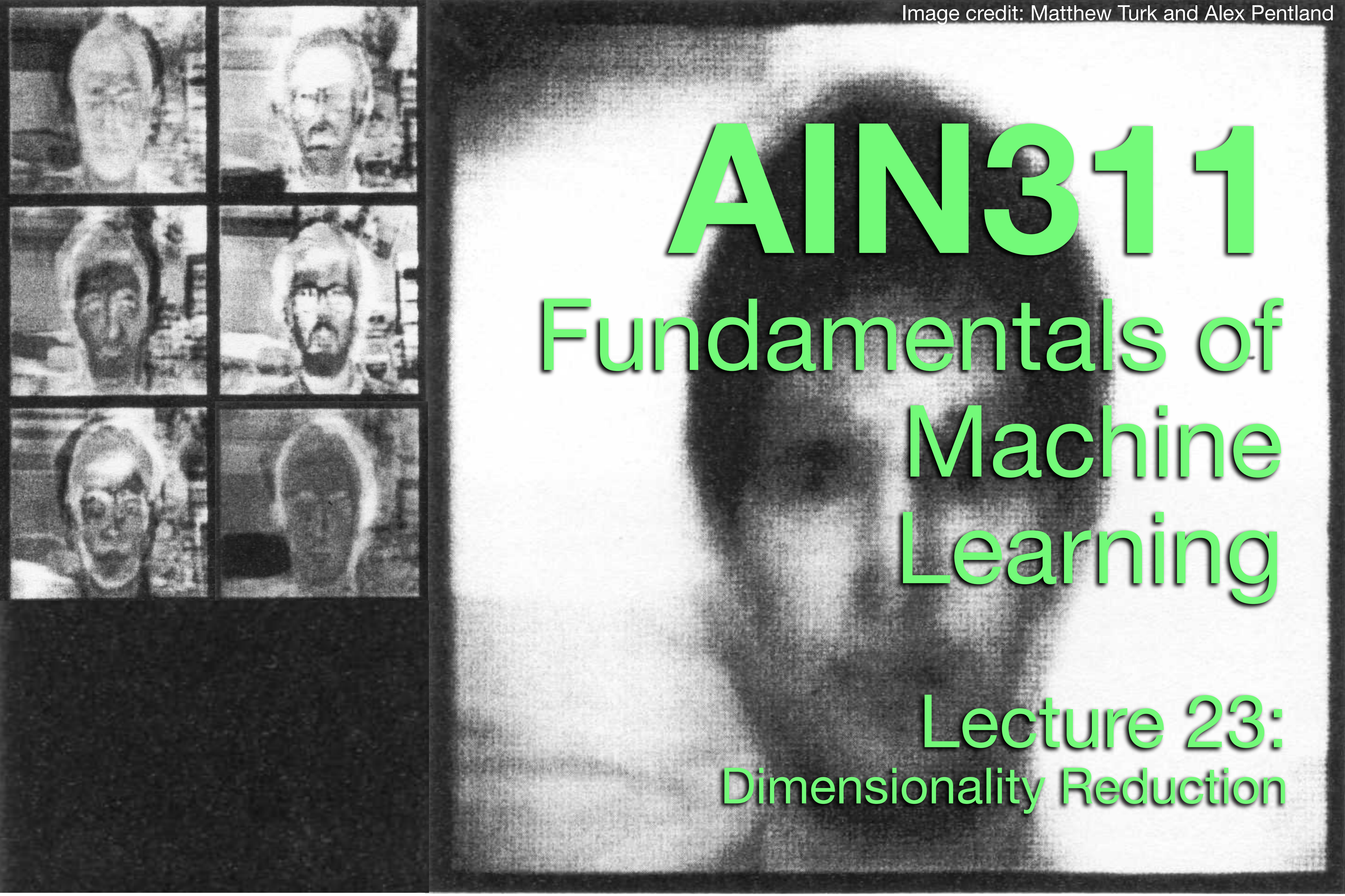


Image credit: Matthew Turk and Alex Pentland

AIN311

Fundamentals of Machine Learning

Lecture 23:

Dimensionality Reduction

HACETTEPE UNIVERSITY COMPUTER VISION LAB

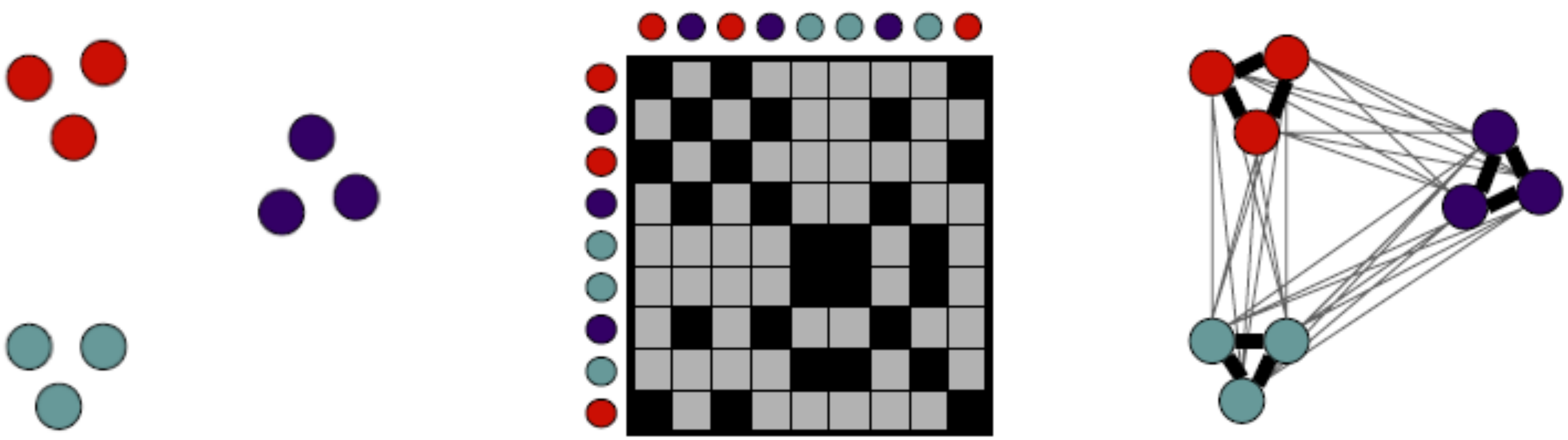
Erkut Erdem // Hacettepe University // Fall 2023

Last time… **Graph-Theoretic Clustering**

Goal: Given data points $X_1, \ldots, X_n$ and similarities $W(X_i, X_j)$, partition the data into groups so that points in a group are similar and points in different groups are dissimilar.

Similarity Graph: G(V,E,W)

V – Vertices (Data points)
E – Edge if similarity > 0
W - Edge weights (similarities)

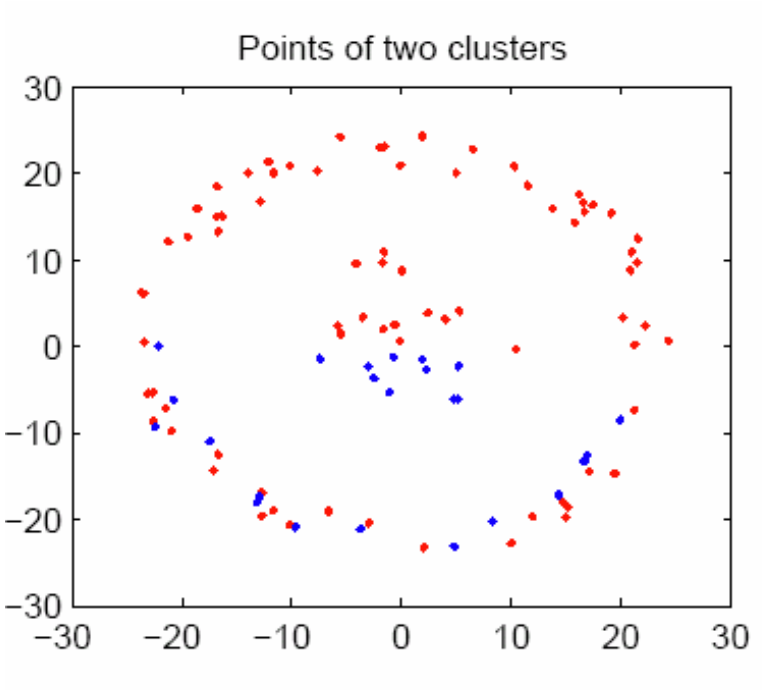


Data   Similarities   Similarity graph

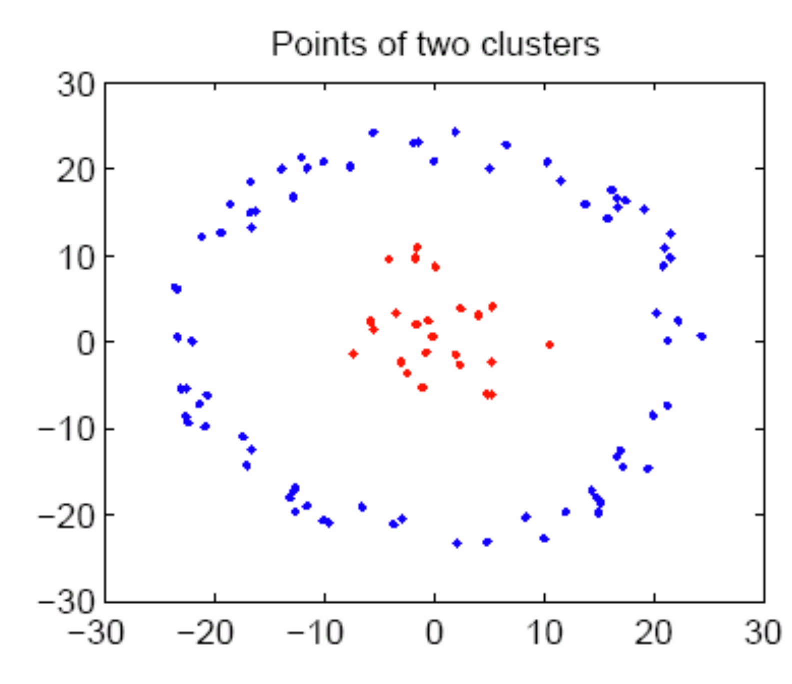
Partition the graph so that edges within a group have large weights and edges across groups have small weights.

slide by Aarti Singh

Last time… **K-Means vs. Spectral Clustering**

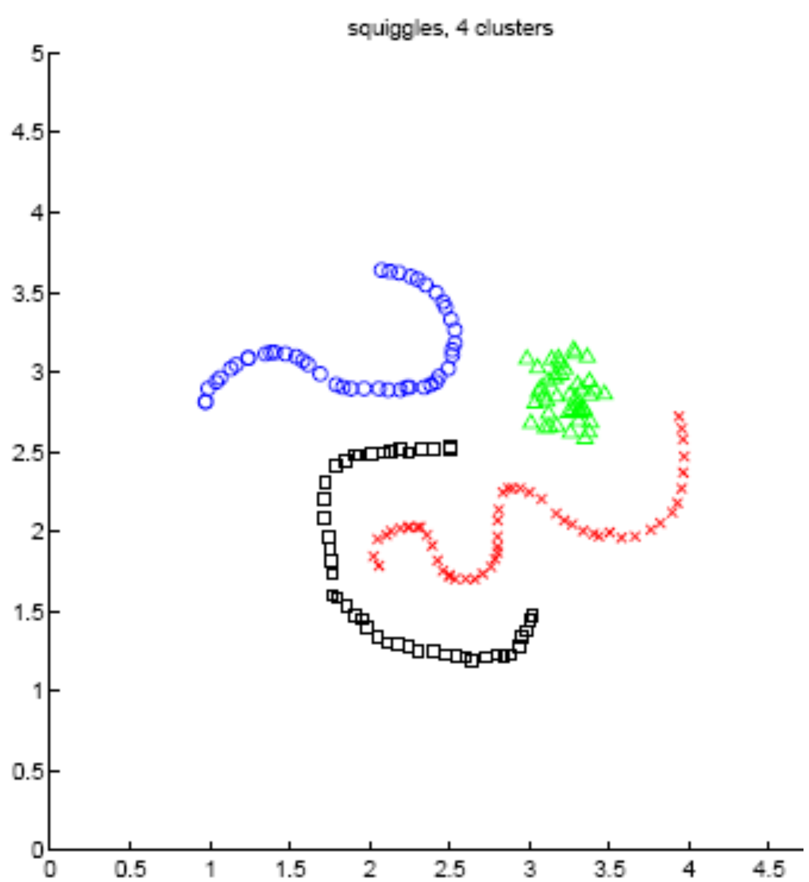


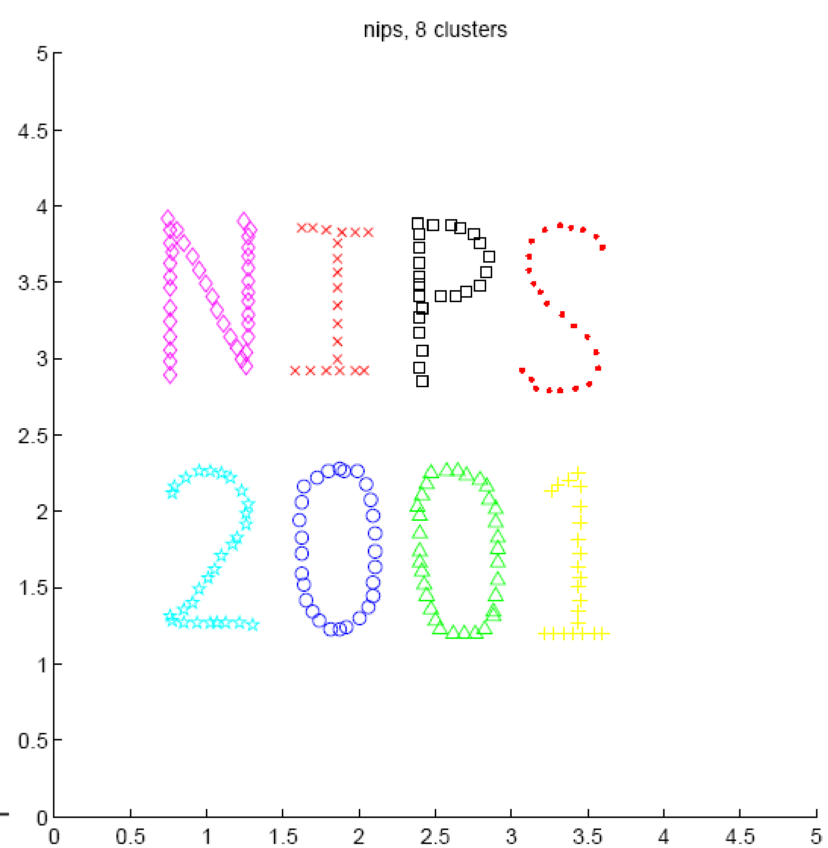
k-means output



Spectral clustering output

- Applying k-means to Laplacian eigenvectors allows us to find cluster with non-convex boundaries.





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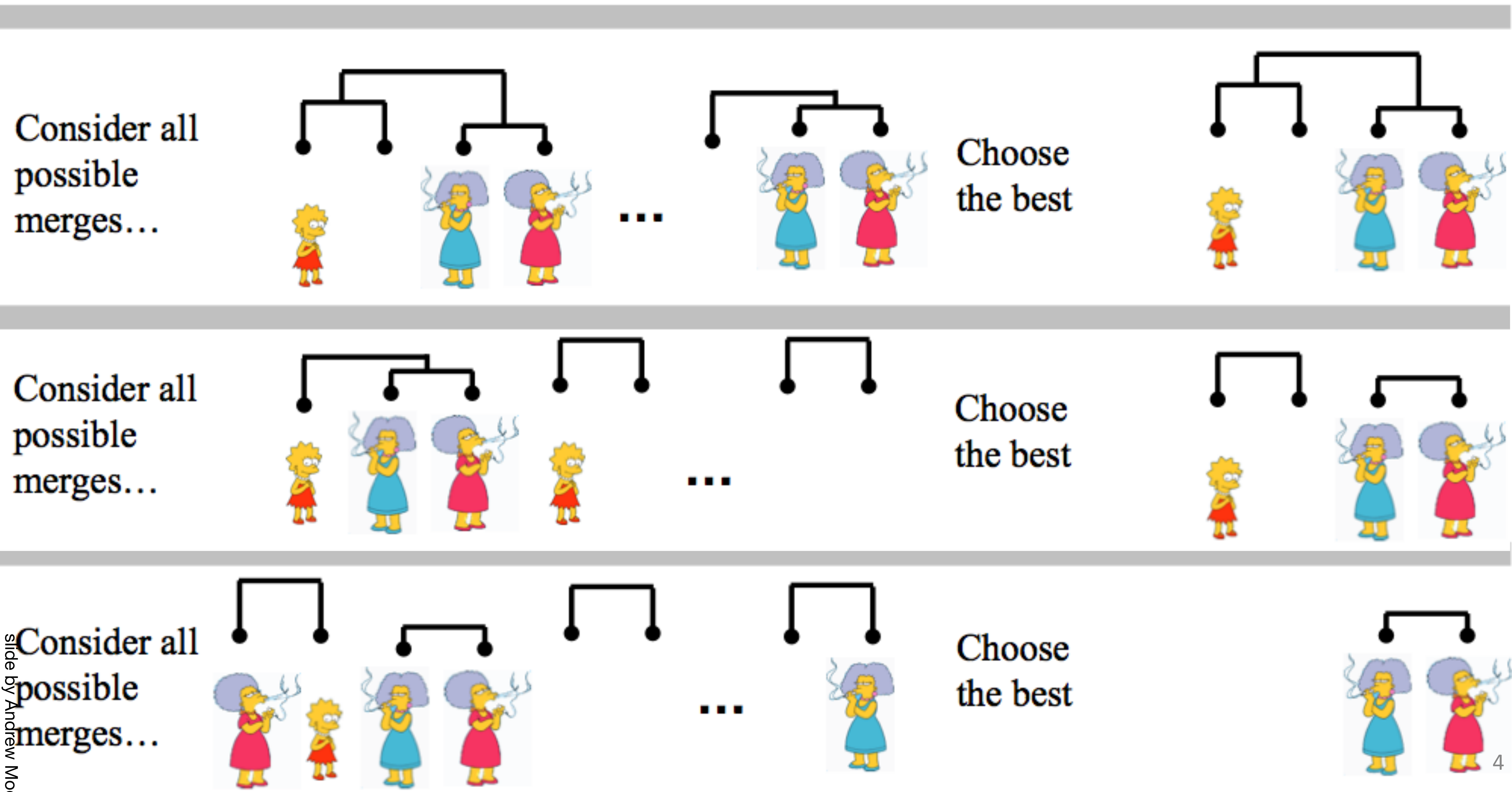
Last time…

Bottom-Up (agglomerative):

Start with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.



slide by Andrew Moore

Today

- Dimensionality Reduction
- Principle Component Analysis (PCA)
- PCA Applications
- PCA Shortcomings
- Autoencoders
- Independent Component Analysis

Dimensionality Reduction

Motivation I: Data Visualization

Instances

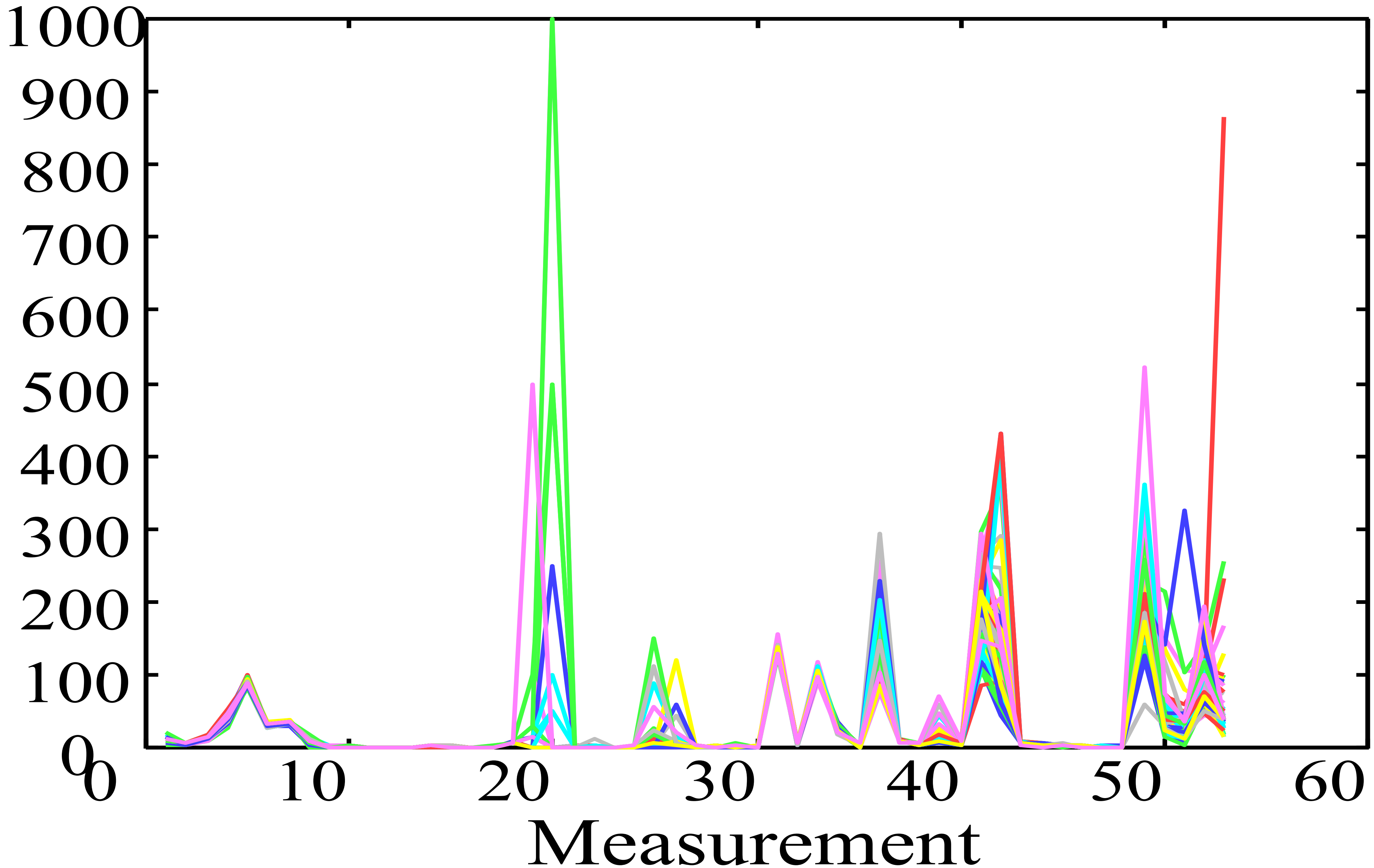
	H-WBC	H-RBC	H-Hgb	H-Hct	H-MCV	H-MCH	H-MCHC
A1	8.0000	4.8200	14.1000	41.0000	85.0000	29.0000	34.0000
A2	7.3000	5.0200	14.7000	43.0000	86.0000	29.0000	34.0000
A3	4.3000	4.4800	14.1000	41.0000	91.0000	32.0000	35.0000
A4	7.5000	4.4700	14.9000	45.0000	101.0000	33.0000	33.0000
A5	7.3000	5.5200	15.4000	46.0000	84.0000	28.0000	33.0000
A6	6.9000	4.8600	16.0000	47.0000	97.0000	33.0000	34.0000
A7	7.8000	4.6800	14.7000	43.0000	92.0000	31.0000	34.0000
A8	8.6000	4.8200	15.8000	42.0000	88.0000	33.0000	37.0000
A9	5.1000	4.7100	14.0000	43.0000	92.0000	30.0000	32.0000

Features

- 53 Blood and urine samples from 65 people
- Difficult to see the correlations between features

slide by Alex Smola

Motivation I: Data Visualization

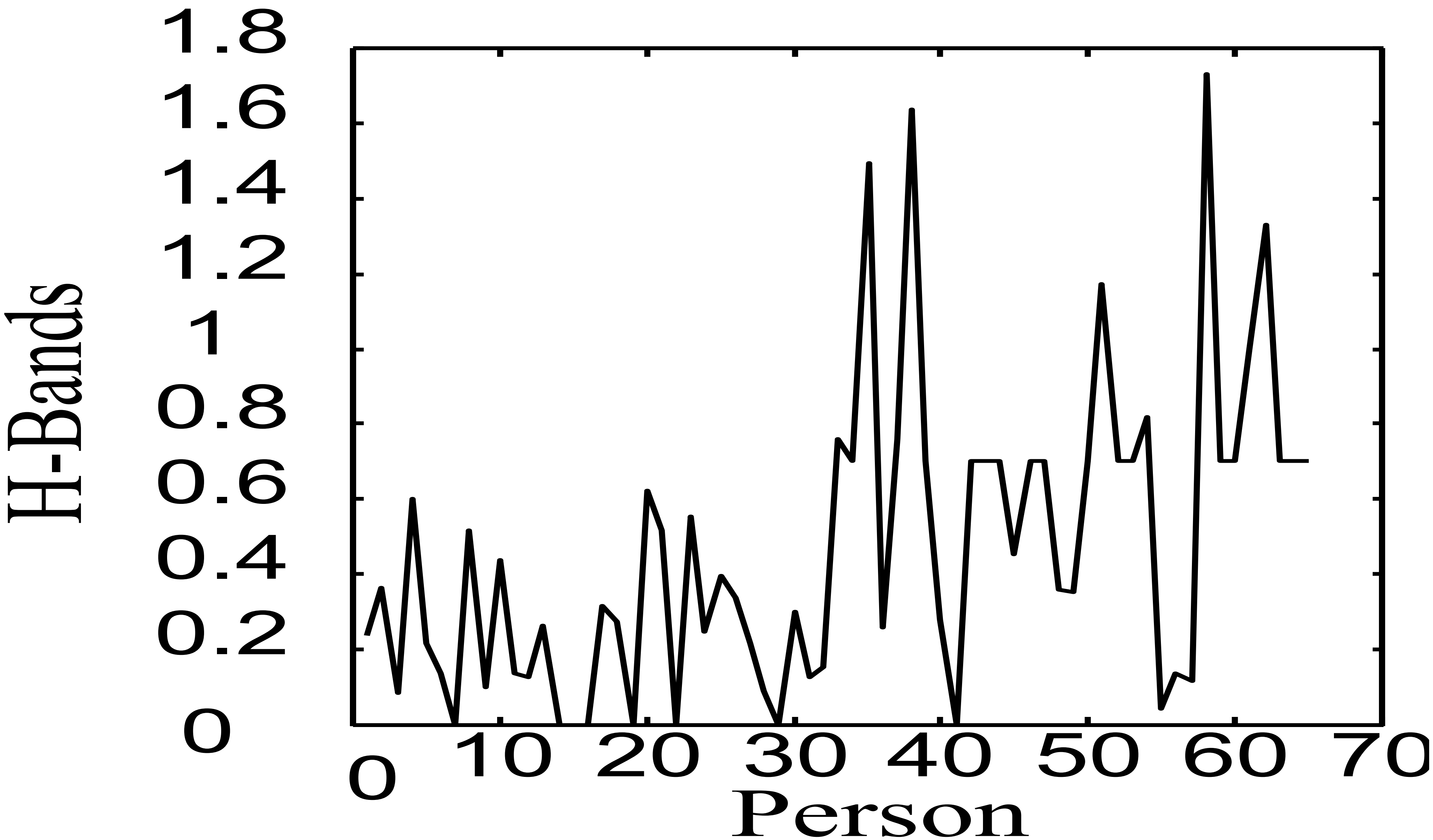


- Spectral format (65 curves, one for each person)
- Difficult to compare different patients

slide by Alex Smola

Motivation I: Data Visualization

- Spectral format (53 pictures, one for each feature)



- Difficult to see the correlations between features

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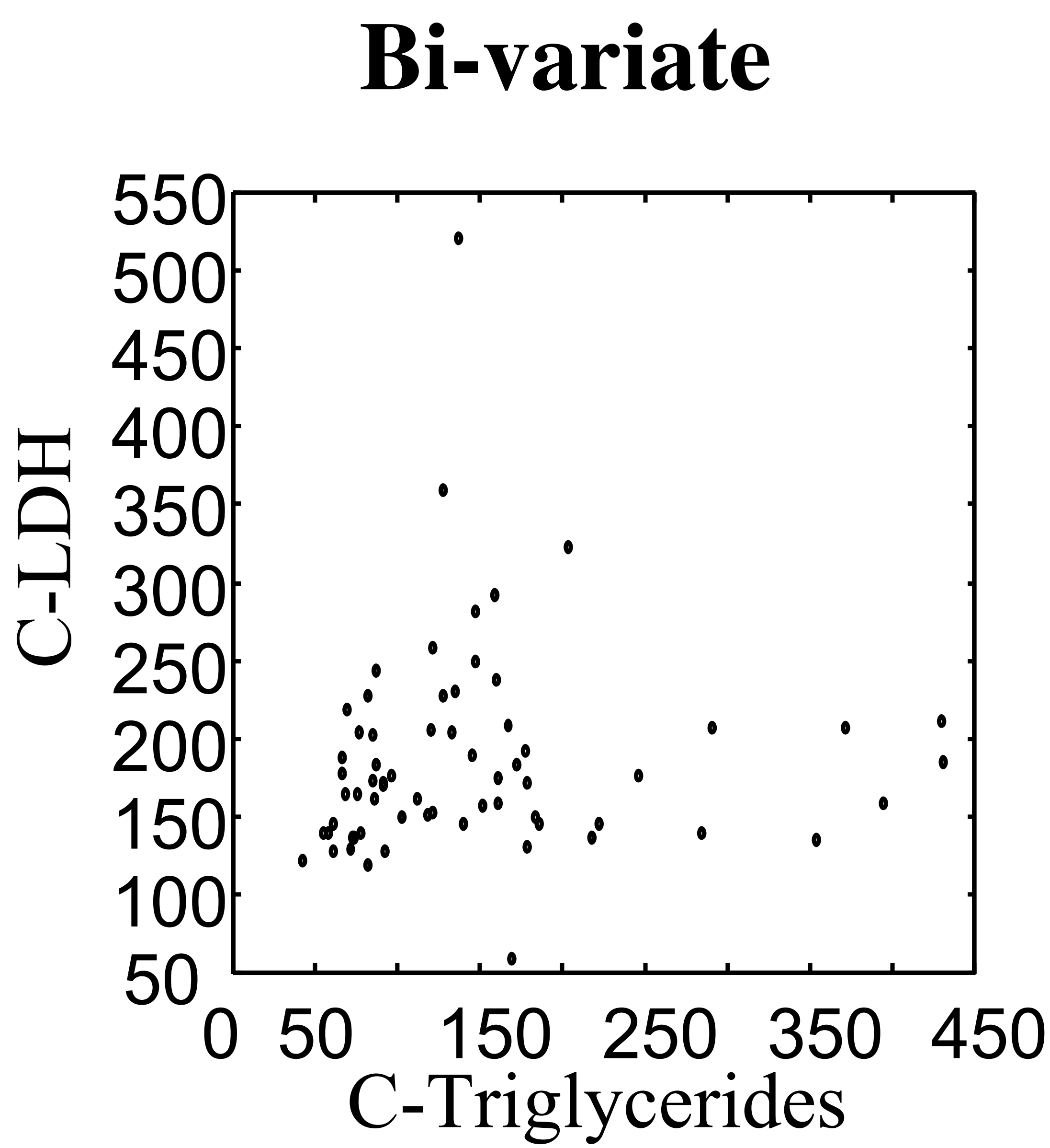
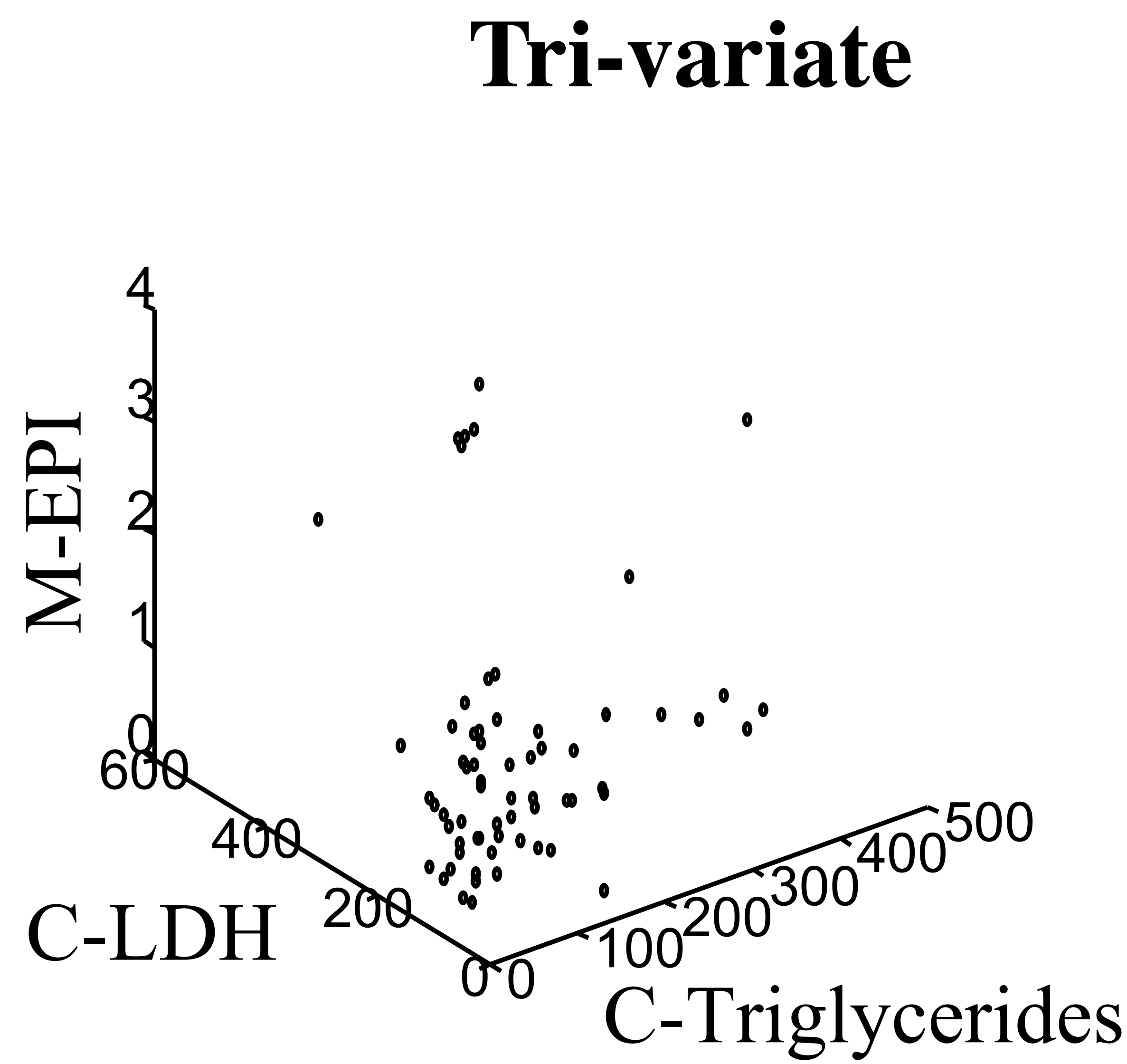
Motivation I: Data Visualization





Even 3 dimensions are already difficult. How to extend this?

slide by Alex Smola

Motivation I: Data Visualization

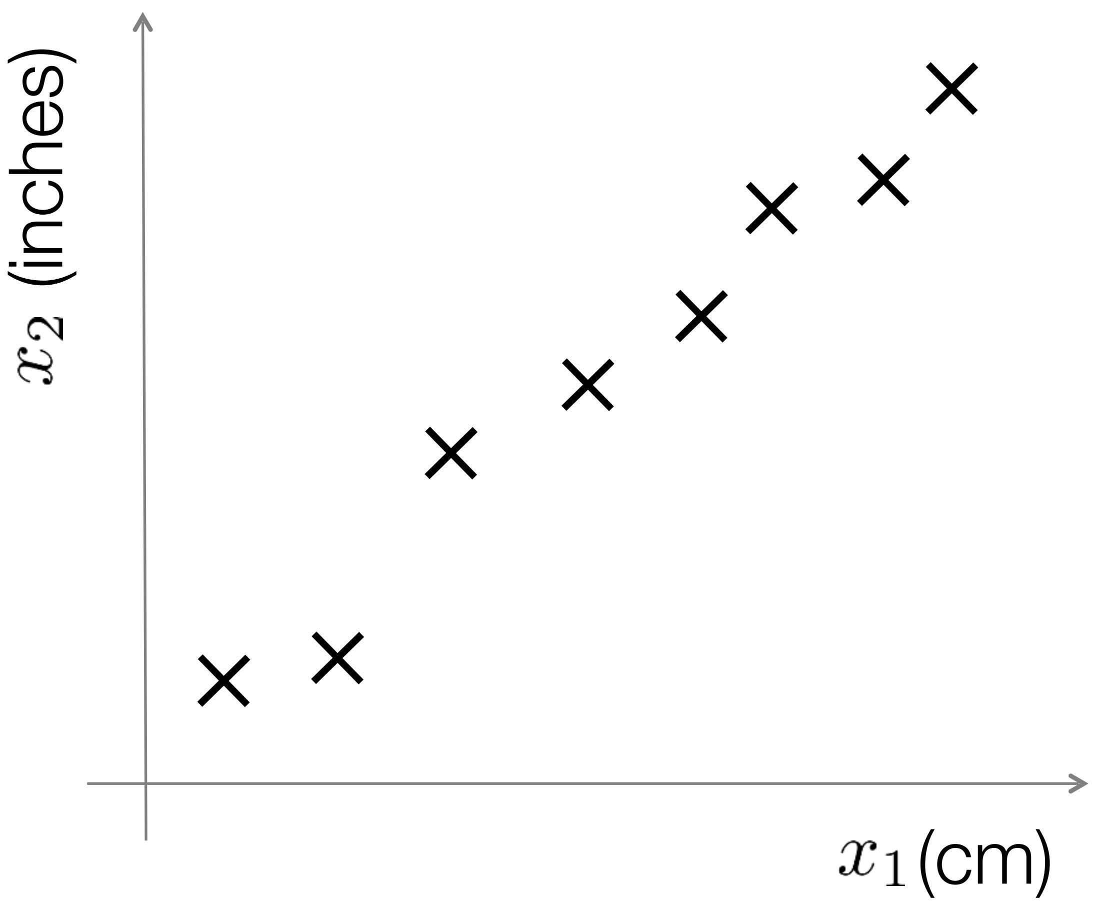
- Is there a representation better than the coordinate axes?

- Is it really necessary to show all the 53 dimensions?
  - ... what if there are strong correlations between the features?

- How could we find the smallest subspace of the 53-D space that keeps the most information about the original data?

slide by Barnabás Póczos and Aarti Singh

Motivation II: Data Compression



Reduce data from 2D to 1D

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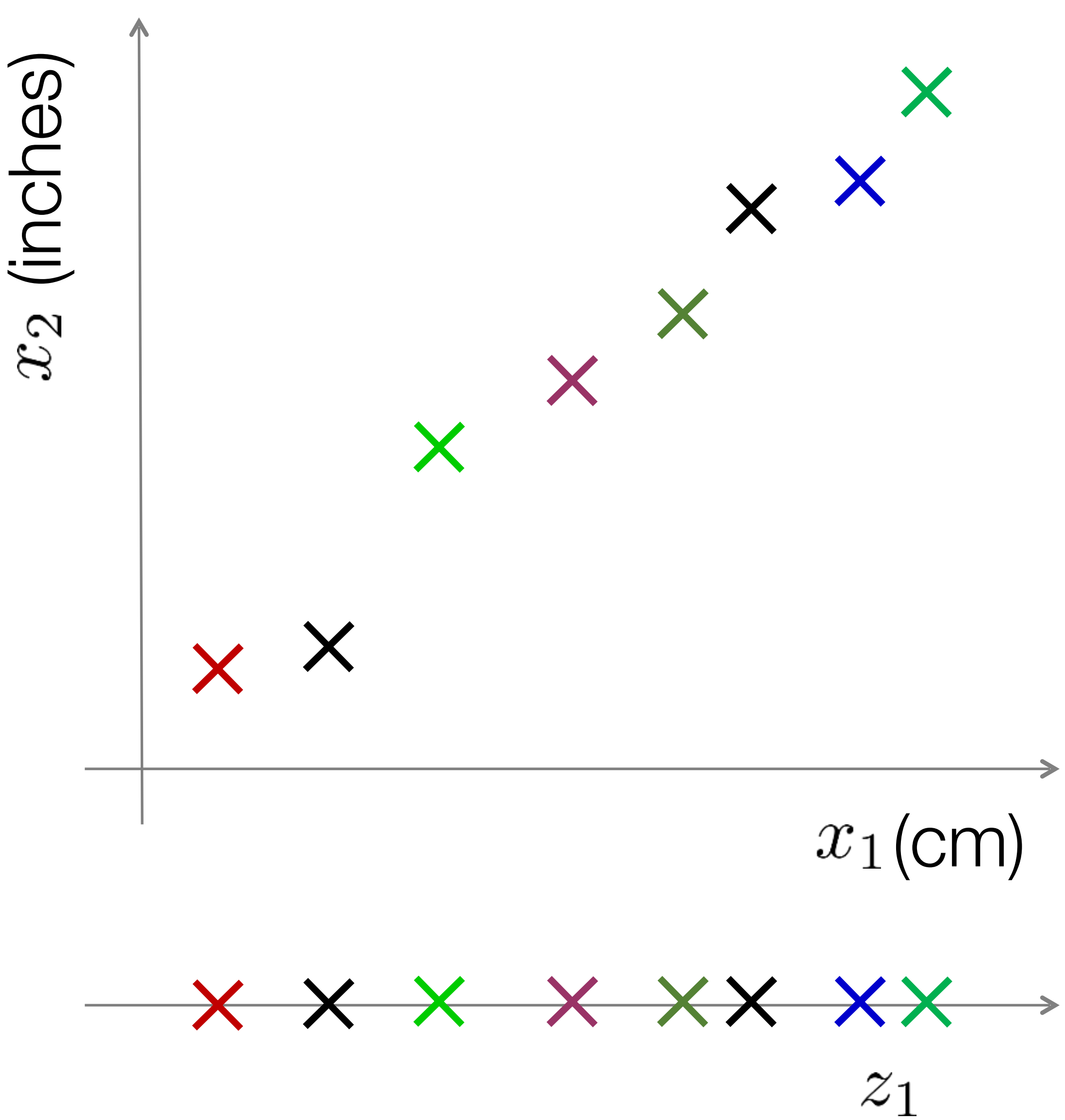
Motivation II: Data Compression



Reduce data from 2D to 1D

$$x^{(1)} \rightarrow z^{(1)}$$
$$x^{(2)} \rightarrow z^{(2)}$$
$$\vdots$$
$$x^{(m)} \rightarrow z^{(m)}$$

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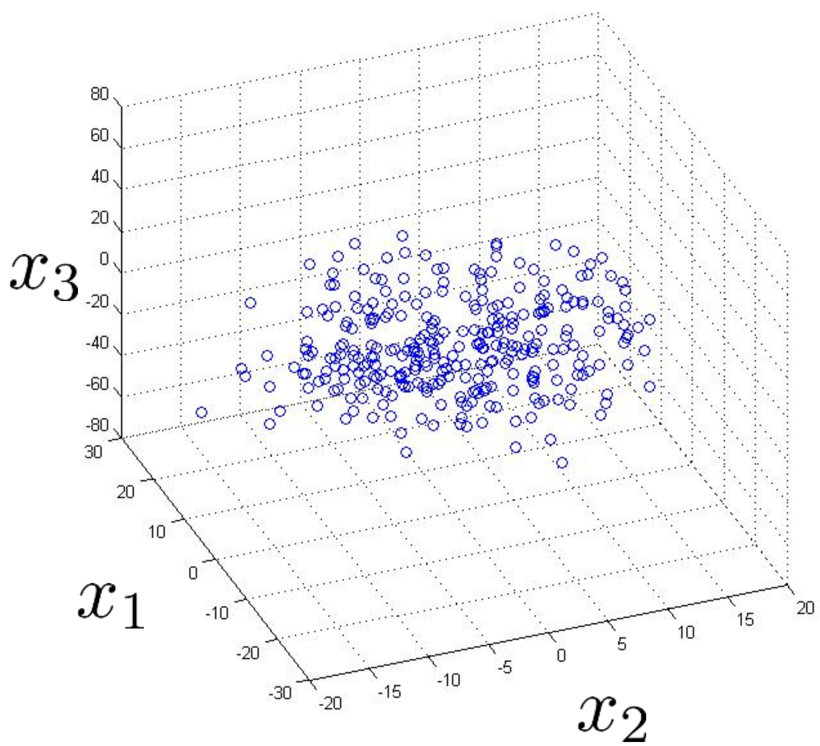
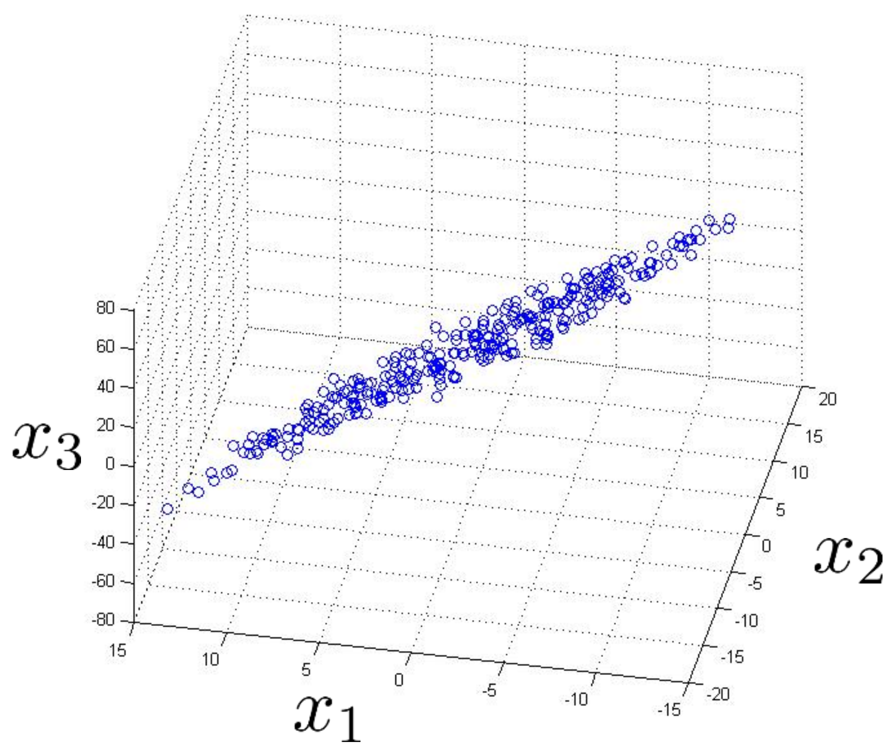
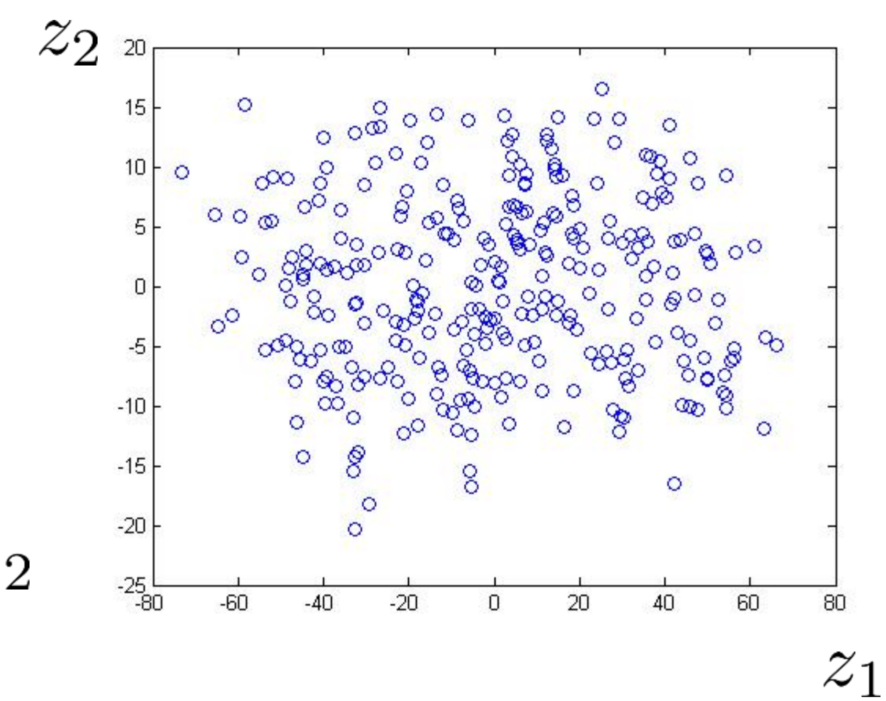
Motivation II: Data Compression

Reduce data from 3D to 2D







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Dimensionality Reduction

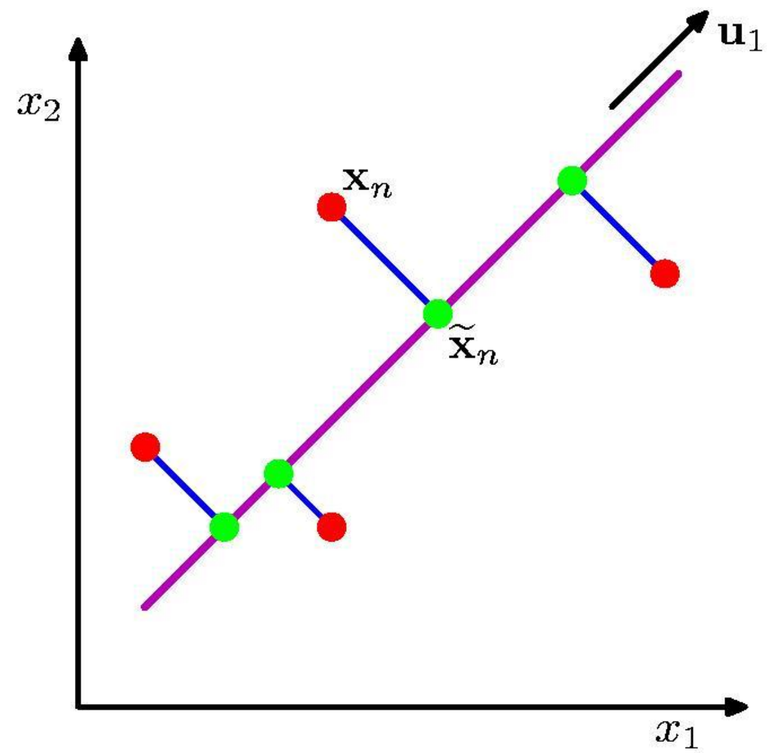
- Clustering
  - One way to summarize a complex real-valued data point with a single categorical variable
- Dimensionality reduction
  - Another way to simplify complex high-dimensional data
  - Summarize data with a lower dimensional real valued vector

- Given data points in *d* dimensions
- Convert them to data points in $r<d$ dims
- With minimal loss of information

slide by Fereshteh Sadeghi

Principal Component Analysis

Principal Component Analysis



PCA:

Orthogonal projection of the data onto a lower-dimension linear space that...

- maximizes variance of projected data (purple line)
- minimizes mean squared distance between
  - data point and
  - projections (sum of blue lines)

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Principal Component Analysis

- **PCA Vectors** originate from the center of mass.

- Principal component #1: points in the direction of the **largest variance**.

- Each subsequent principal component
  - is **orthogonal** to the previous ones, and
  - points in the directions of the **largest variance of the residual subspace**

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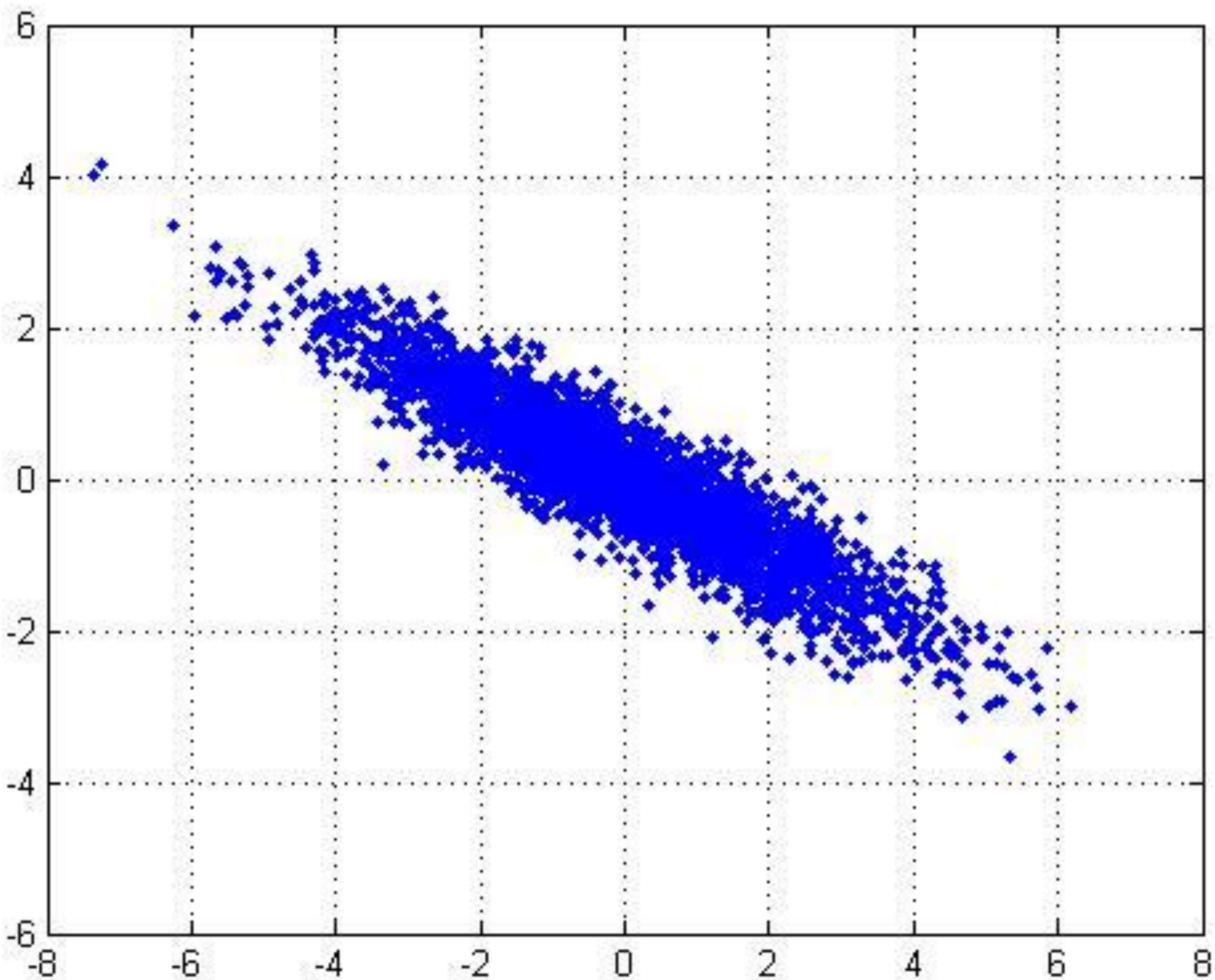
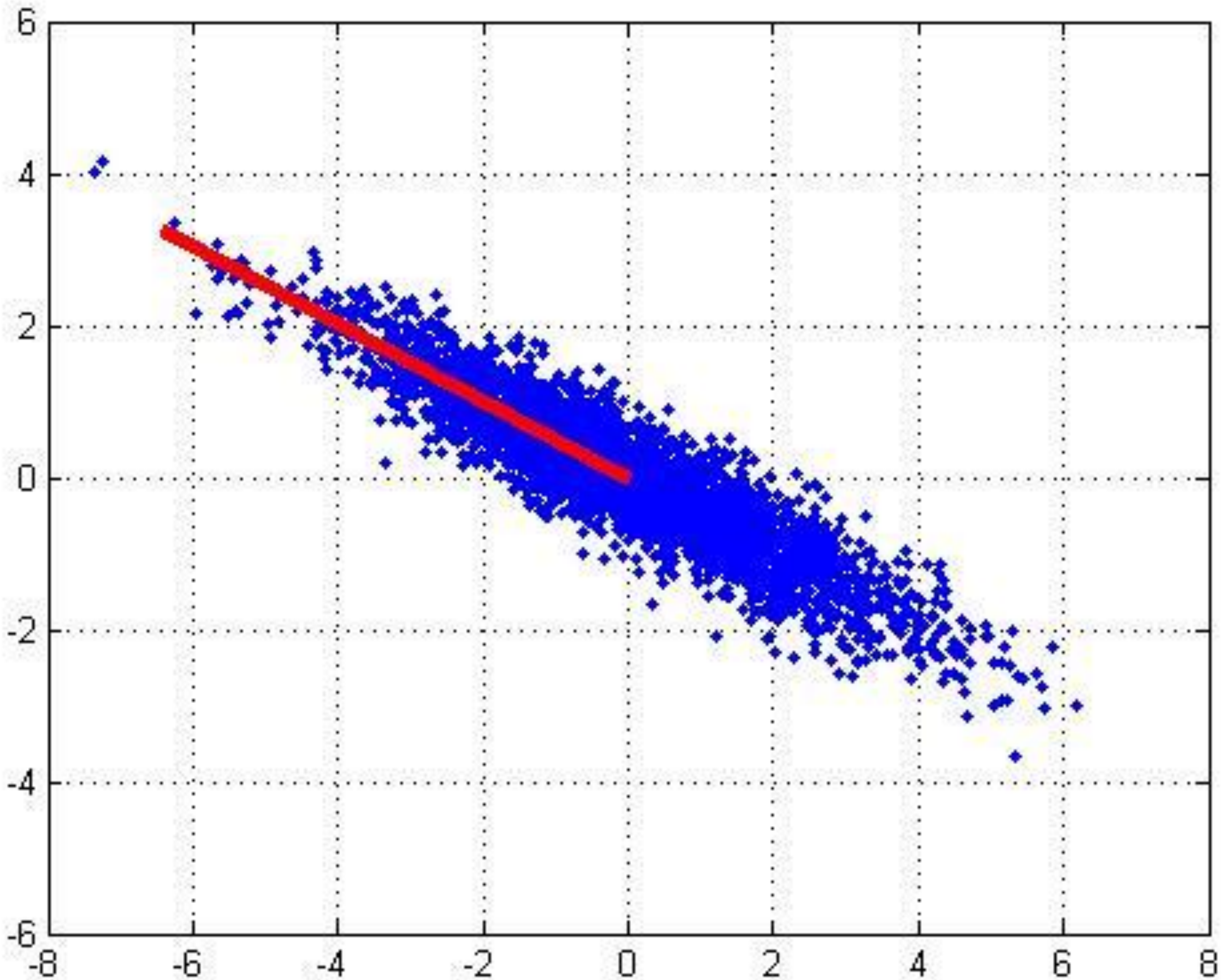
2D Gaussian dataset



1^{st} PCA axis



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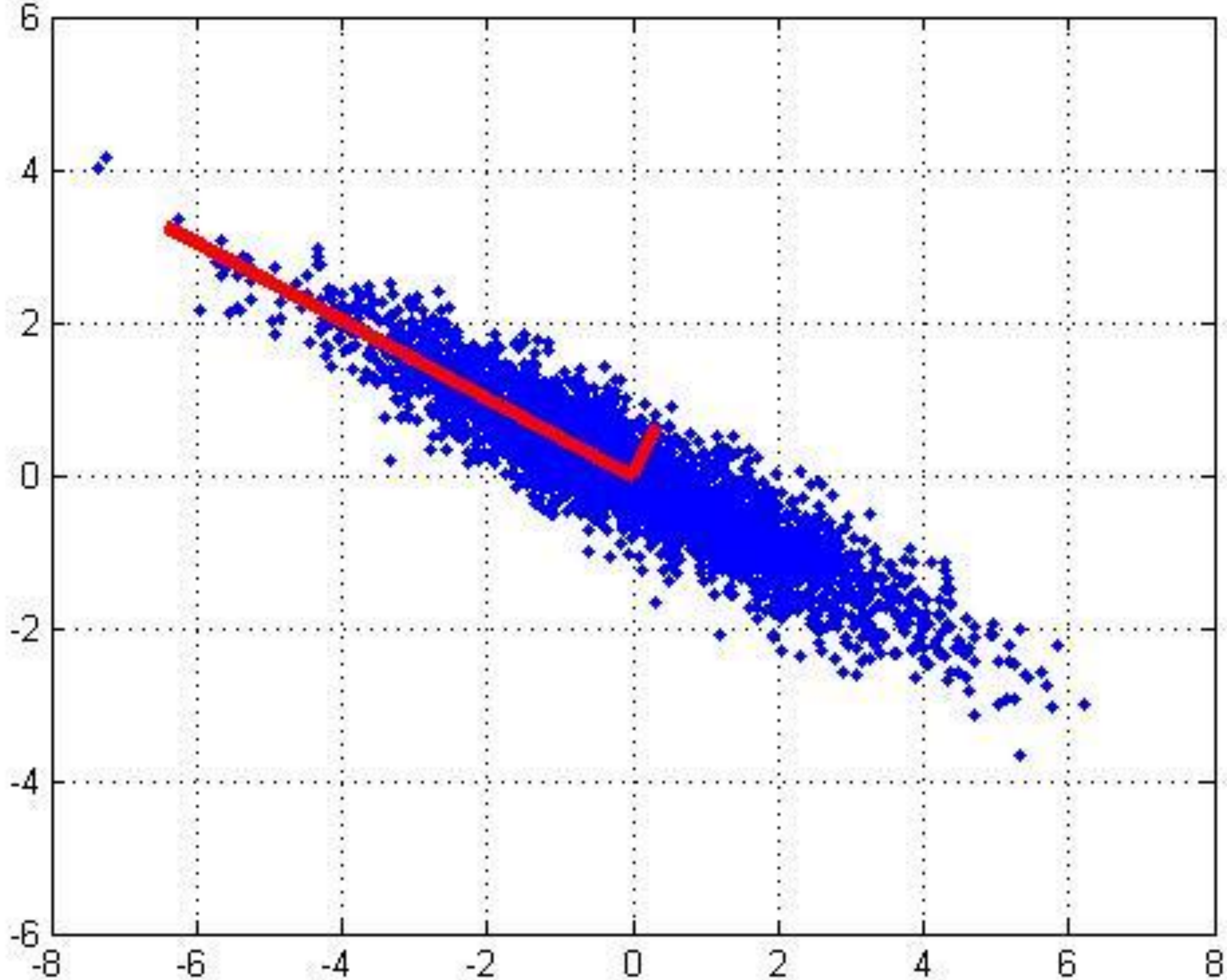
2^{nd} PCA axis



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PCA algorithm I (sequential)

Given the **centered** data $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, compute the principal vectors:

$$\mathbf{w}_1 = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m} \sum_{i=1}^{m} \{(\mathbf{w}^T \mathbf{x}_i)^2\}$$

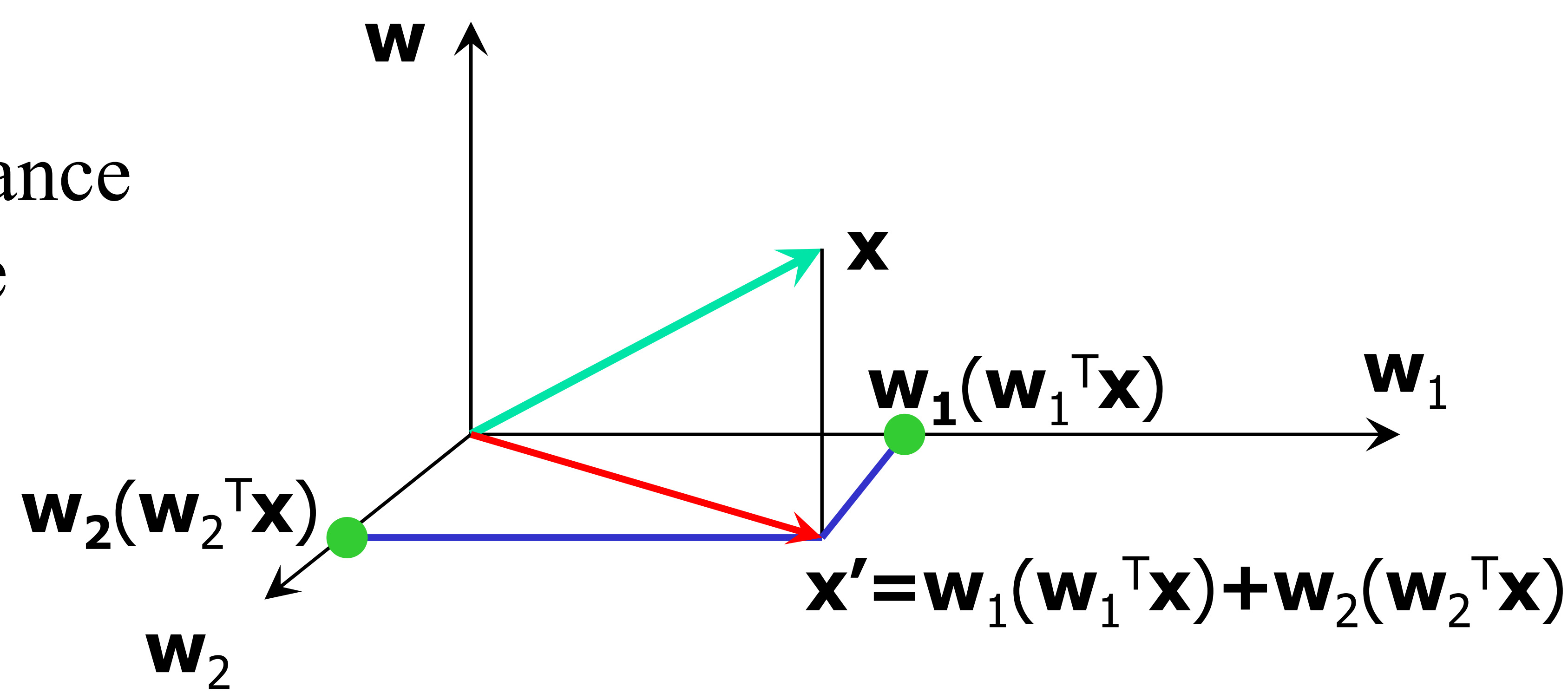
1st PCA vector

We maximize the variance of projection of $\mathbf{x}$

$$\mathbf{w}_k = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m} \sum_{i=1}^{m} \{[\mathbf{w}^T (\underbrace{\mathbf{x}_i - \sum_{j=1}^{k-1} \mathbf{w}_j \mathbf{w}_j^T \mathbf{x}_i}_{\mathbf{x}' \text{ PCA reconstruction}})]^2\}$$

kth PCA vector

We maximize the variance of the projection in the residual subspace



PCA algorithm II
(sample covariance matrix)

- Given data $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, compute covariance matrix Σ

$$\boxed{\Sigma = \frac{1}{m}\sum_{i=1}^{m}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^T}$$

where

$$\boxed{\bar{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i}$$

- **PCA** basis vectors = the eigenvectors of Σ

- Larger eigenvalue $\Rightarrow$ more important eigenvectors

Reminder: Eigenvector and Eigenvalue

$$\mathrm{A}x = \lambda x$$

A: Square matrix
λ: Eigenvector or characteristic vector
x: Eigenvalue or characteristic value

$$Show\ \ x = \begin{bmatrix} 2 \\ 1 \end{bmatrix} is\,an\,eigenvector\ for\ A = \begin{bmatrix} 2 & -4 \\ 3 & -6 \end{bmatrix}$$

$$Solution: Ax = \begin{bmatrix} 2 & -4 \\ 3 & -6 \end{bmatrix}\begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$But\quad for\ \ \lambda = 0,\ \ \lambda x = 0\begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$Thus, x\,is\,an\,eigenvector\,of\ A, and\,\lambda = 0\ is\,an\,eigenvalue.$$

Reminder: Eigenvector and Eigenvalue

$$\mathbf{A}x = \lambda\mathbf{x} \longrightarrow \begin{array}{l}\mathbf{Ax - \lambda x = 0}\\ \mathbf{(A - \lambda I)x = 0}\end{array}$$

If we define a new matrix B: $\longrightarrow$ $\begin{array}{l}\mathbf{B = A - \lambda I}\\ \mathbf{Bx = 0}\end{array}$

If B has an inverse: $\longrightarrow$ $\mathbf{x = B^{-1}0 = 0}$ ✘ BUT! an eigenvector cannot be zero!!

x will be an eigenvector of A if and only if B does not have an inverse, or equivalently det(B)=0 :

$$\boxed{\mathbf{det(A - \lambda I) = 0}}$$

Reminder: Eigenvector and Eigenvalue

Example 1: Find the eigenvalues of

$$A = \begin{bmatrix} 2 & -12 \\ 1 & -5 \end{bmatrix}$$

$$|\lambda I - A| = \begin{vmatrix} \lambda - 2 & 12 \\ -1 & \lambda + 5 \end{vmatrix} = (\lambda - 2)(\lambda + 5) + 12$$

$$= \lambda^2 + 3\lambda + 2 = (\lambda + 1)(\lambda + 2)$$

two eigenvalues: $-1, -2$

Note: The roots of the characteristic equation can be repeated. That is, $\lambda_1 = \lambda_2 = \ldots = \lambda_k$. If that happens, the eigenvalue is said to be of multiplicity k.

Example 2: Find the eigenvalues of

$$A = \begin{bmatrix} 2 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

$$|\lambda I - A| = \begin{vmatrix} \lambda - 2 & -1 & 0 \\ 0 & \lambda - 2 & 0 \\ 0 & 0 & \lambda - 2 \end{vmatrix} = (\lambda - 2)^3 = 0$$

$\lambda = 2$ is an eigenvector of multiplicity 3.

PCA algorithm II (sample covariance matrix)

Goal: Find r-dim projection that best preserves variance

1. Compute mean vector μ and covariance matrix Σ of original points

2. Compute eigenvectors and eigenvalues of Σ

3. Select top r eigenvectors

4. Project points onto subspace spanned by them:

$$y = A(x - \mu)$$

   where y is the new point, x is the old one, and the rows of A are the eigenvectors

PCA algorithm III
(SVD of the data matrix)

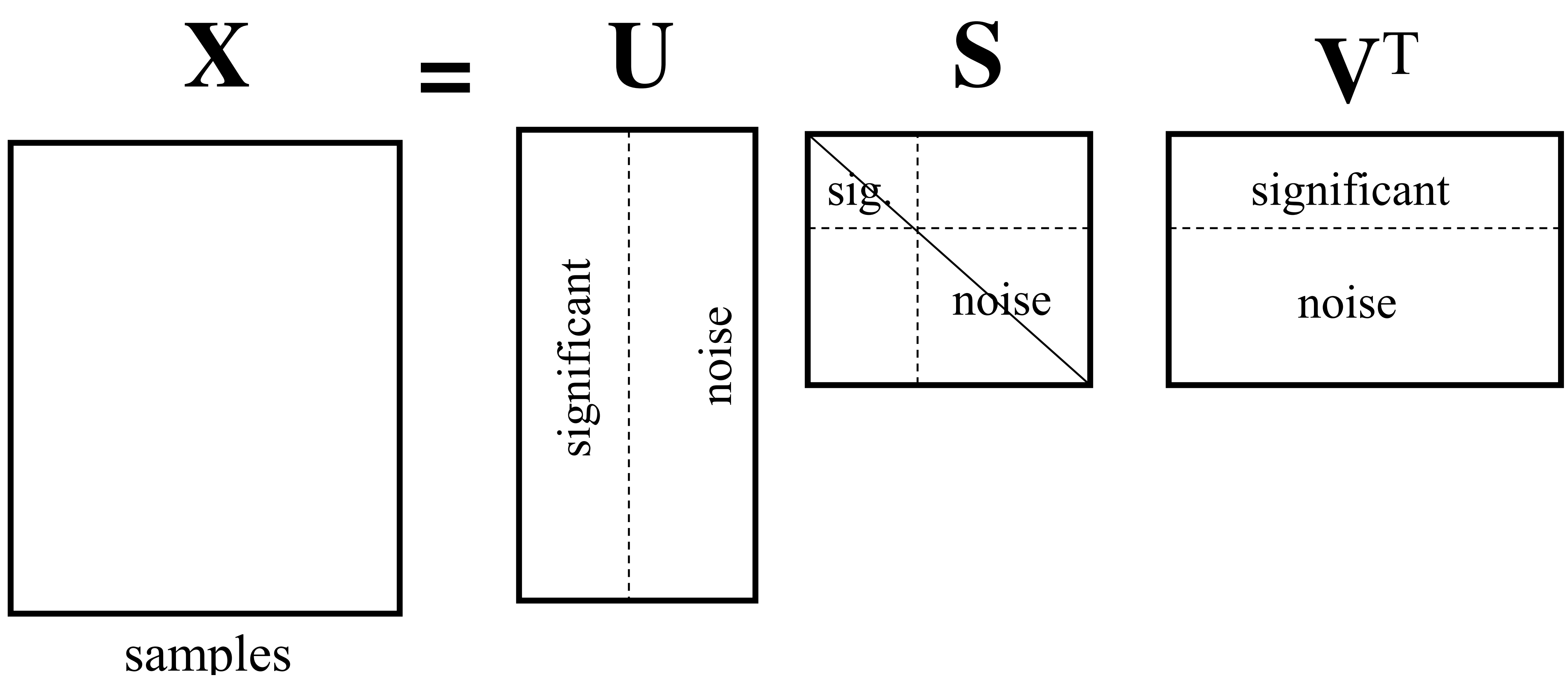
Singular Value Decomposition of the **centered** data matrix **X.**

$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_m] \in \mathbb{R}^{N \times m}$,

m: number of instances,

N: dimension

$$\mathbf{X}_{\text{features} \times \text{samples}} = \mathbf{USV}^{\mathrm{T}}$$



PCA algorithm III

- **Columns of U**
  - the principal vectors, $\{\ \mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(k)}\ \}$
  - orthogonal and has unit norm – so $U^T U = I$
  - Can reconstruct the data using linear combinations of $\{\ \mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(k)}\ \}$

- **Matrix S**
  - Diagonal
  - Shows importance of each eigenvector

- **Columns of V^T**
  - The coefficients for reconstructing the samples

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Applications

Face Recognition

Face Recognition

- Want to identify specific person, based on facial image
- Robust to glasses, lighting, …
  - Can’t just use the given 256 x 256 pixels

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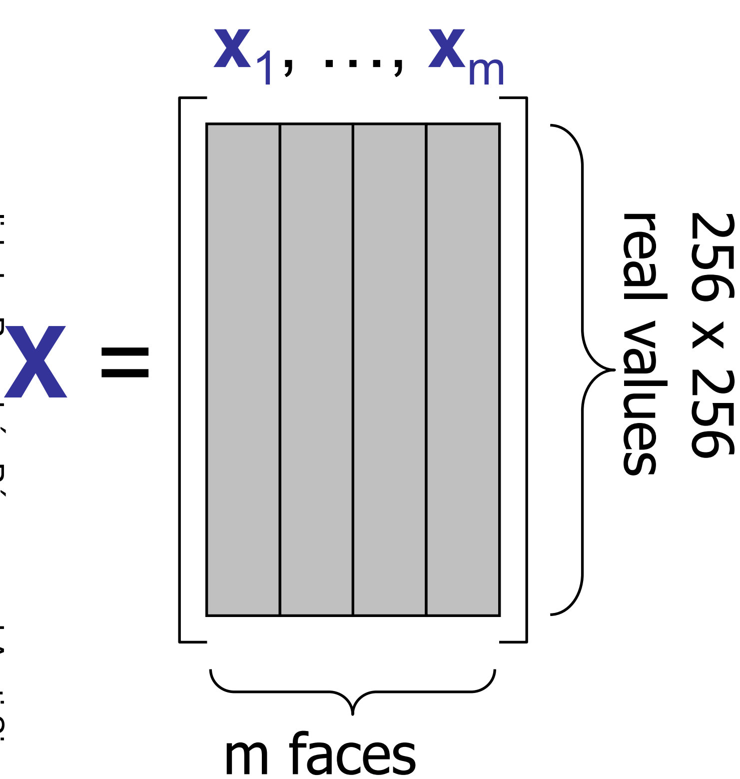
Applying PCA: Eigenfaces

Method A: Build a PCA subspace for each person and check which subspace can reconstruct the test image the best

Method B: Build one PCA database for the whole dataset and then classify based on the weights.

- ❑ Example data set: Images of faces
  - Famous Eigenface approach
    [Turk & Pentland], [Sirovich & Kirby]
- ❑ Each face $\mathbf{x}$ is …
  - 256×256 values (luminance at location)
  - $\mathbf{x}$ in $\Re^{256\times256}$ (view as 64K dim vector)
- ❑ Form $\mathbf{X} = [\ \mathbf{x}_1, \dots, \mathbf{x}_m\ ]$ **centered** data mtx
- ❑ Compute $\Sigma = \mathbf{X}\mathbf{X}^T$
- ❑ Problem: Σ is $64K \times 64K$ … HUGE!!!



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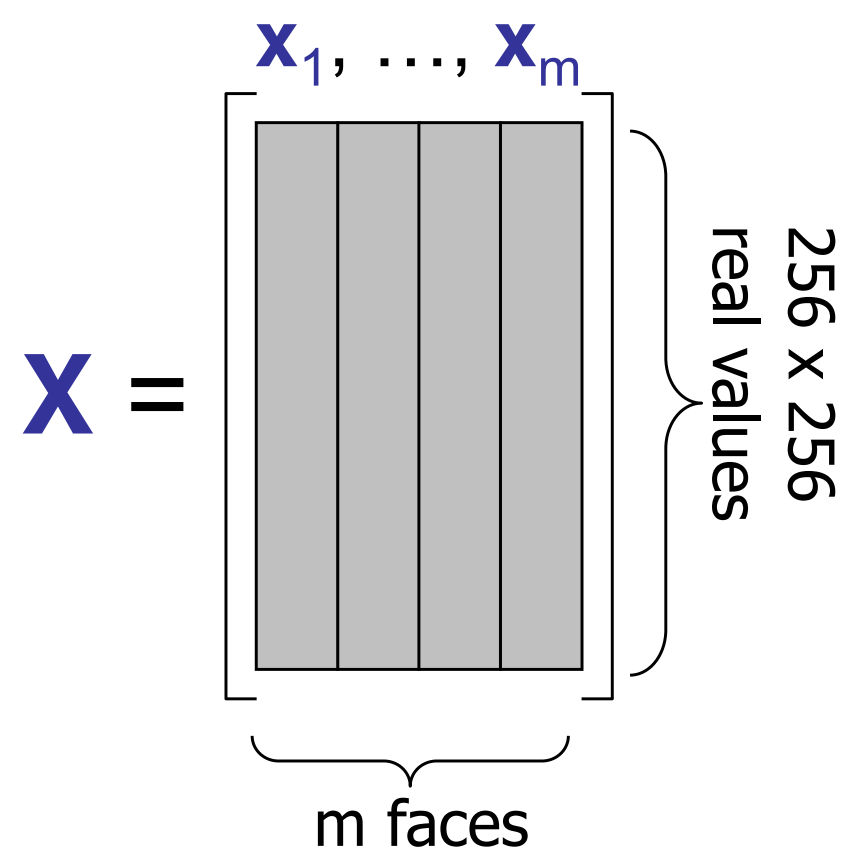
A Clever Workaround

- Note that $m << 64K$
- Use $\mathbf{L=X^TX}$ instead of $\mathbf{\Sigma=XX^T}$
- If $\mathbf{v}$ is eigenvector of $\mathbf{L}$
  then $\mathbf{Xv}$ is eigenvector of Σ



Proof:

$$\mathbf{L\ v} = \gamma\ \mathbf{v}$$

$$\mathbf{X^TX\ v} = \gamma\ \mathbf{v}$$

$$\mathbf{X\ (X^TX\ v)} = \mathbf{X}(\gamma\ \mathbf{v}) = \gamma\ \mathbf{Xv}$$

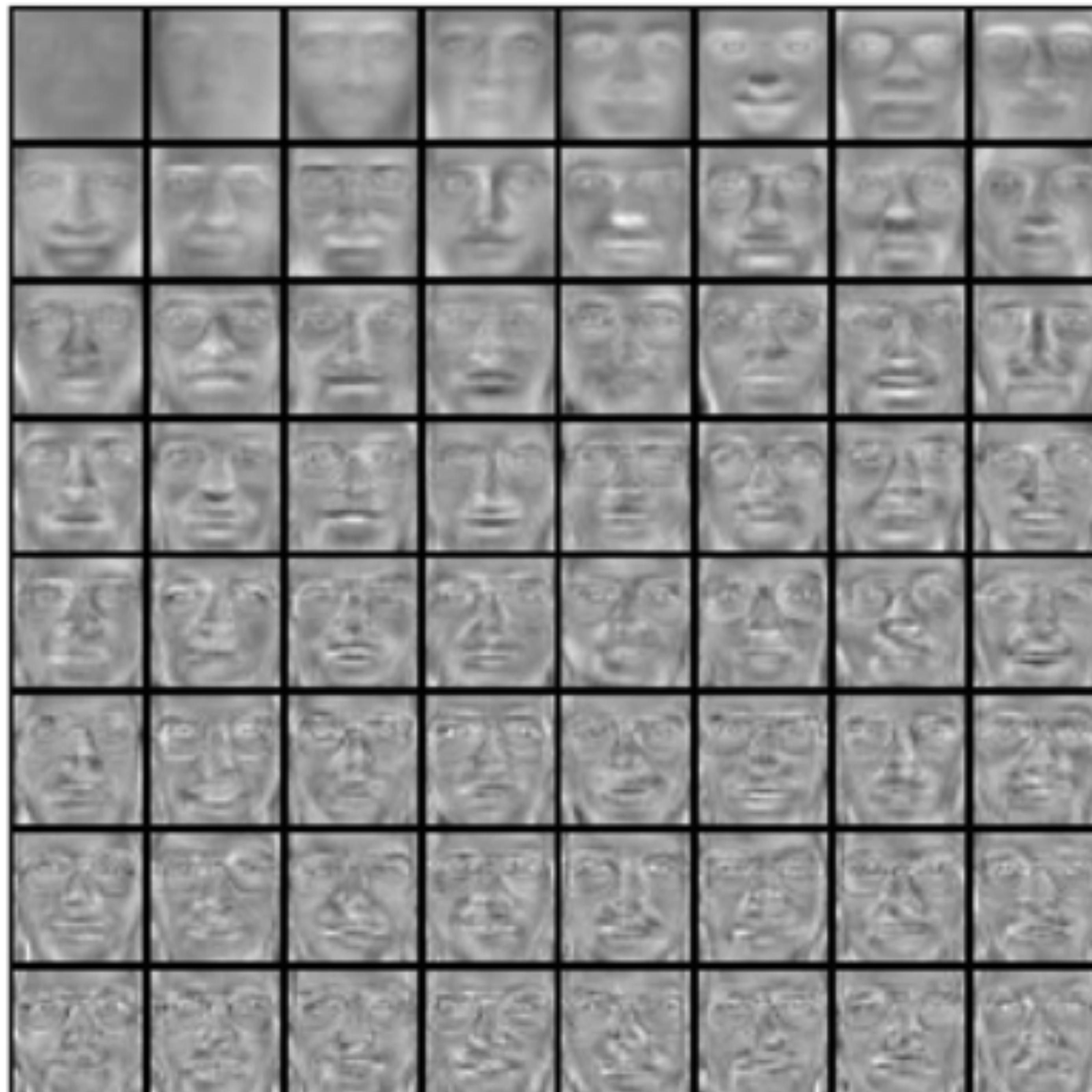
$$\mathbf{(XX^T)X\ v} = \gamma\ \mathbf{(Xv)}$$

$$\Sigma\ \mathbf{(Xv)} = \gamma\ \mathbf{(Xv)}$$

Eigenfaces Example

Mean: μ

Top eigenvectors: $u_1, \ldots u_k$



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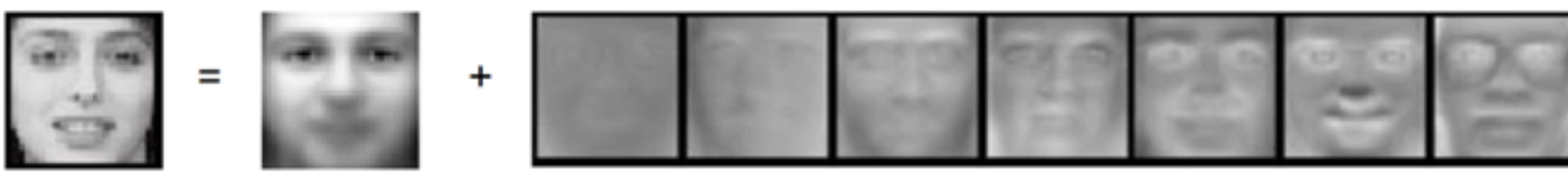
Representation and Reconstruction

- Face $\mathbf{x}$ in "face space" coordinates:

$$\mathbf{x} \rightarrow [\mathbf{u}_1^{\mathrm{T}}(\mathbf{x} - \mu), \ldots, \mathbf{u}_k^{\mathrm{T}}(\mathbf{x} - \mu)]$$
$$= \quad w_1, \ldots, w_k$$

- Reconstruction:



$\hat{x} = \mu + w_1u_1 + w_2u_2 + w_3u_3 + w_4u_4 + \ldots$

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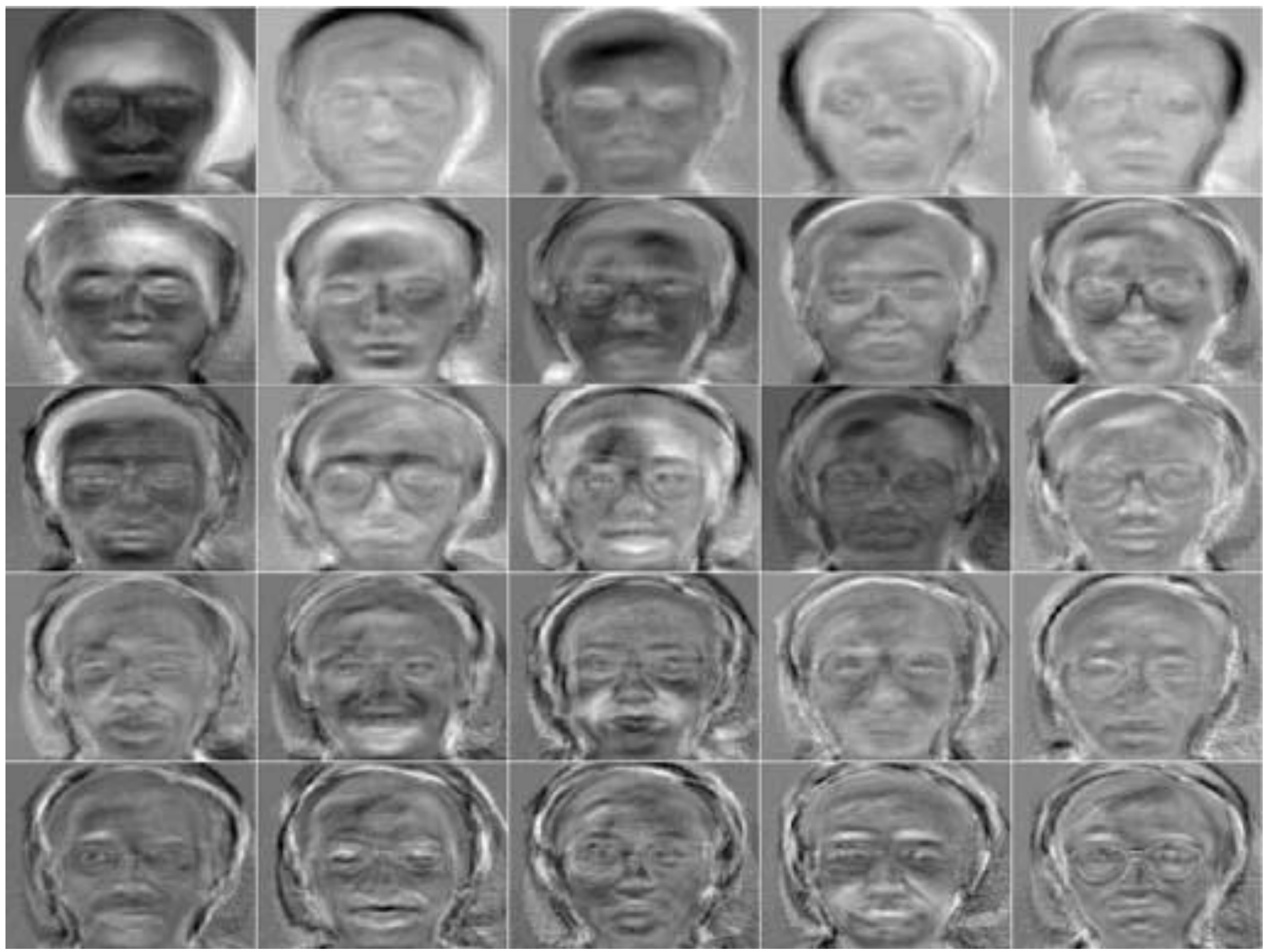
Principle Components (Method B)



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Principle Components (Method B)

- … faster if train with …
  - only people w/out glasses
  - same lighting conditions

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When projecting strange data

- Original images
- Reconstruction doesn't look like the original

slide by Alex Smola

Happiness subspace (method A)

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Disgust subspace (method A)

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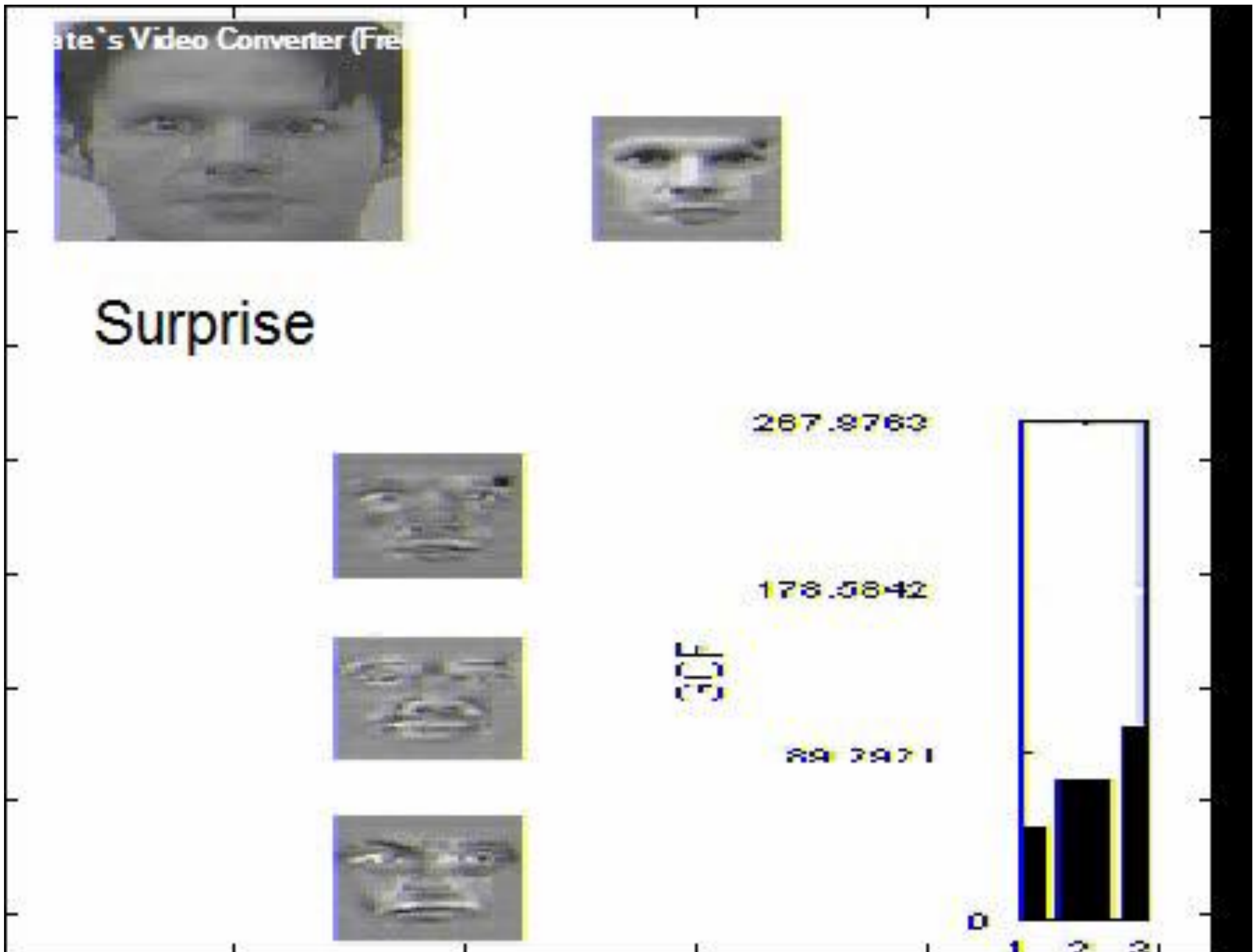
Facial Expression Recognition Movies



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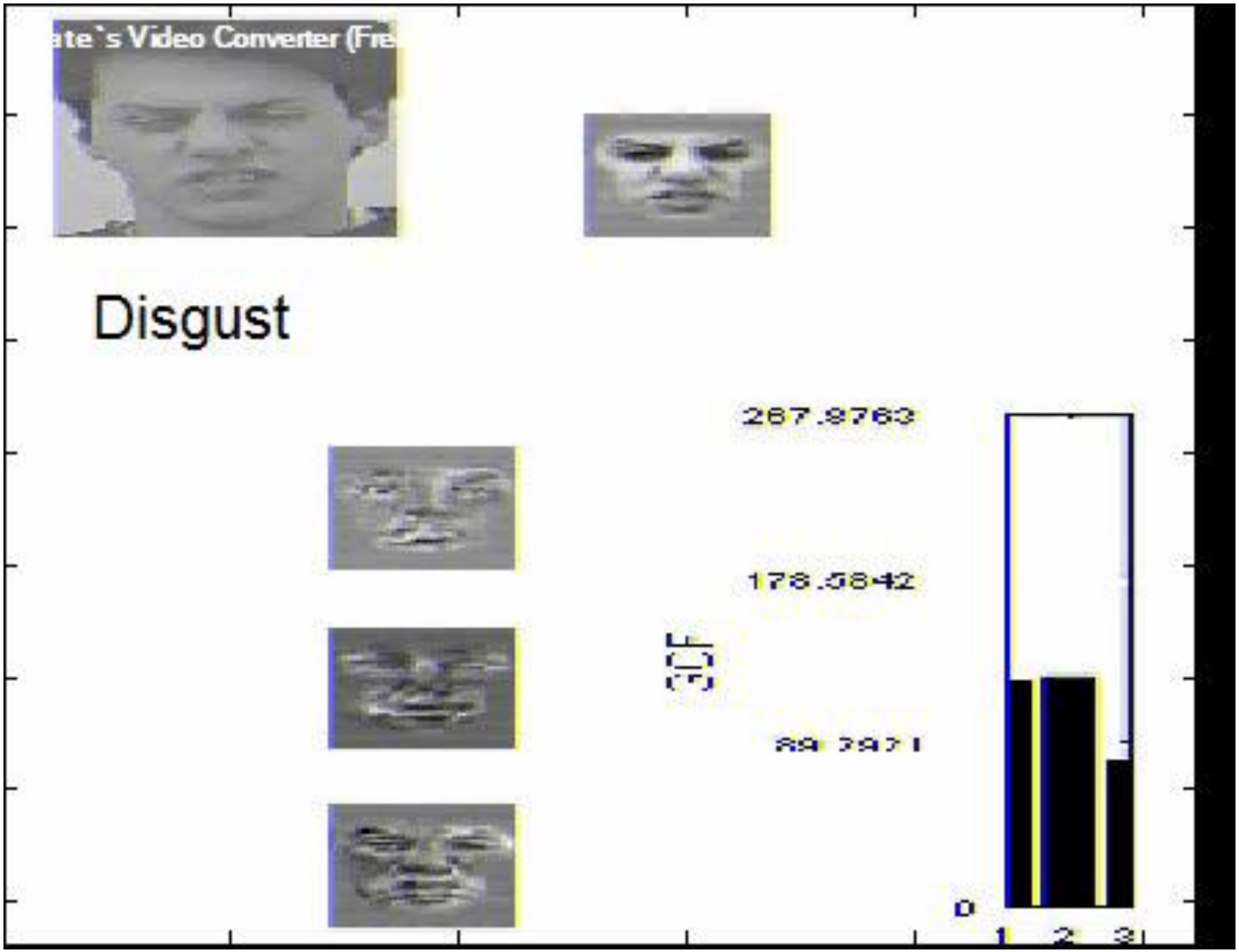
Facial Expression Recognition Movies

Facial Expression Recognition Movies



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Shortcomings

- Requires carefully controlled data:
  - All faces centered in frame
  - Same size
  - Some sensitivity to angle
- Method is completely knowledge free
  - (sometimes this is good!)
  - Doesn't know that faces are wrapped around 3D objects (heads)
  - Makes no effort to preserve class distinctions

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Image Compression

Original Image

- Divide the original 372x492 image into patches:
  - Each patch is an instance
- View each as a 144-D vector

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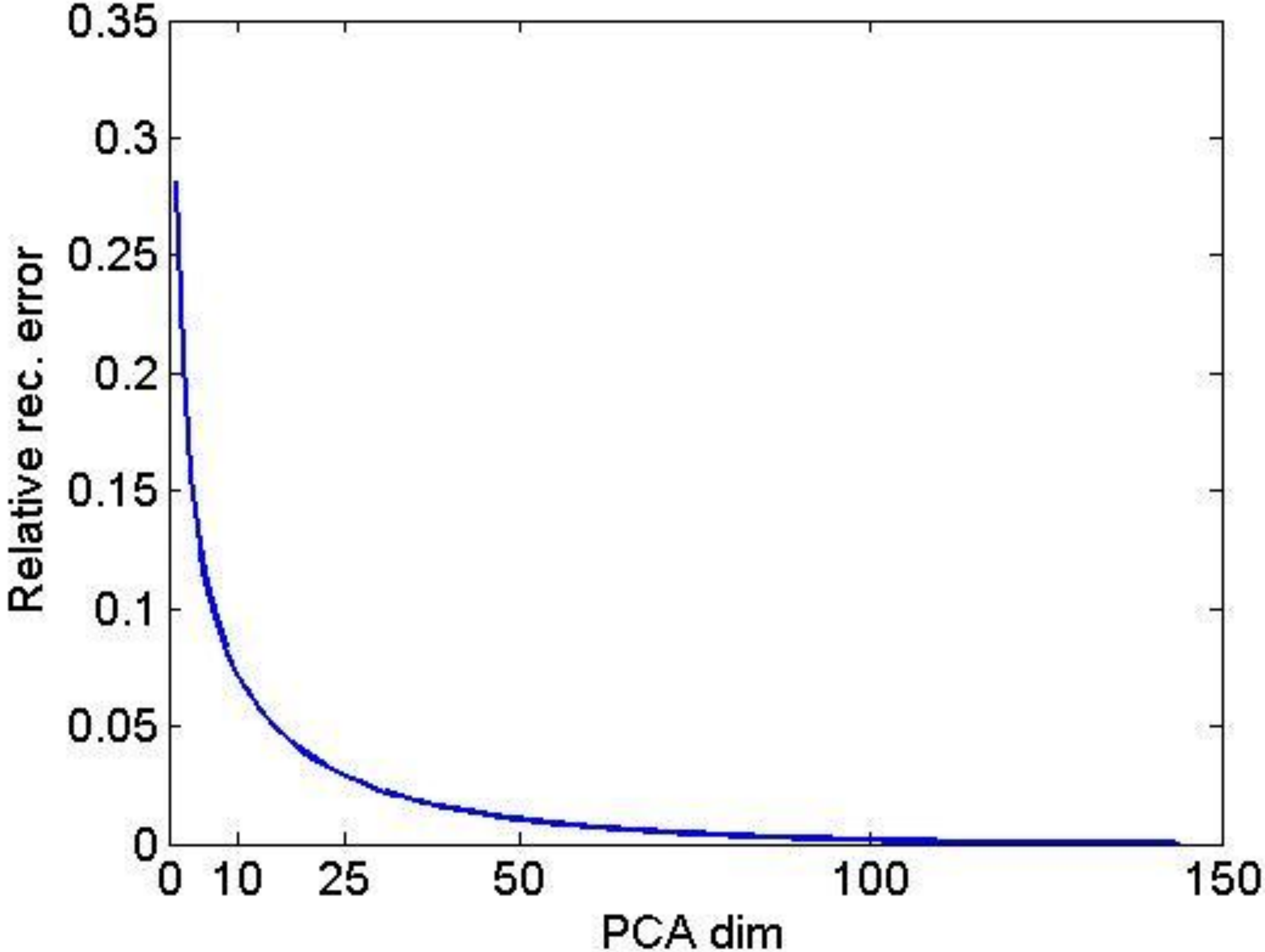
L_2 error and PCA dim



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PCA compression: 144D => 60D

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PCA compression: 144D => 16D

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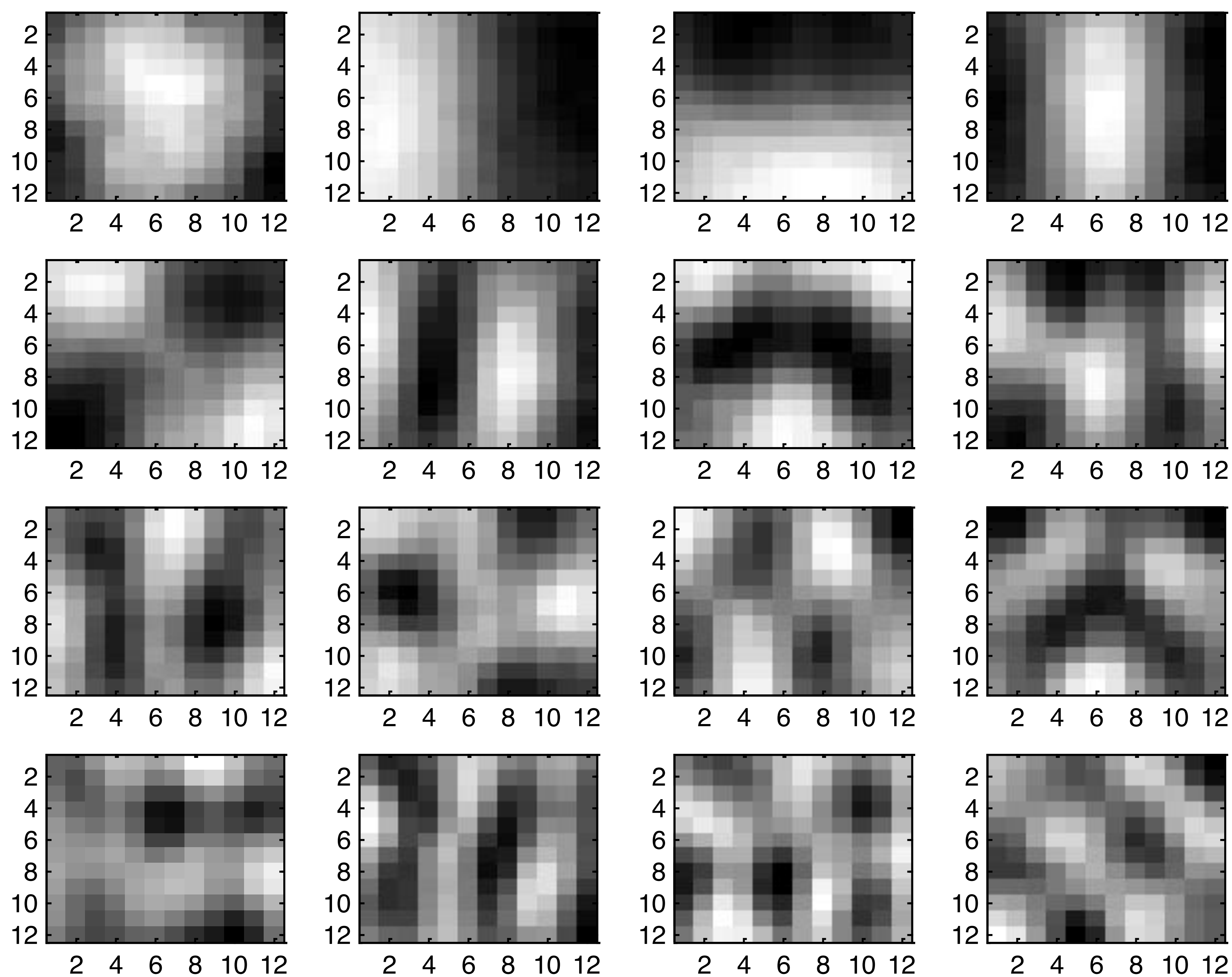
16 most important eigenvectors



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PCA compression: 144D => 6D

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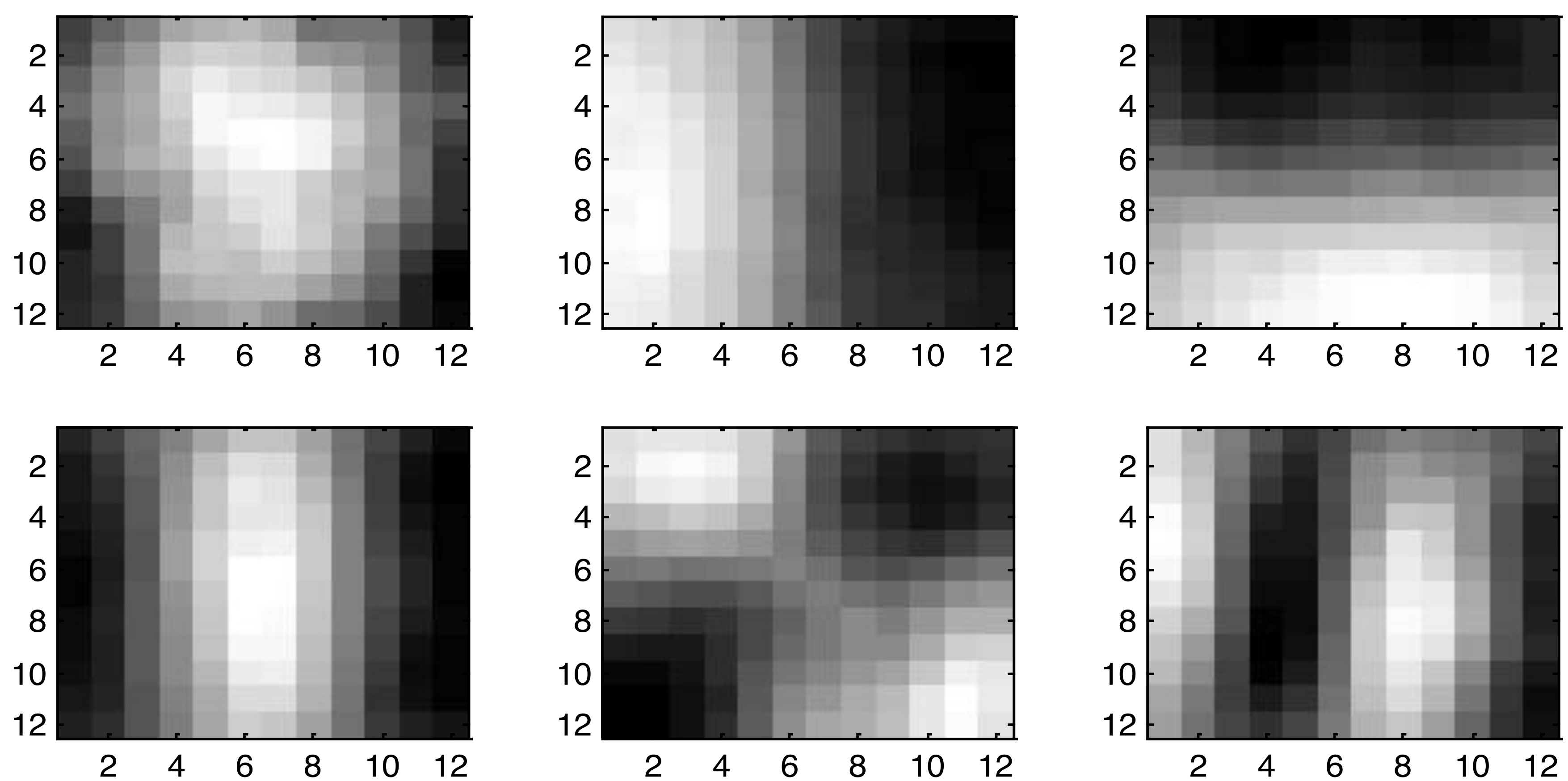
6 most important eigenvectors



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PCA compression: 144D => 3D

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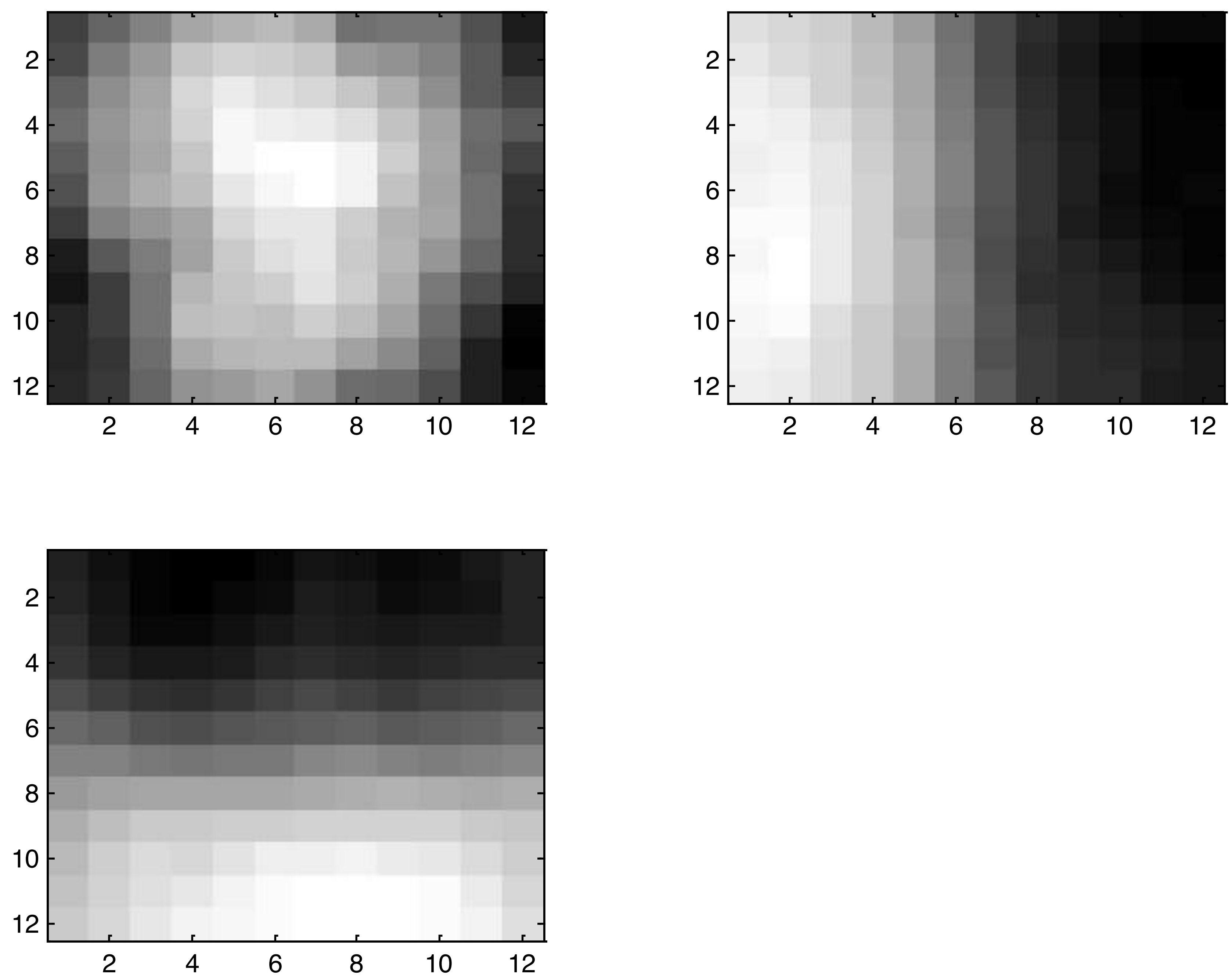
3 most important eigenvectors



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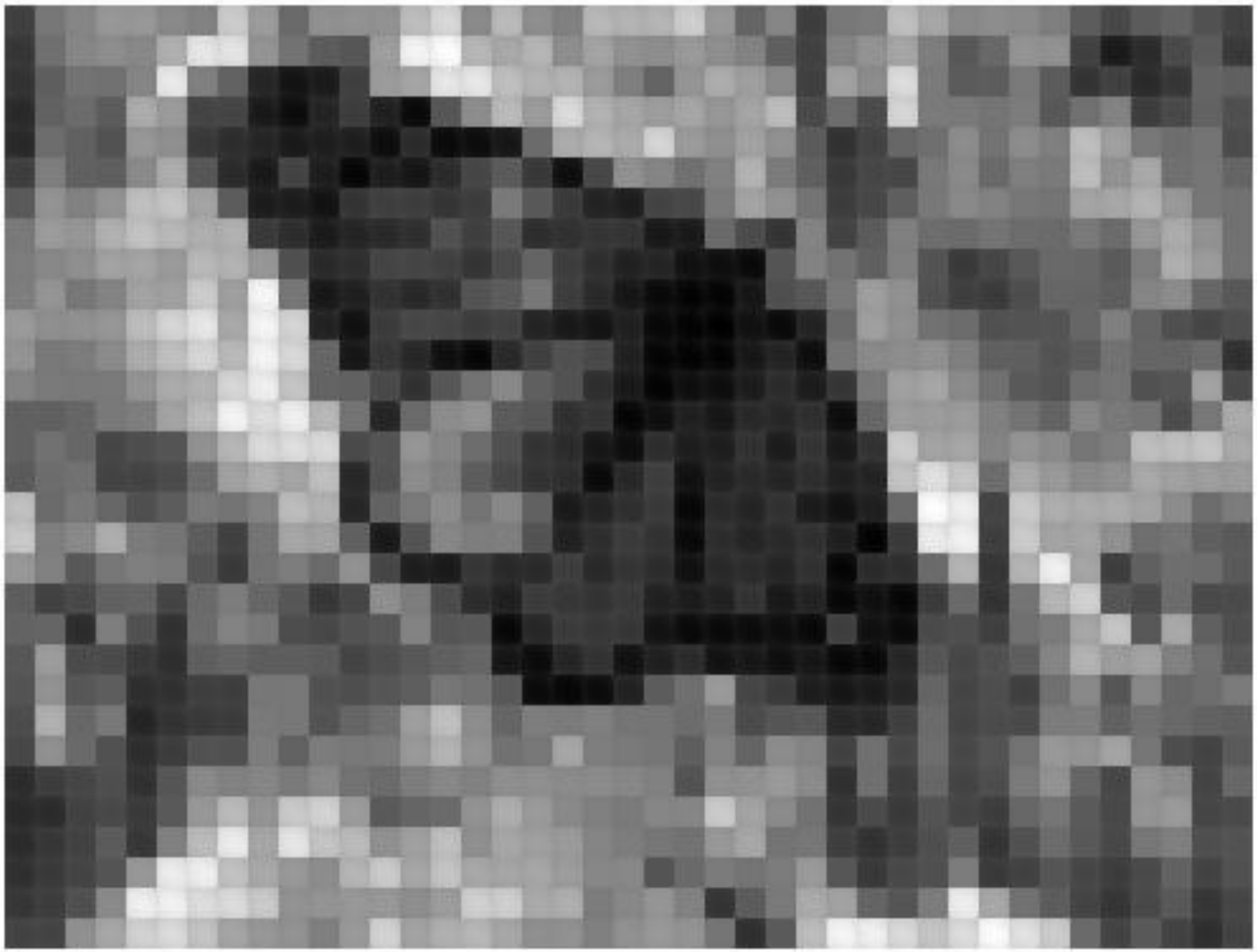
PCA compression: 144D => 1D



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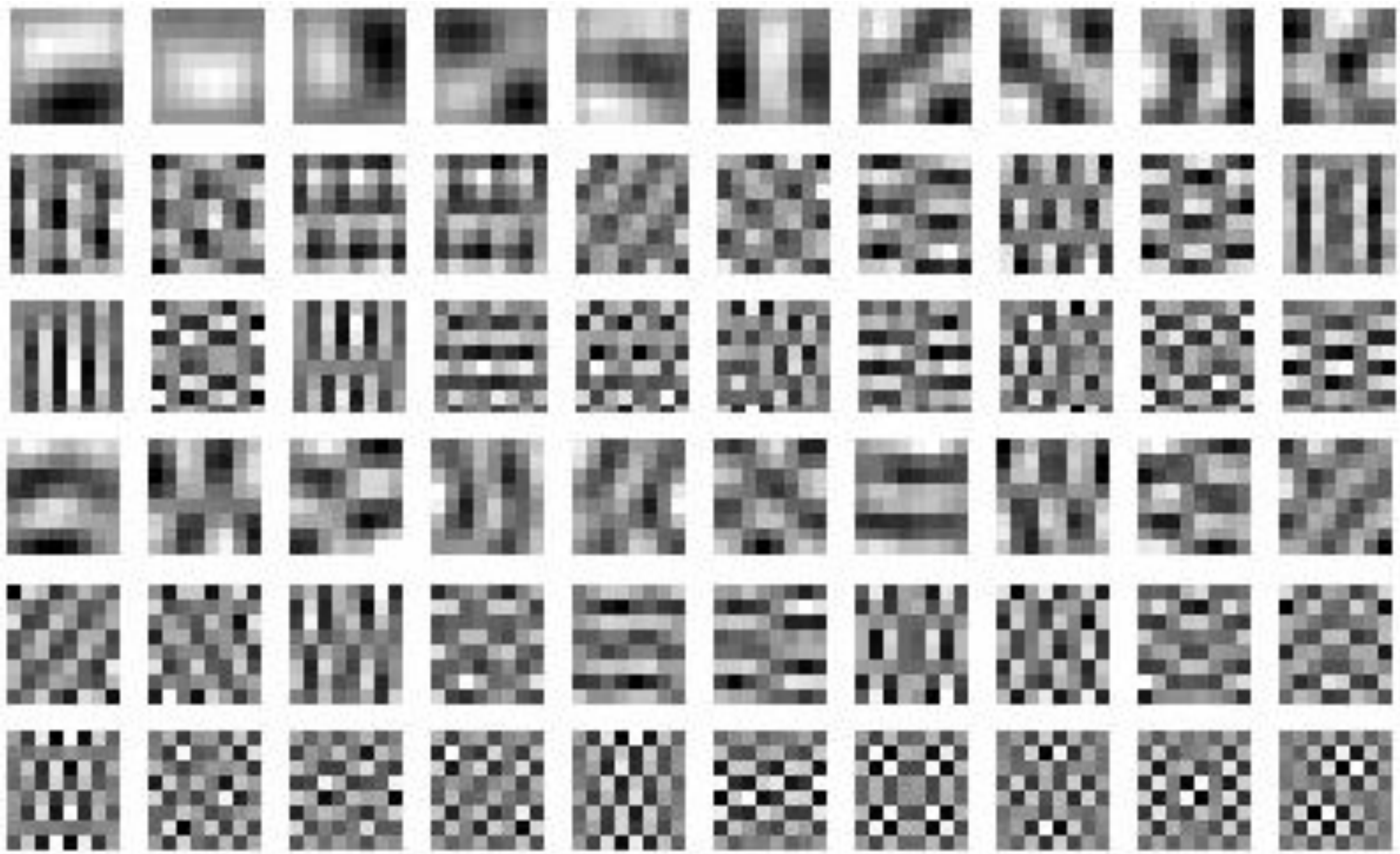
60 most important eigenvectors



- Looks like the discrete cosine bases of JPG!…

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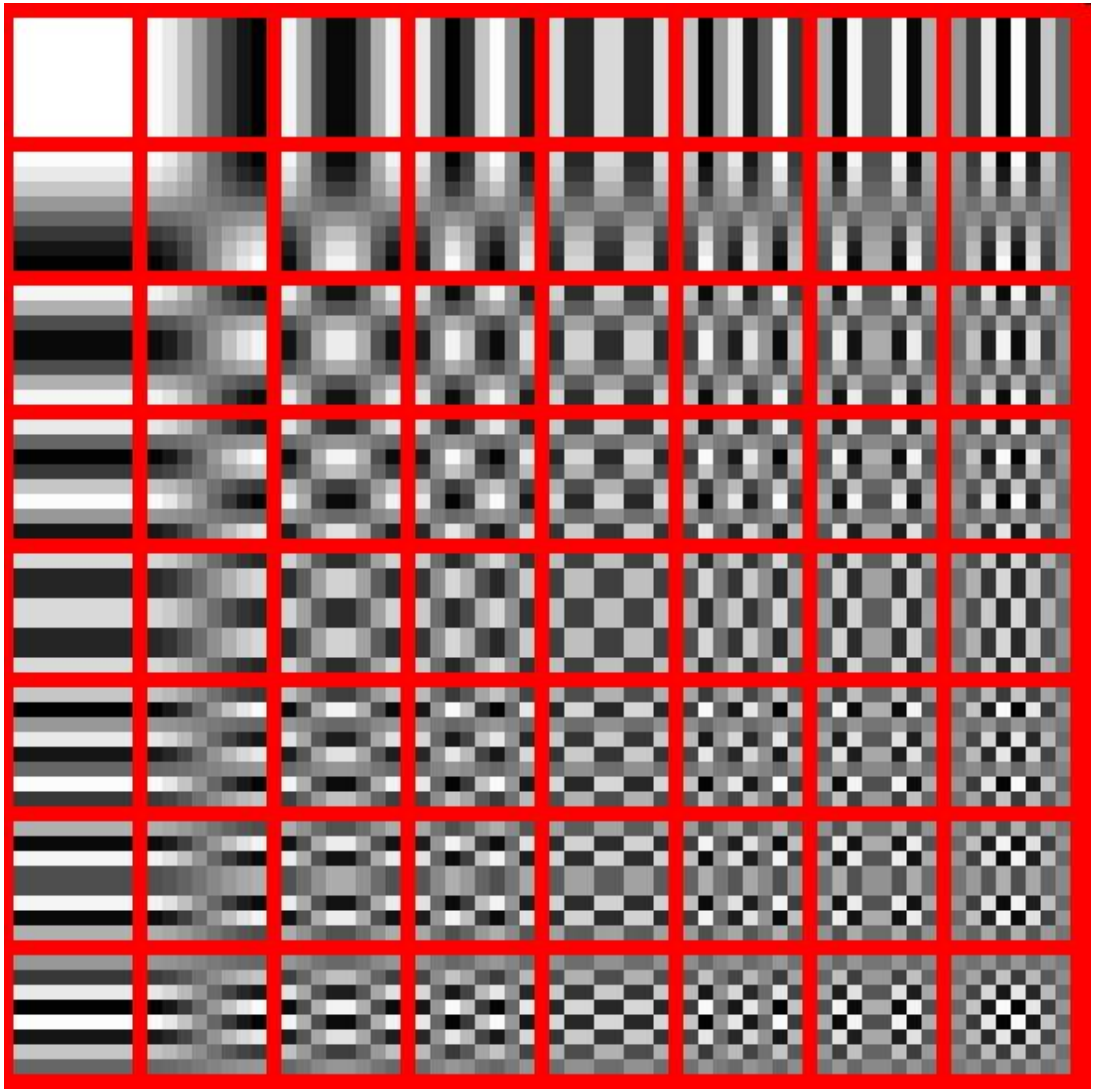
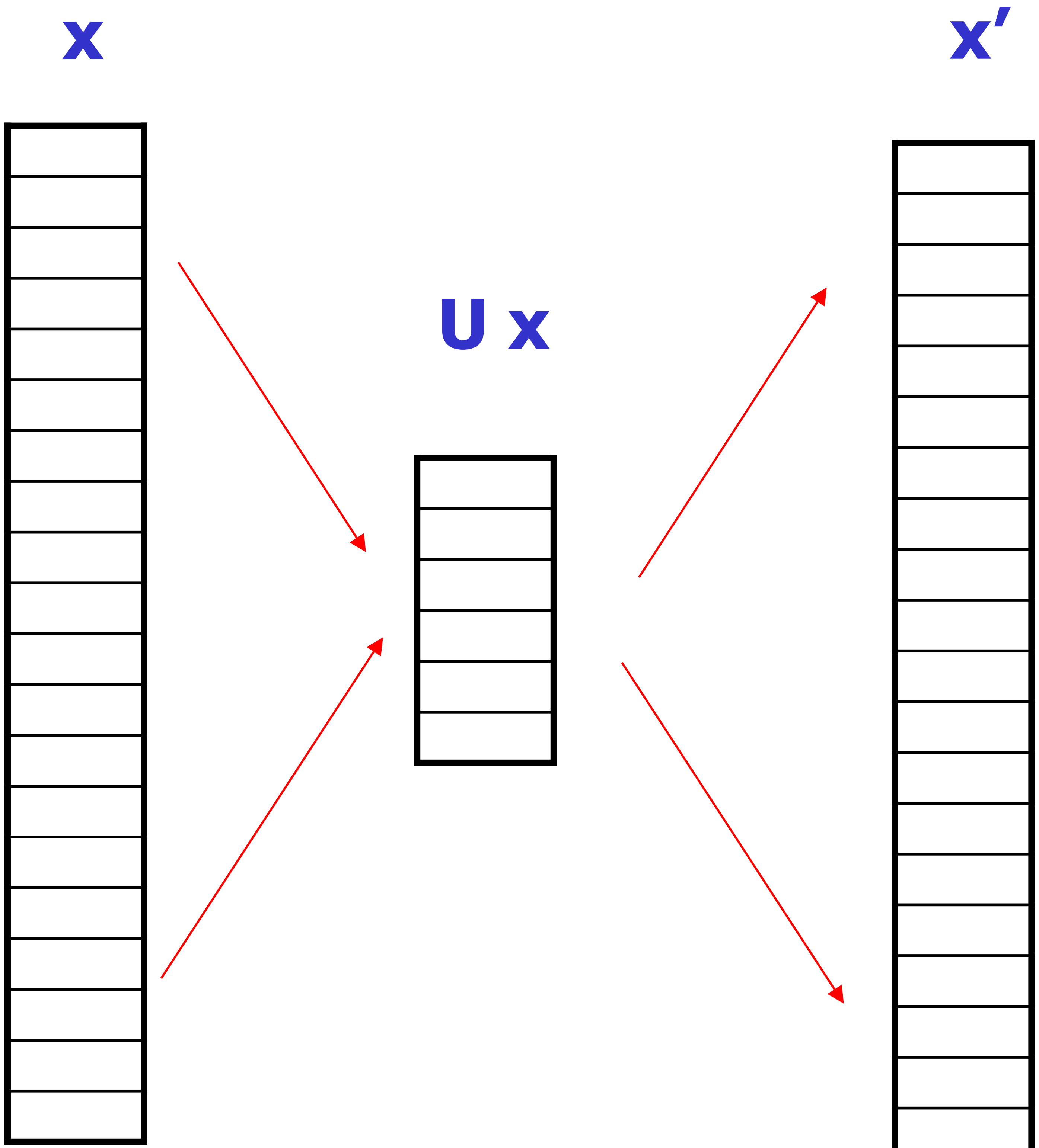
2D Discrete Cosine Basis



http://en.wikipedia.org/wiki/Discrete_cosine_transform

Noise Filtering

Noise Filtering



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Noisy image

Denoised image using 15 PCA components

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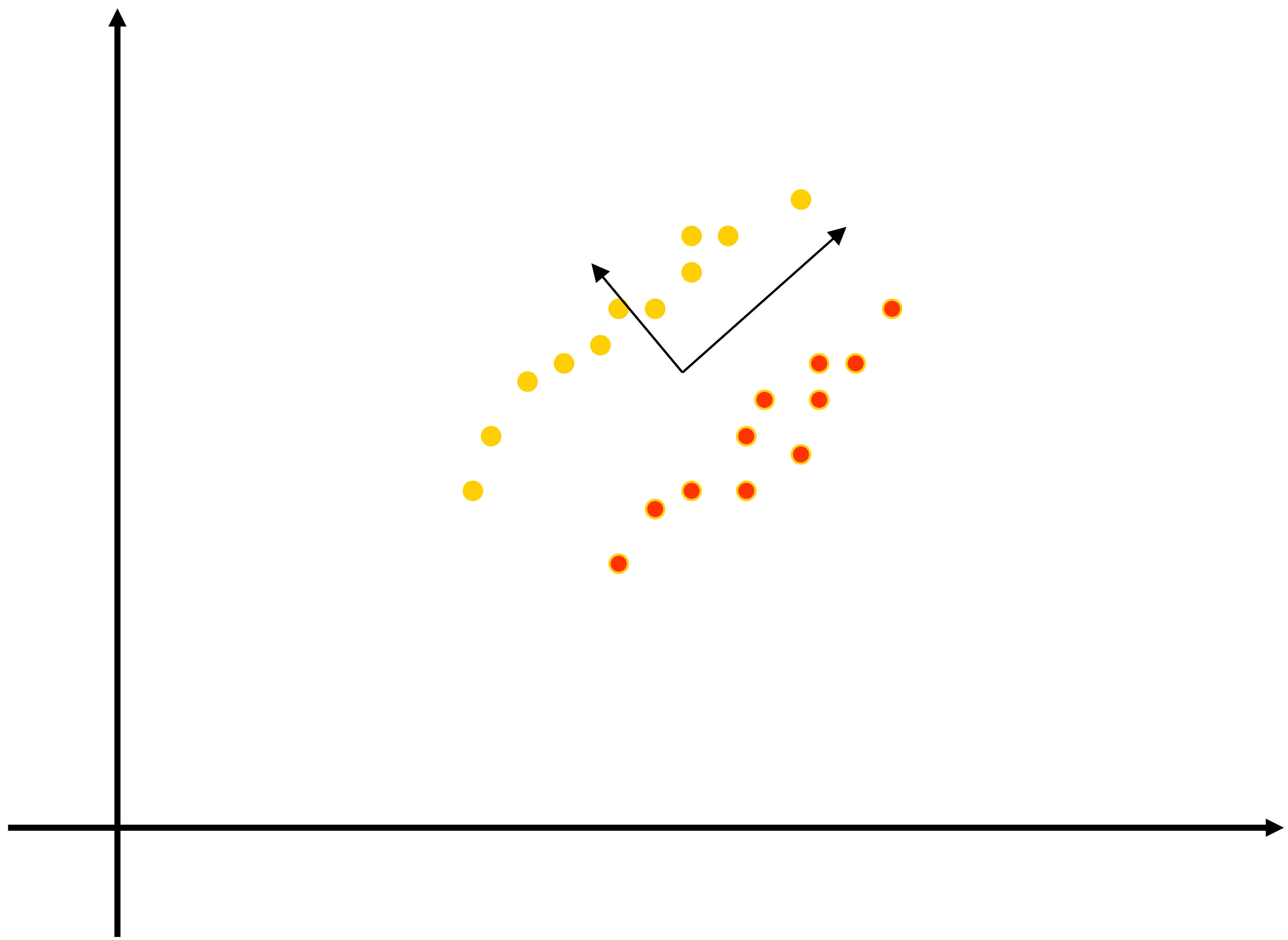
PCA Shortcomings

Problematic Data Set for PCA

- PCA doesn't know labels!



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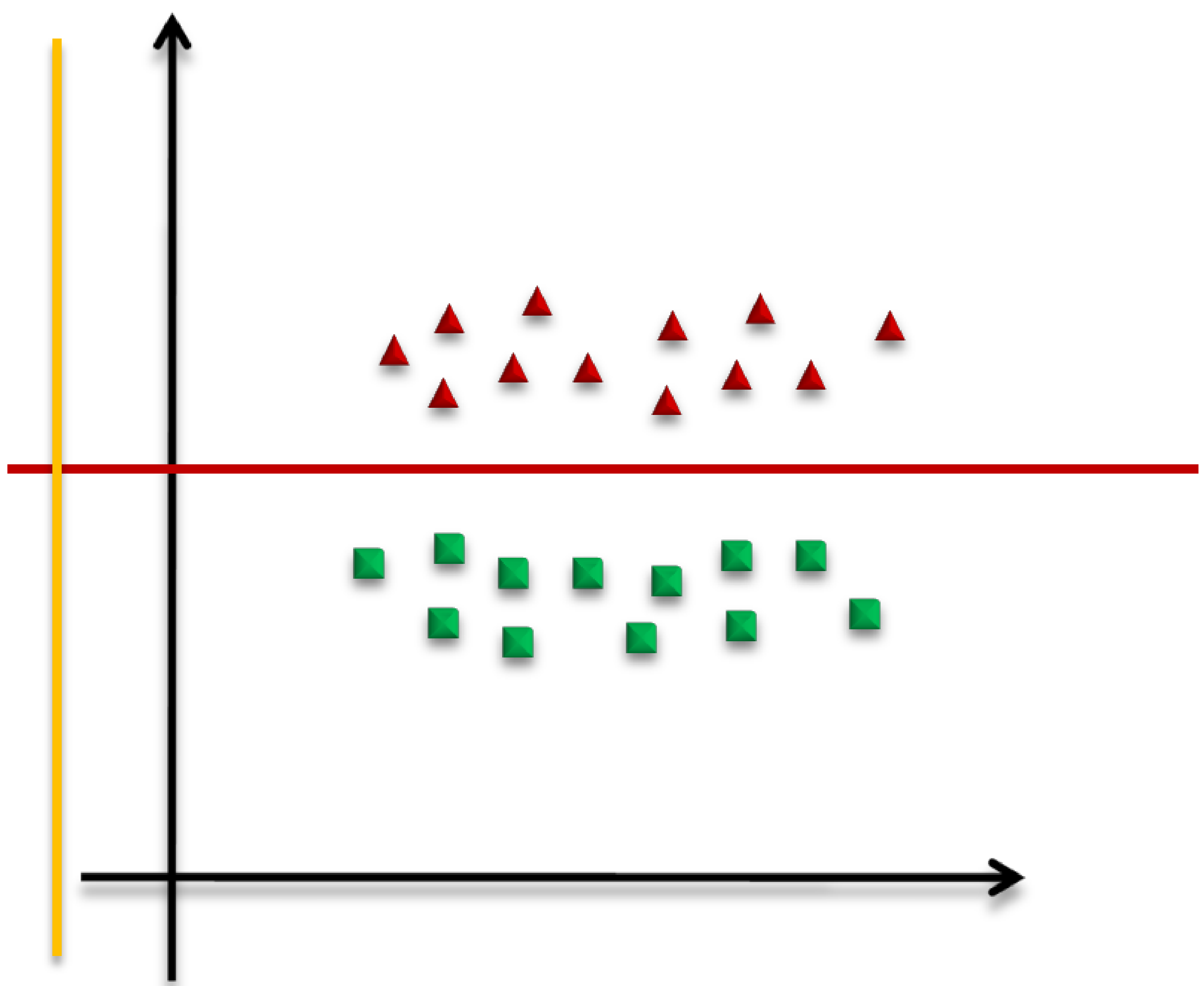
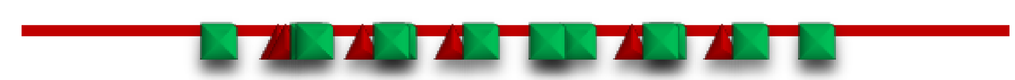
PCA vs. Fisher Linear Discriminant



Principal Component Analysis

- higher variance
- bad for discriminability



Fisher Linear Discriminant

- smaller variance
- good discriminability

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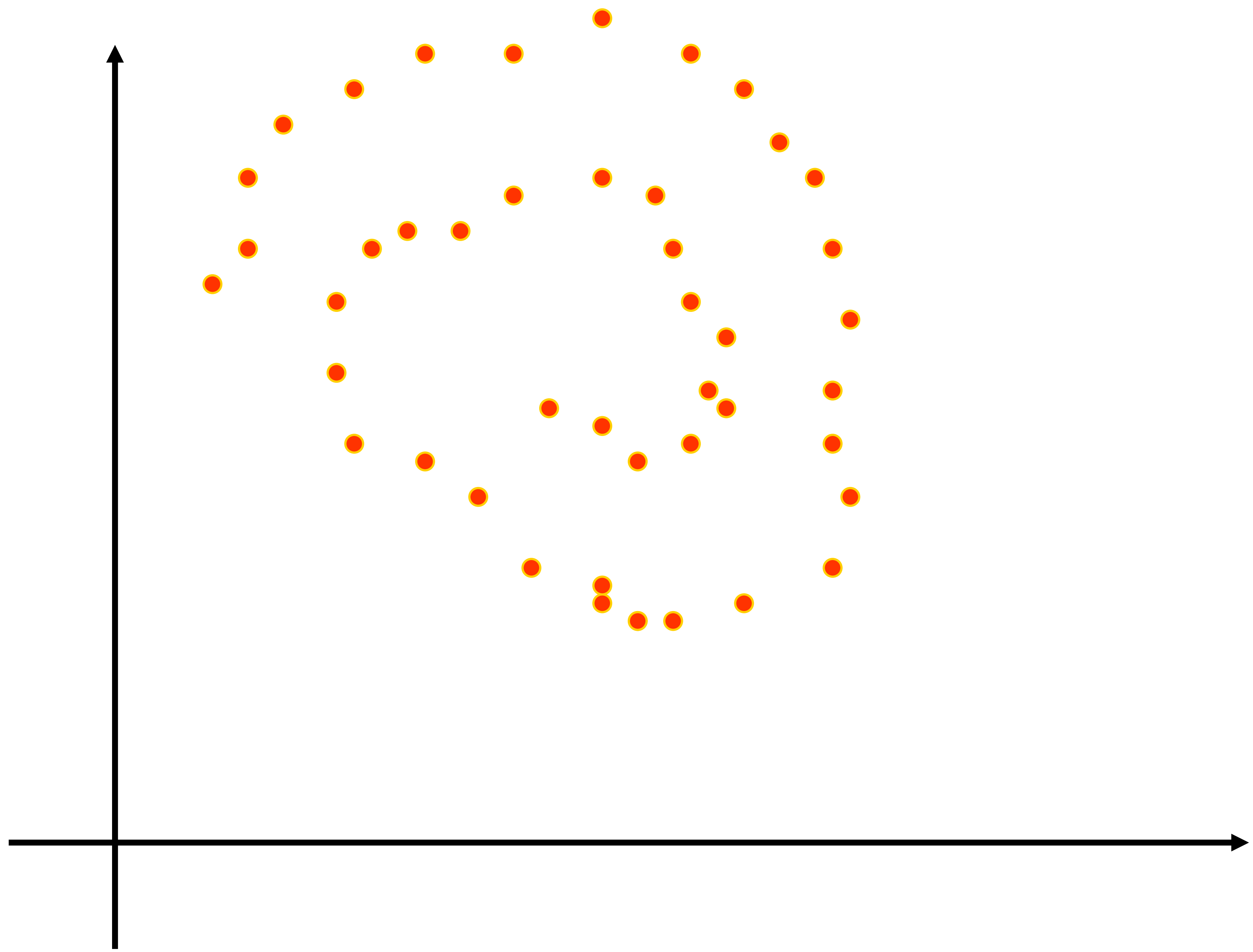
Problematic Data Set for PCA

- PCA cannot capture NON-LINEAR structure!



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PCA Conclusions

- 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)
- Not magic:
  - Doesn’t know class labels
  - Can only capture linear variations
- One of many tricks to reduce dimensionality!

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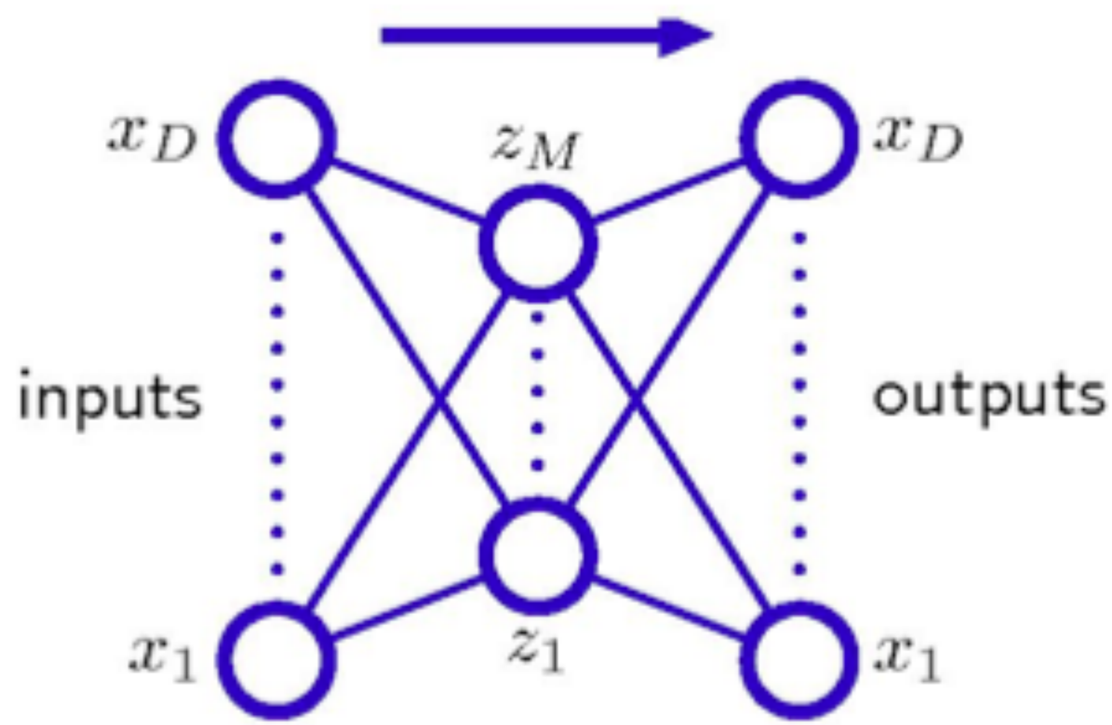
Autoencoders

Relation to Neural Networks

- PCA is closely related to a particular form of neural network
- An autoencoder is a neural network whose outputs are its own inputs



- The goal is to minimize reconstruction error

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Auto encoders

- Define

$$\mathbf{z} = f(W\mathbf{x}); \quad \hat{\mathbf{x}} = g(V\mathbf{z})$$

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Auto encoders

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$$\mathbf{z} = f(W\mathbf{x}); \quad \hat{\mathbf{x}} = g(V\mathbf{z})$$

- Goal:

$$\min_{\mathbf{W},\mathbf{V}} \ \frac{1}{2N}\sum_{n=1}^{N}||\mathbf{x}^{(n)} - \hat{\mathbf{x}}^{(n)}||^2$$

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Auto encoders

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- Goal:

$$\min_{\mathbf{W},\mathbf{V}} \frac{1}{2N} \sum_{n=1}^{N} ||\mathbf{x}^{(n)} - \hat{\mathbf{x}}^{(n)}||^2$$

- If g and f are linear

$$\min_{\mathbf{W},\mathbf{V}} \frac{1}{2N} \sum_{n=1}^{N} ||\mathbf{x}^{(n)} - VW\mathbf{x}^{(n)}||^2$$

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Auto encoders

- Define

$$\mathbf{z} = f(W\mathbf{x}); \quad \hat{\mathbf{x}} = g(V\mathbf{z})$$

- Goal:

$$\min_{\mathbf{W},\mathbf{V}} \frac{1}{2N} \sum_{n=1}^{N} ||\mathbf{x}^{(n)} - \hat{\mathbf{x}}^{(n)}||^2$$

- If *g* and *f* are linear

$$\min_{\mathbf{W},\mathbf{V}} \frac{1}{2N} \sum_{n=1}^{N} ||\mathbf{x}^{(n)} - VW\mathbf{x}^{(n)}||^2$$

- In other words, the optimal solution is PCA

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Auto encoders: Nonlinear PCA

- What if *g*( ) is not linear?
- Then we are basically doing **nonlinear PCA**
- Some subtleties but in general this is an accurate description

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Comparing Reconstructions

Real data

30-d deep autoencoder

30-d logistic PCA

30-d PCA

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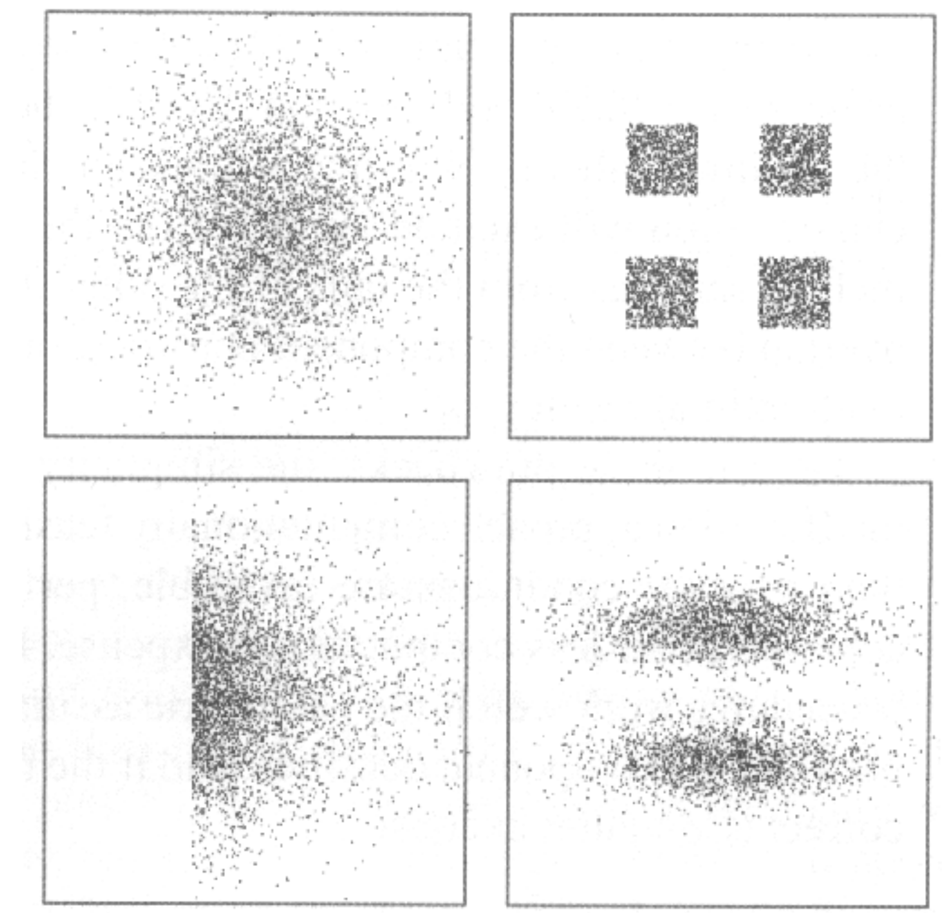
Independent Component Analysis (ICA)

A Serious Limitation of PCA

- Recall that PCA looks at the covariance matrix only. What if the data is not well described by the covariance matrix?



- The only distribution which is uniquely specified by its covariance (with the subtracted mean) is the Gaussian distribution. Distributions which deviate from the Gaussian are poorly described by their covariances.

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Faithful vs Meaningful Representations

- Even with non-Gaussian data, variance maximization leads to the most faithful representation in a reconstruction error sense (recall that we trained our autoencoder network using a mean-square error in an input reconstruction layer).

- The mean-square error measure implicitly assumes Gaussianity, since it penalizes datapoints close to the mean less that those that are far away.

- But it does not in general lead to the most meaningful representation.

- We need to perform gradient descent in some function other than the reconstruction error.

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A Criterion Stronger than Decorrelation

- The way to circumvent these problems is to look for components which are statistically independent, rather than just uncorrelated.

- For statistical independence, we require that

$$p(\xi_1, \xi_2, \cdots, \xi_N) \;=\; \prod_{i=1}^{N} p(\xi_i)$$

- For uncorrelatedness, all we required was that

$$\langle \xi_i \xi_j \rangle - \langle \xi_i \rangle \langle \xi_j \rangle \;=\; 0\,, \quad i \neq j$$

- Independence is a stronger requirement; under independence,

$$\langle g_1(\xi_i) g_2(\xi_j) \rangle - \langle g_1(\xi_i) \rangle \langle g_2(\xi_j) \rangle \;=\; 0\,, \quad i \neq j$$

for any functions g_1 and g_2.

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Independent Component Analysis (ICA)

- Like PCA, except that we're looking for a transformation subject to the stronger requirement of independence, rather than uncorrelatedness.
- In general, no analytic solution (like eigenvalue decomposition for PCA) exists, so ICA is implemented using neural network models.
- To do this, we need an architecture and an objective function to descend/climb in.
- Leads to *N* independent (or as independent as possible) components in *N*-dimensional space; they need not be orthogonal.
- When are independent components identical to uncorrelated (principal) components? When the generative distribution is uniquely determined by its first and second moments. This is true of only the Gaussian distribution.

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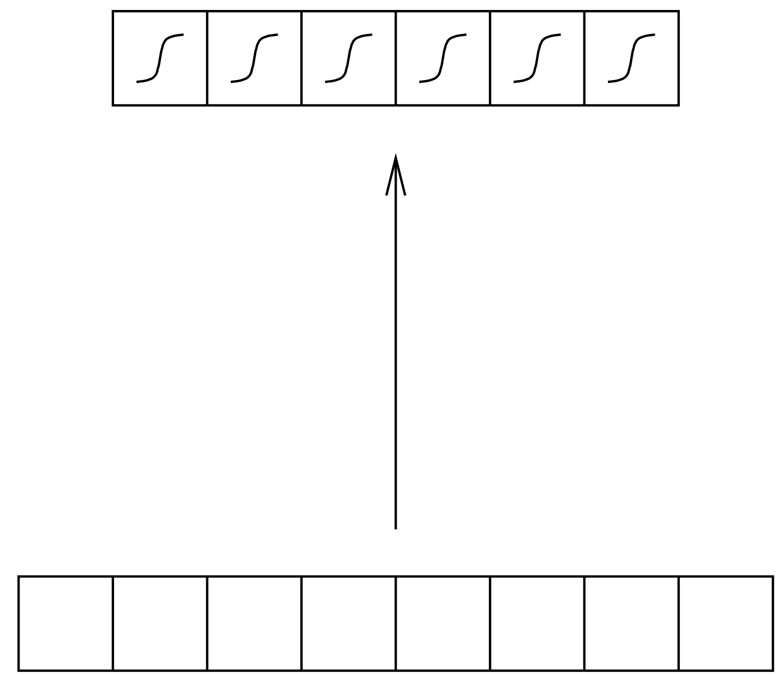
Neural Network for ICA

- Single layer network:



- Patterns $\{\xi\}$ are fed into the input layer.
- Inputs multiplied by weights in matrix **W**.
- Output logistic (vector notation here):

$$\bar{y} = \frac{1}{1 + e^{\mathbf{W}^T \bar{\xi}}}$$

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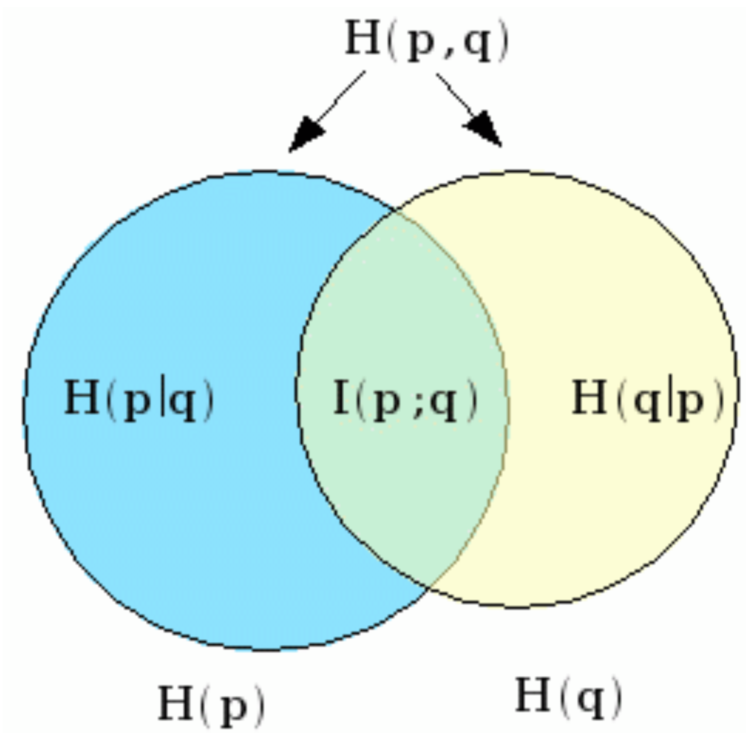
Objective Function for ICA

- Want to ensure that the outputs y_i are maximally independent.
- This is identical to requiring that the mutual information be small. Or alternately that the joint entropy be large.



$$
\begin{aligned}
H(p) &= \text{entropy of distribution } p \text{ of first neuron's output} \\
H(p|q) &= \text{conditional entropy} \\
I(p;q) &= H(p) - H(q|p) \\
&= H(q) - H(p|q) \\
&= \text{mutual information}
\end{aligned}
$$

- Gradient ascent in this objective function is called infomax (we're trying to maximize the enclosed area representing information quantities).

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Blind Source Separation (BSS)

- The most famous application of ICA.
- Have K sources $\{s_k[t]\}$, and K signals $\{x_k[t]\}$. Both $\{s_k[t]\}$ and $\{x_k[t]\}$ are time series (t is a discrete time index).
- Each signal is a linear mixture of the sources

$$x_k[t] \;=\; \mathbf{A}s_k[t] + n_k[t]$$

  where $n_k[t]$ is the noise contribution in the kth signal $x_k[t]$, and $\mathbf{A}$ is a mixture matrix.

- The problem: given $x_k[n]$, determine $\mathbf{A}$ and $s_k[n]$.

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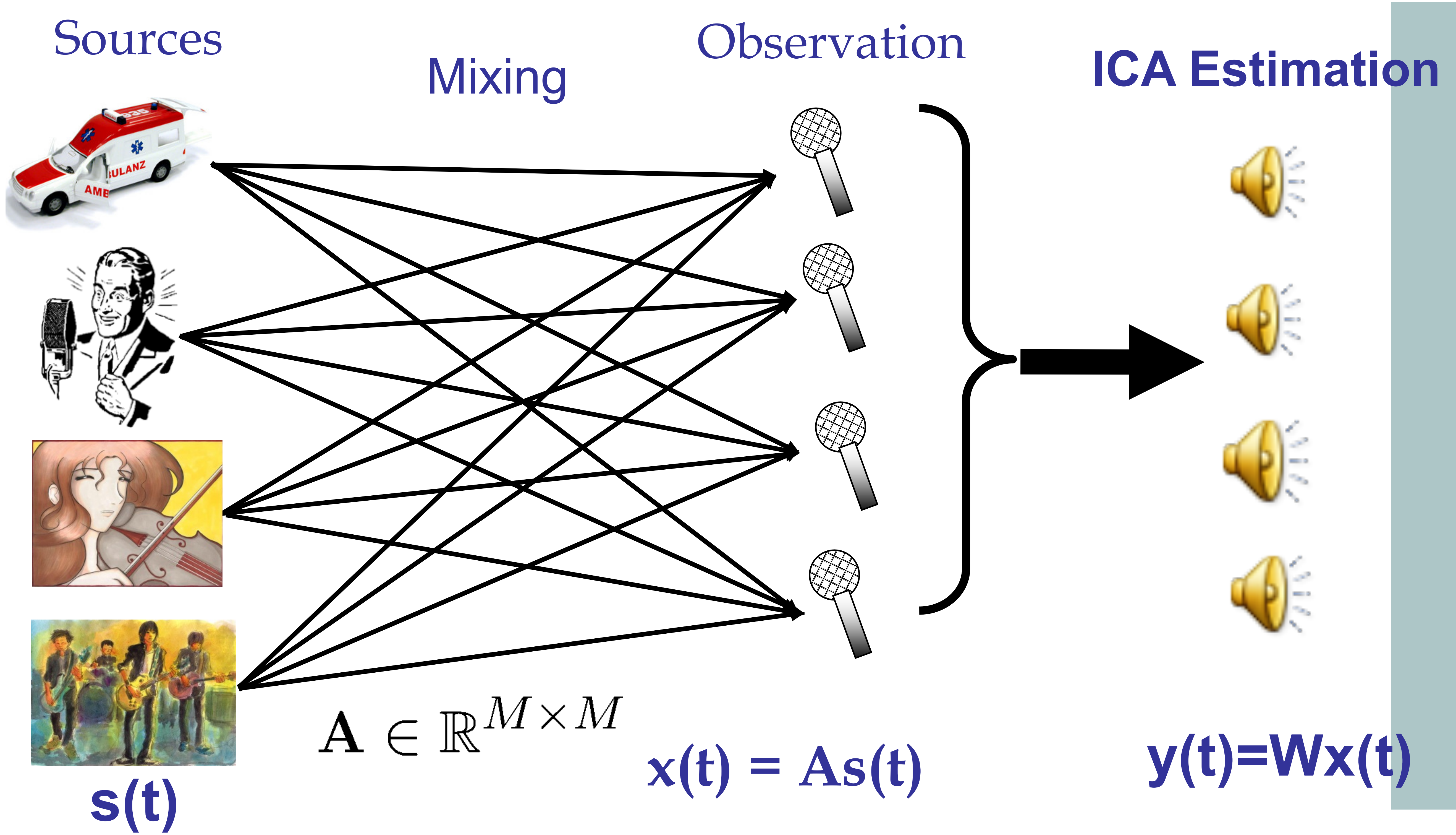
The Cocktail Party



Demo: The Cocktail Party

- Frequency domain ICA (1995)

Input mix:

Extracted speech: