Dimensionality Reduction

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Contents

Question 1

1) In the standard PCA pipeline, what is the *first* operation you should do on the data matrix X?

A. Compute the SVD of X directly

B. Subtract the mean of each feature (center the data)

C. Normalize every feature to unit variance

D. Build the kernel matrix K

Question 2

2) In PCA, each eigenvalue of the covariance matrix represents:

A. The covariance between pairs of features
B. The variance captured along its corresponding principal component
C. The reconstruction error of the model
D. The correlation between the first two principal components

Question 3

3) Which statement best captures the relationship between SVD and PCA?

A. PCA is done by applying SVD to the *covariance* matrix

B. PCA and SVD are unrelated

C. SVD is done by applying PCA to X

D. PCA returns the left singular vectors of X as principal components

Question 4

4) Lloyd's K-means algorithm minimizes which objective?

A. Sum of absolute distances to cluster medoids

B. Sum of squared distances of each point to its assigned centroid

C. Sum of pairwise distances inside each cluster

D. Negative log-likelihood under a Gaussian mixture

Question 5

5) In the assignment step of K-means with fixed centroids, each point is assigned to the cluster whose centroid is:

A. Farthest in Euclidean distance
B. Closest in Euclidean distance
C. Most probable under a learned density
D. Randomly chosen to encourage exploration

Question 6

6) In K-means++ initialization, after choosing the first center at random, each subsequent center is chosen with probability proportional to:

A. Uniform probability over remaining points

B. The (unsquared) distance to the *nearest* chosen center

C. The **squared** distance to the nearest chosen center

D. The inverse of the distance to the nearest chosen center

Question 7

7) A well-known limitation of basic K-means is that it effectively assumes clusters are:

A. Arbitrarily shaped with nonlinear boundaries

B. Spherical and of roughly similar size, leading to linear decision boundaries

C. Nested hierarchies with tree-structured boundaries

D. Determined by a Mahalanobis metric by default

Question 8

8) Learning with Prototypes (LwP), using Euclidean distances for binary classes with means $\mu_+$and μ_- ,leads to a linear decision function $f(x) = w^\top x + b$ .What are $w$and b?

A. $w = \mu_+ - \mu_-, \ b = \| \mu_- \|^2 - \| \mu_+ \|^2$

B. $w = 2(\mu_+ - \mu_-), \ b = \| \mu_- \|^2 - \| \mu_+ \|^2$

C. $w = \mu_+ + \mu_-, \ b = 0$

D. $w = 2(\mu_- - \mu_+), \ b = \| \mu_+ \|^2 - \| \mu_- \|^2$

Question 9

9) In K-nearest neighbors (KNN) classification, increasing K generally tends to:

A. Make the decision boundary more jagged (higher variance)
B. Make the decision boundary smoother (lower variance)
C. Have no effect on the decision boundary
D. Always improve accuracy regardless of data

Question 10

10) When pairwise distances are Euclidean, classical Multi-Dimensional Scaling (MDS) is equivalent to:

A. Locally Linear Embedding (LLE)

B. Principal Component Analysis (PCA)

C. Kernel PCA with an RBF kernel

D. Independent Component Analysis (ICA)

Motivation I: Data Visualization

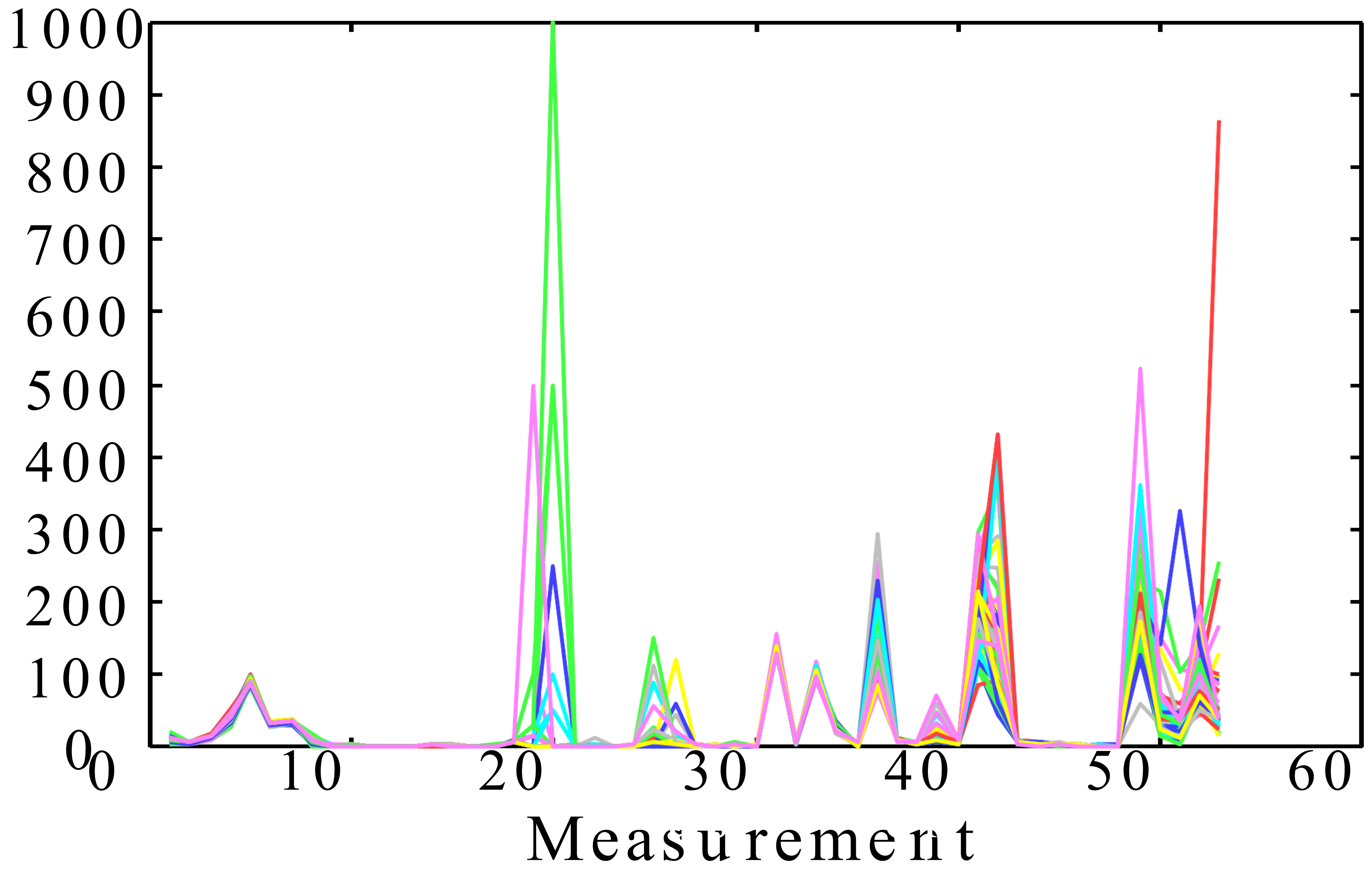
Instances

	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

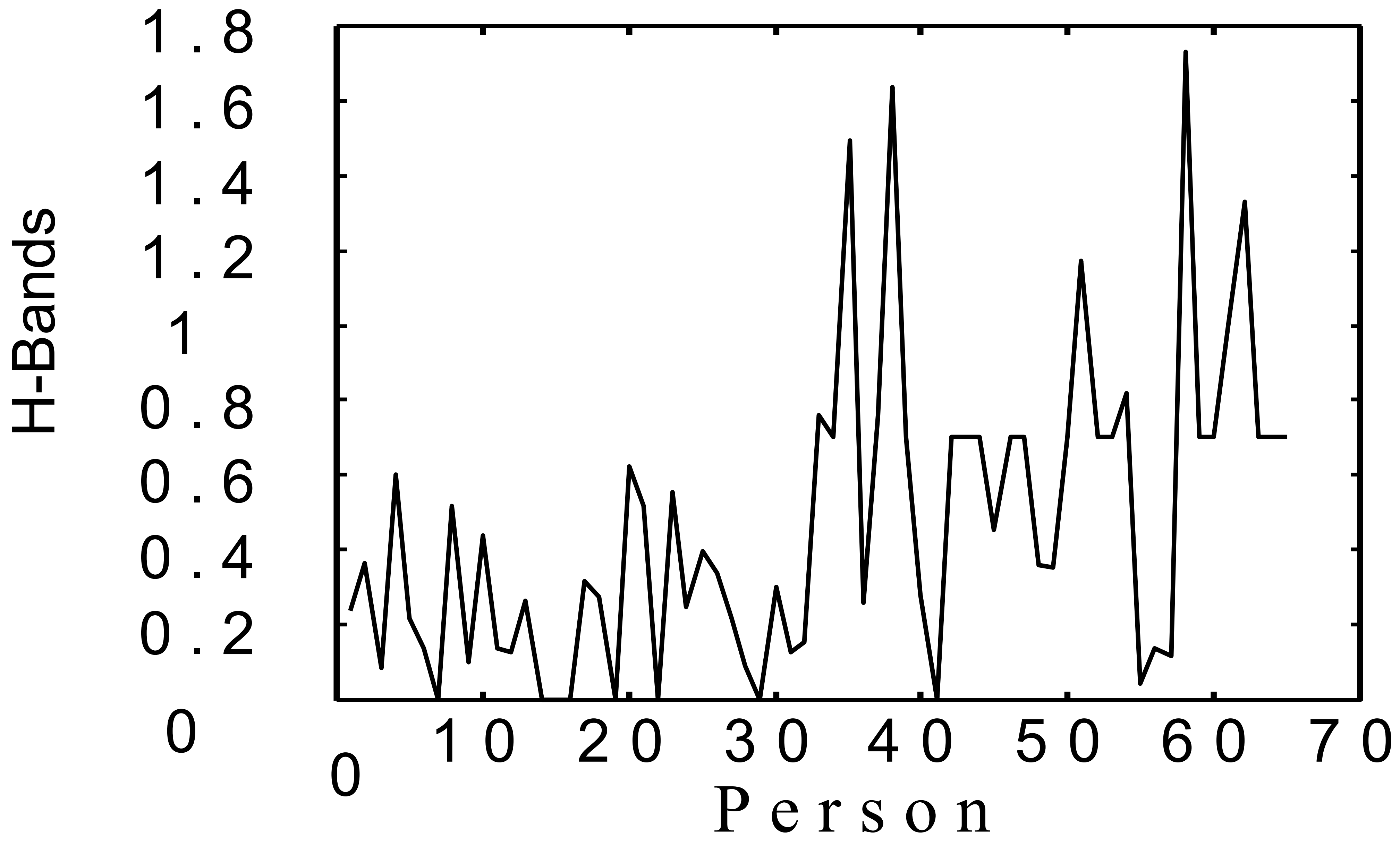
Motivation I: Data Visualization



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

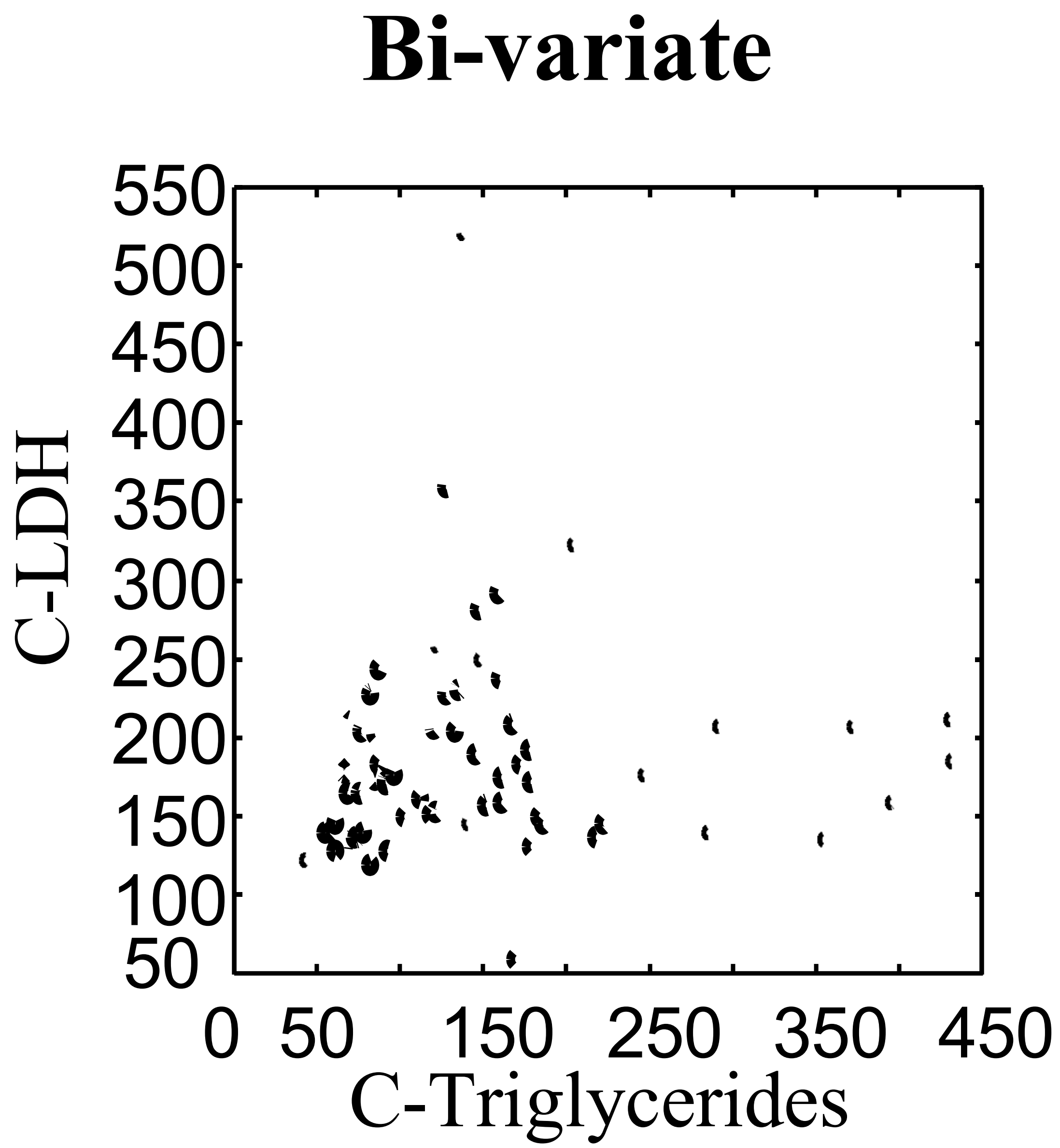
Motivation I: Data Visualization

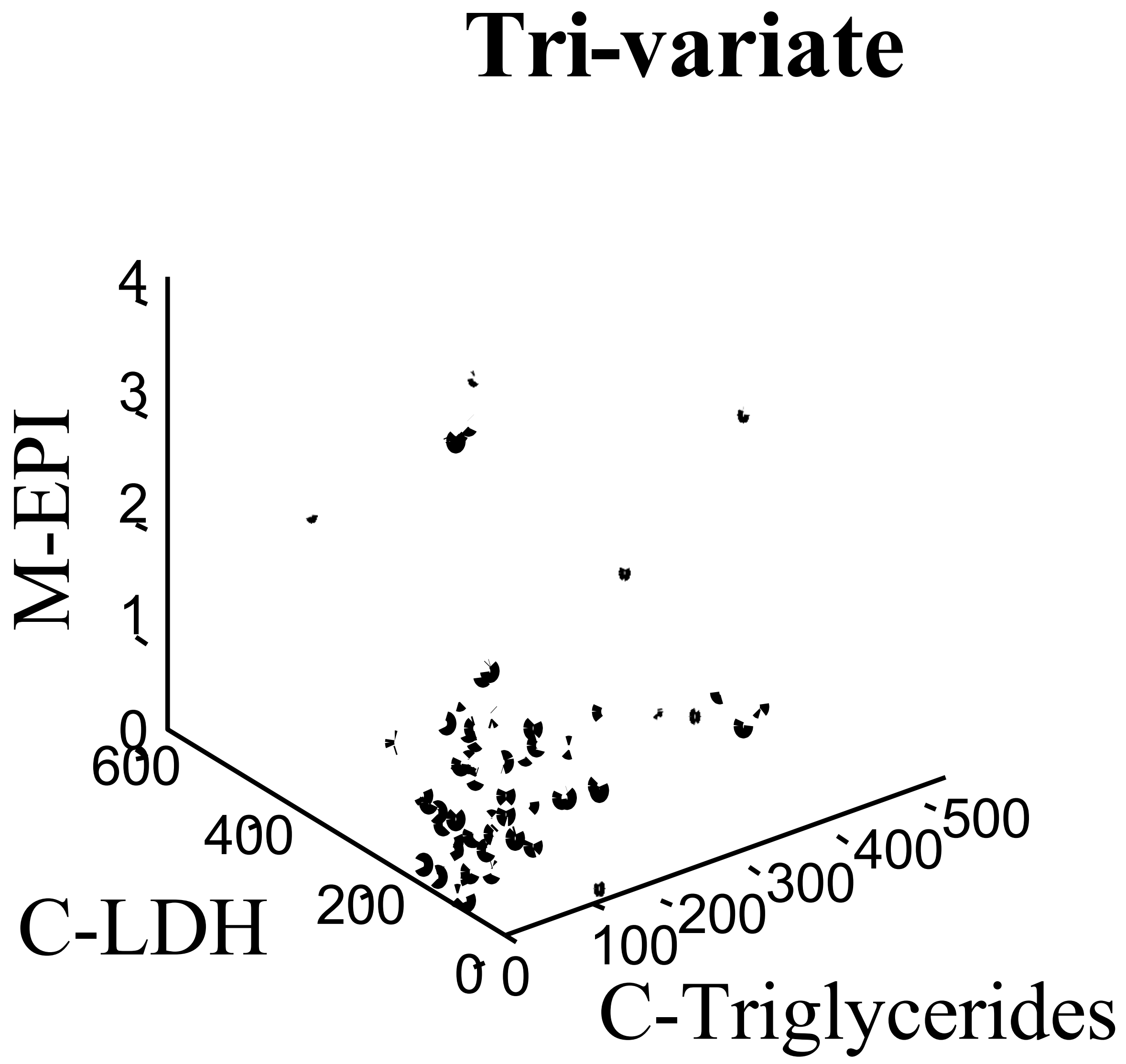
- Spectral format (53 pictures, one for each feature)



- Difficult to see the correlations between features

Motivation I: Data Visualization





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

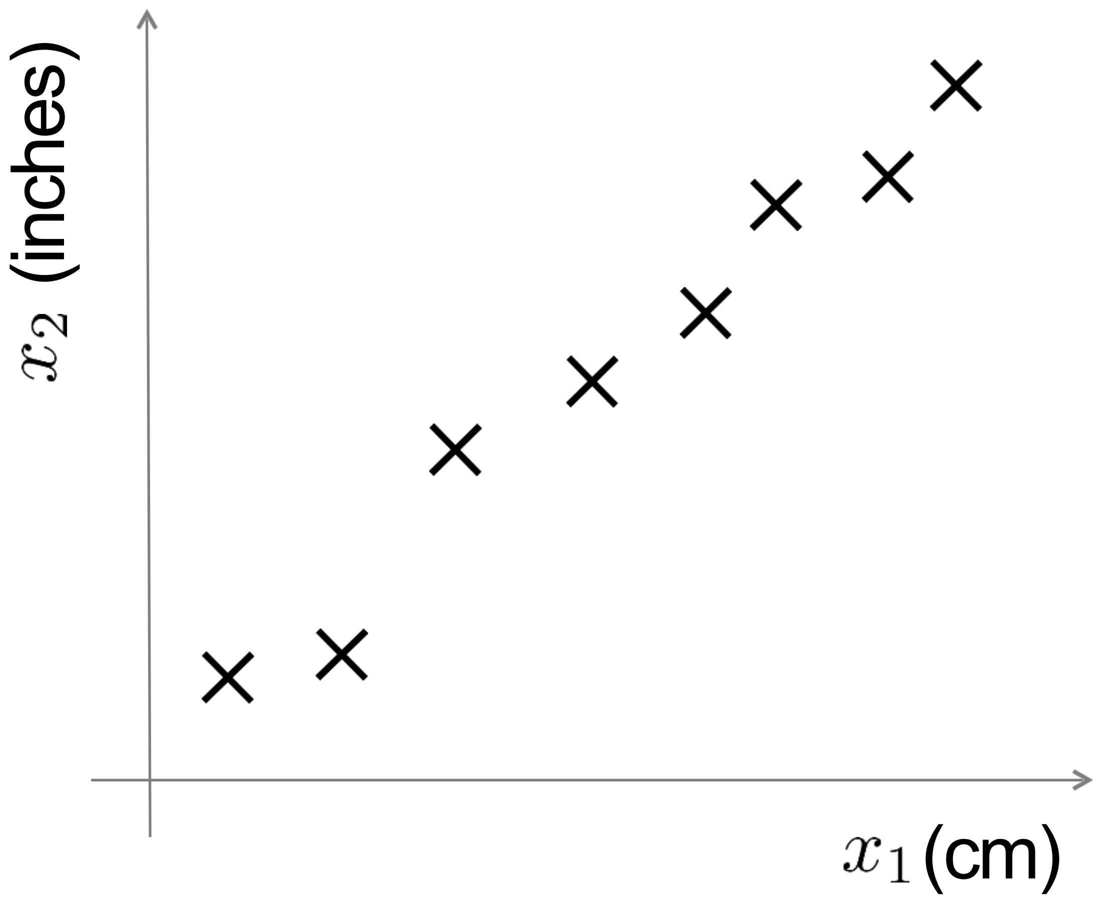
Motivation I: Data Visualization

- Is there a representation better than the coordinate axes?

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

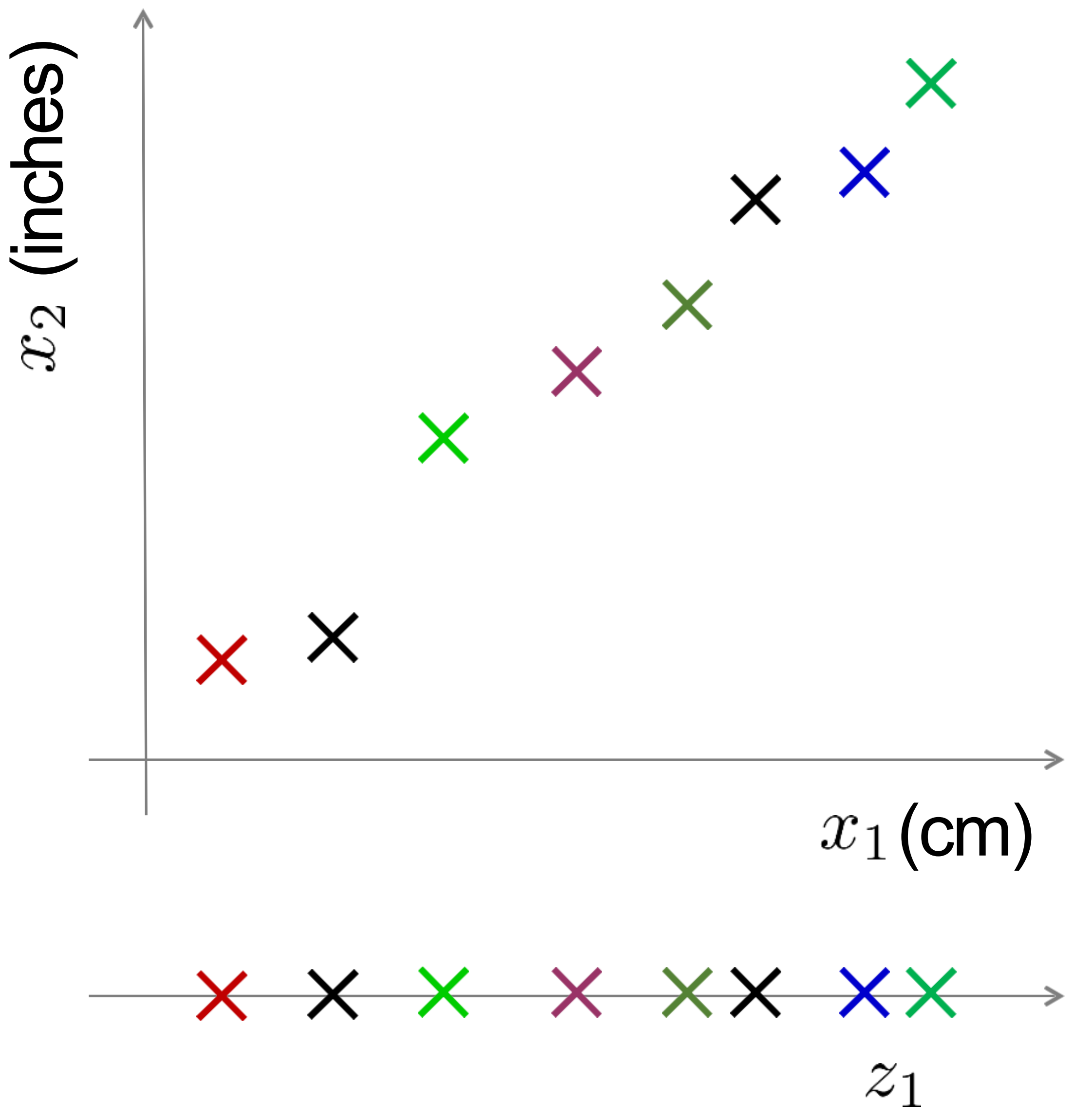
- How could we find the smallest subspace of the 53-D space that keeps the most information about the original data?

Motivation II: Data Compression



Reduce data from 2D to 1D

Motivation II: Data Compression

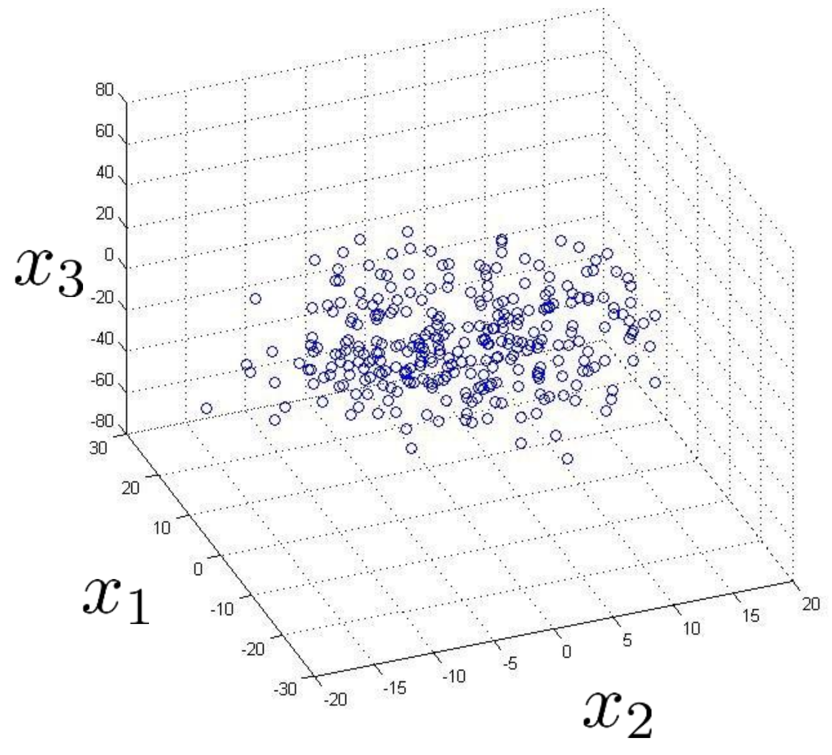


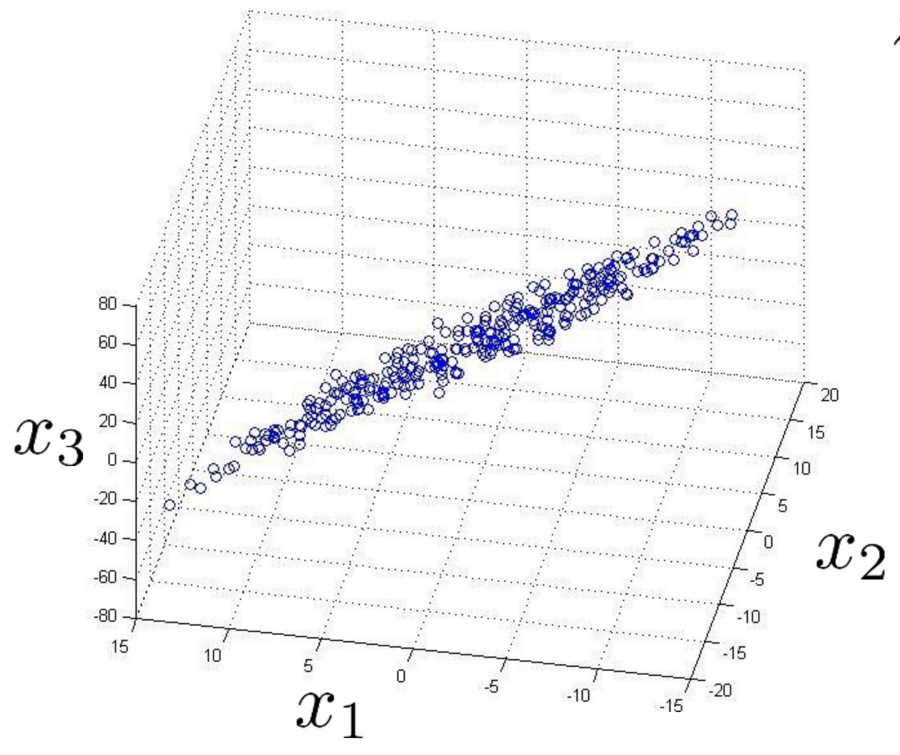
Reduce data from 2D to 1D

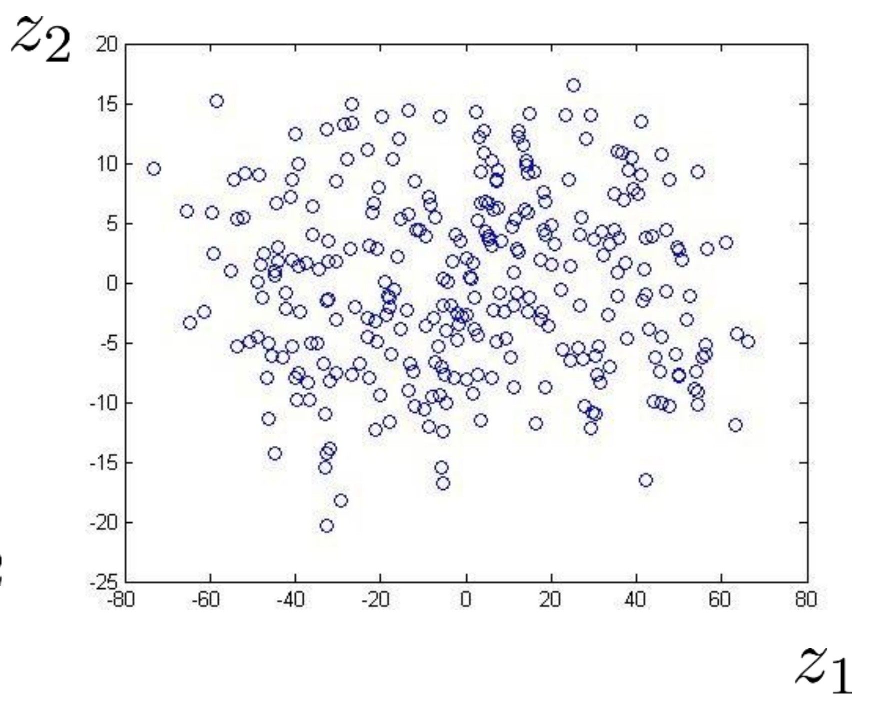
$$
\begin{aligned}
x^{(1)} &\rightarrow z^{(1)} \\
x^{(2)} &\rightarrow z^{(2)} \\
&\vdots \\
x^{(m)} &\rightarrow z^{(m)}
\end{aligned}
$$

Motivation II: Data Compression

Reduce data from 3D to 2D







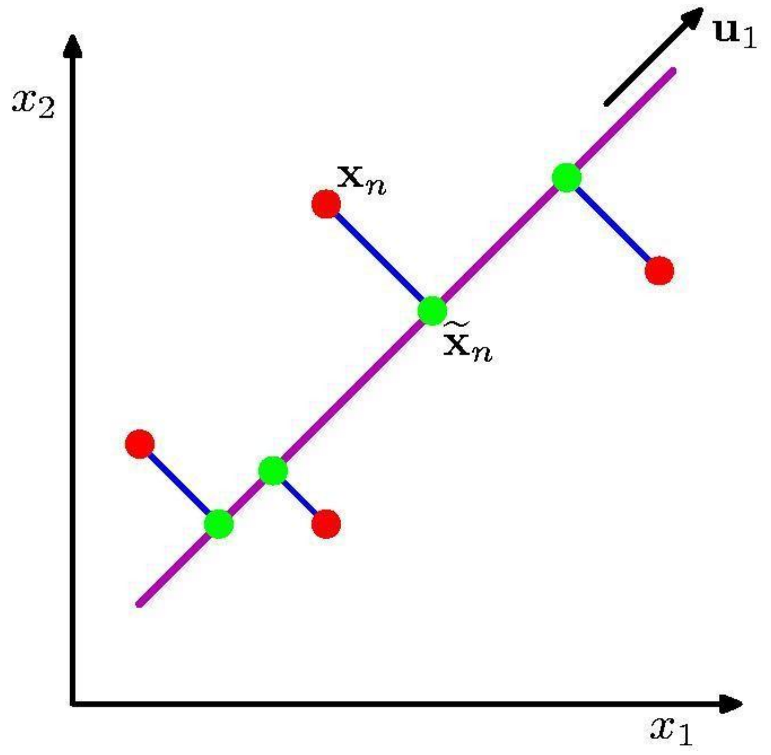
Dimensionality Reduction

- 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

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)

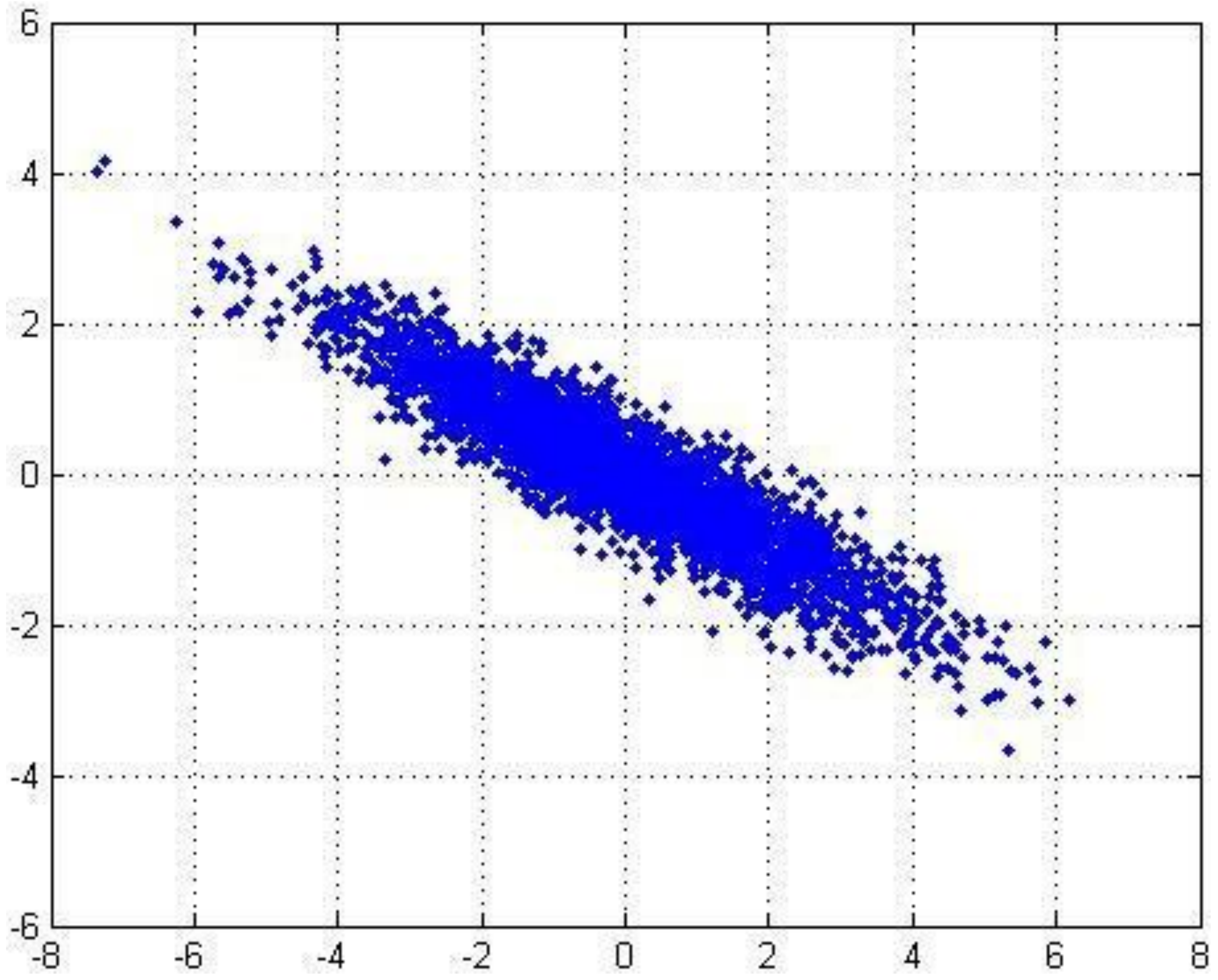
Principal Component Analysis

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

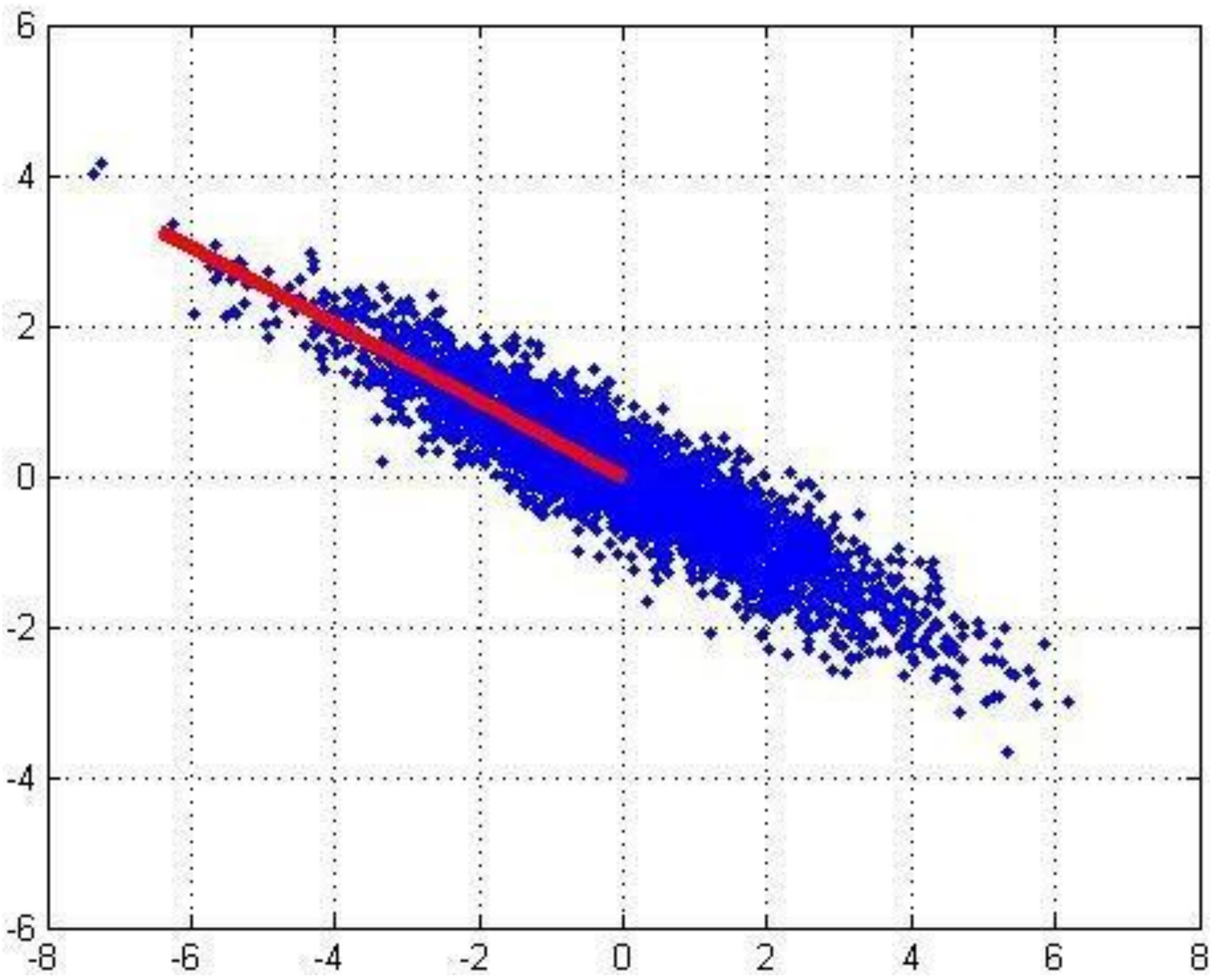
- Principal component #1: points in the direction of the **largest variance**.

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

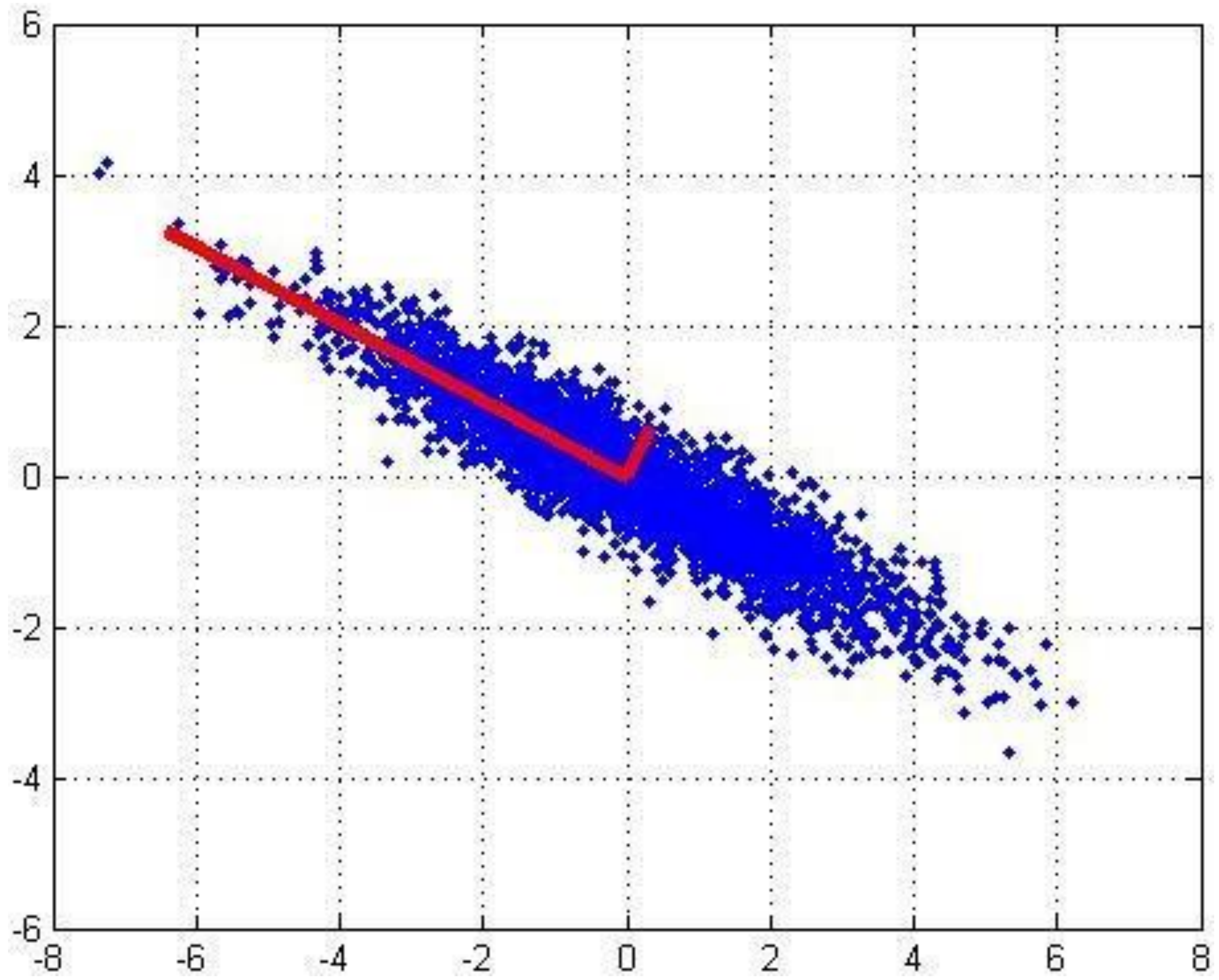
2D Gaussian dataset



1st PCA axis



2nd PCA axis



PCA algorithm I (sequential)

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

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

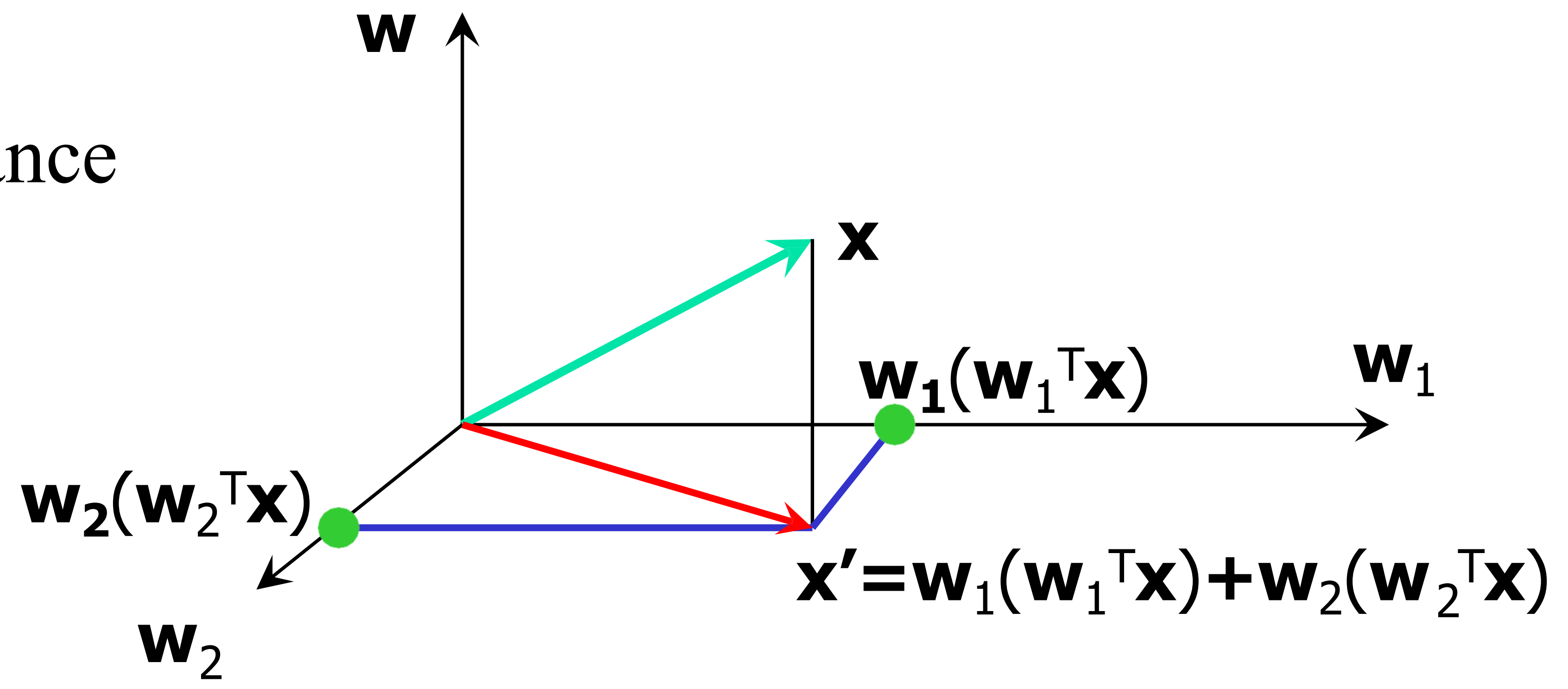
1st PCA vector

We maximize the variance of projection of **x**

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

*k*th PCA vector

We maximize the variance of the projection in the residual subspace



w
x
$\mathbf{w}_1(\mathbf{w}_1^T\mathbf{x})$
$\mathbf{w}_1$
$\mathbf{w}_2(\mathbf{w}_2^T\mathbf{x})$
$\mathbf{x}'=\mathbf{w}_1(\mathbf{w}_1^T\mathbf{x})+\mathbf{w}_2(\mathbf{w}_2^T\mathbf{x})$
$\mathbf{w}_2$

PCA algorithm II (sample covariance matrix)

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

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

- **PCA** basis vectors = the eigenvectors of $\boldsymbol{\Sigma}$

- 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

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

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

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

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!!

$\Rightarrow$ 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)

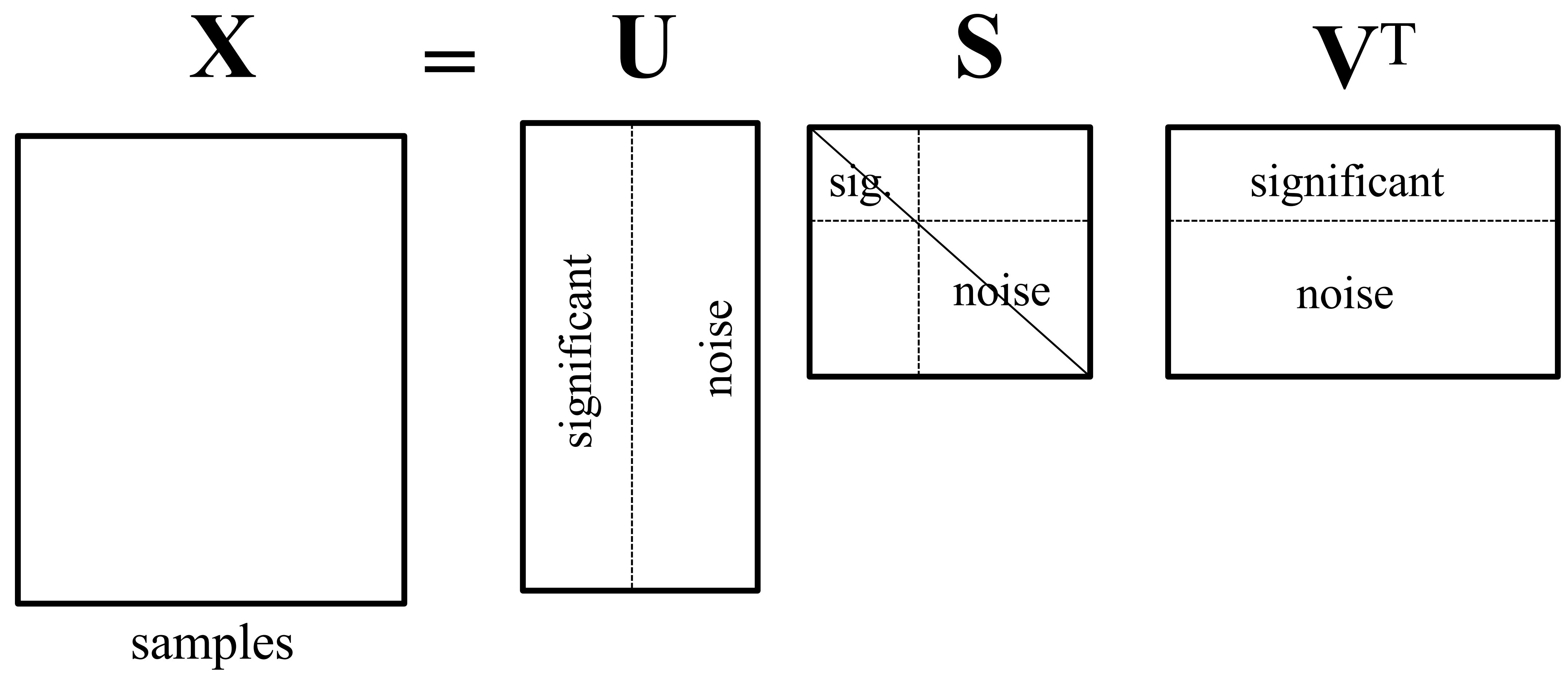
Singular Value Decomposition of the **centered** data matrix **X**.

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

m: number of instances,

N: dimension

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



PCA algorithm III

- **Columns of U**
  - the principal vectors, $\{ \mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(k)} \}$
  - orthogonal and has unit norm – so $U^TU = I$
  - 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

Applications

Face Recognition

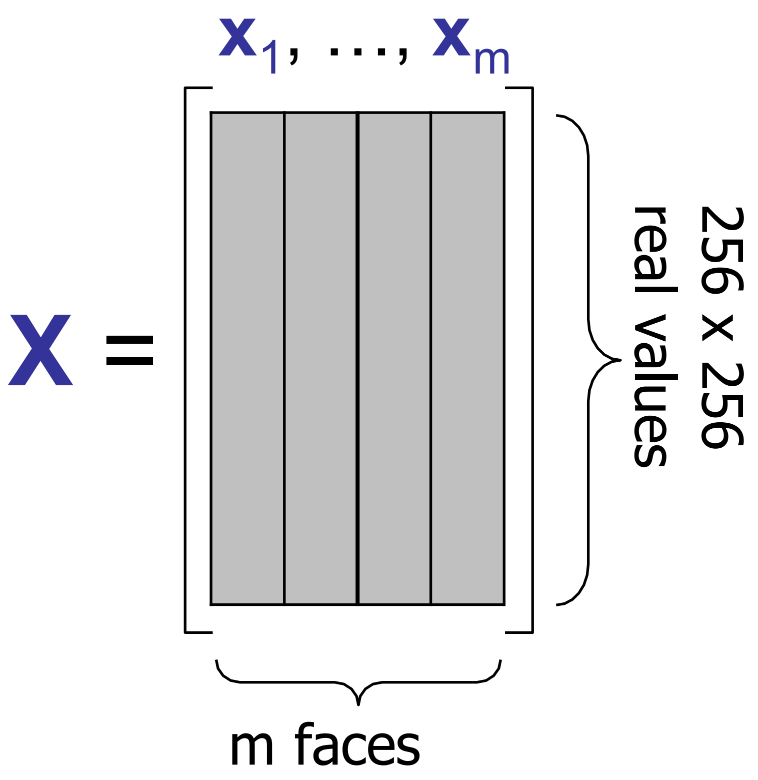
Face Recognition

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

Applying PCA: Eigenfaces

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

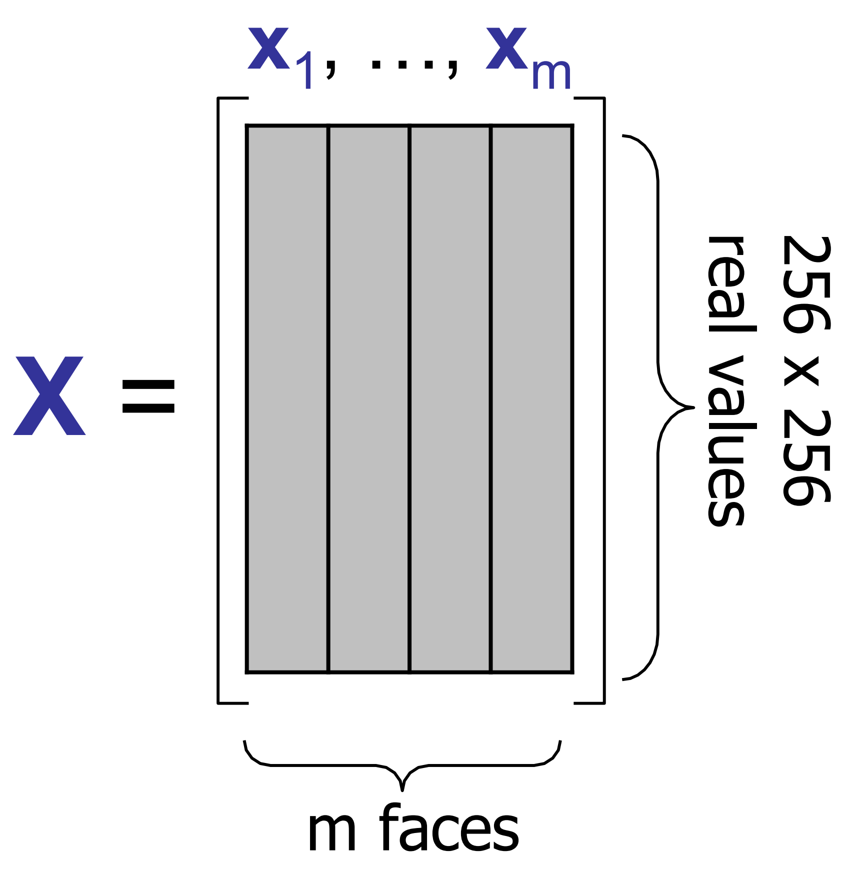
Method B: Build one PCA database for the whole dataset and then classify based on the weights.



- 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 $\mathbf{X} = [\, \mathbf{x}_1 , \ldots, \mathbf{x}_m \,]$ **centered** data mtx
- Compute $\boldsymbol{\Sigma} = \mathbf{X}\mathbf{X}^T$
- Problem: $\boldsymbol{\Sigma}$ is $64K \times 64K$ … HUGE!!!

A Clever Workaround

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



Proof:

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

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

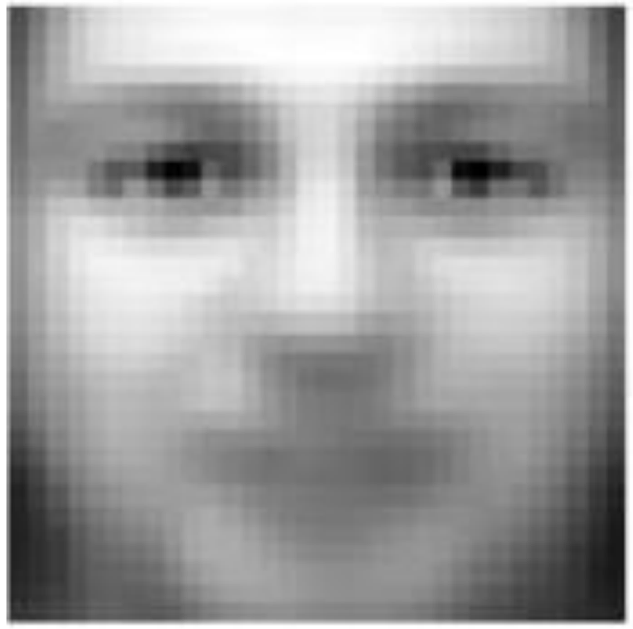
$$\mathbf{X}\ (\mathbf{X}^T\mathbf{X}\ \mathbf{v}) = \mathbf{X}(\gamma\ \mathbf{v}) = \gamma\ \mathbf{X}\mathbf{v}$$

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

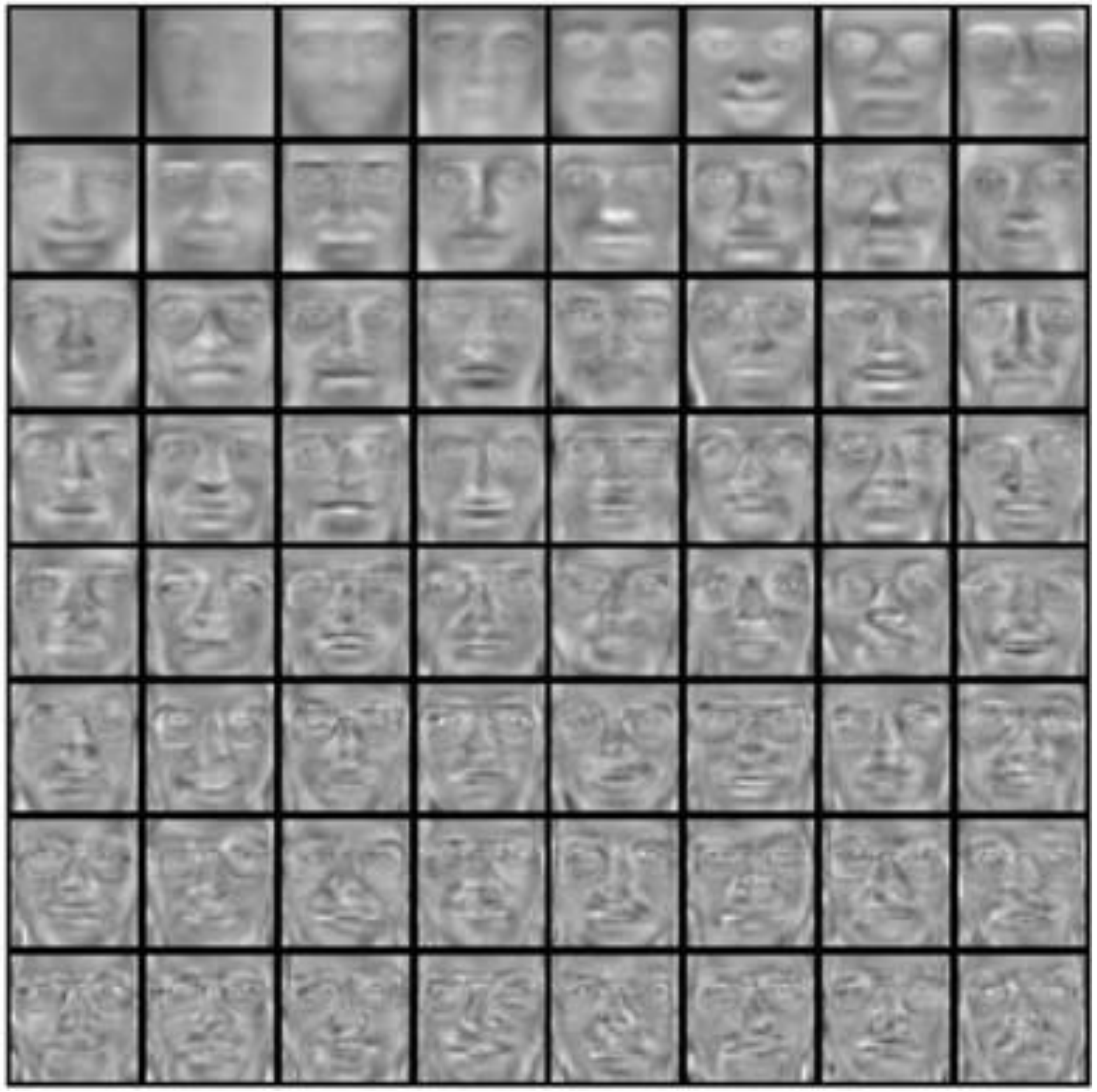
$$\Sigma\ (\mathbf{X}\mathbf{v}) = \gamma\ (\mathbf{X}\mathbf{v})$$

Eigenfaces Example

Mean: μ



Top eigenvectors: $u_1, \ldots u_k$

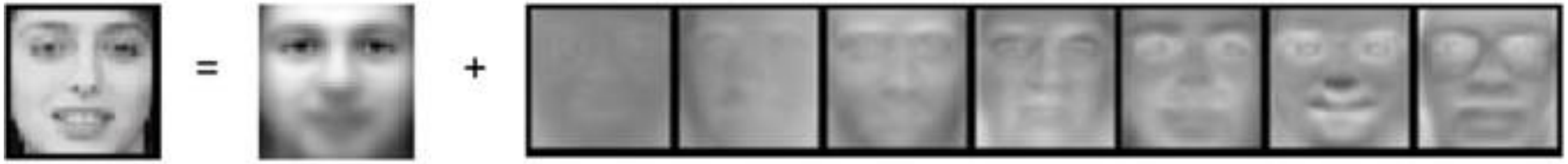


Representation and Reconstruction

- Face **x** in "face space" coordinates:

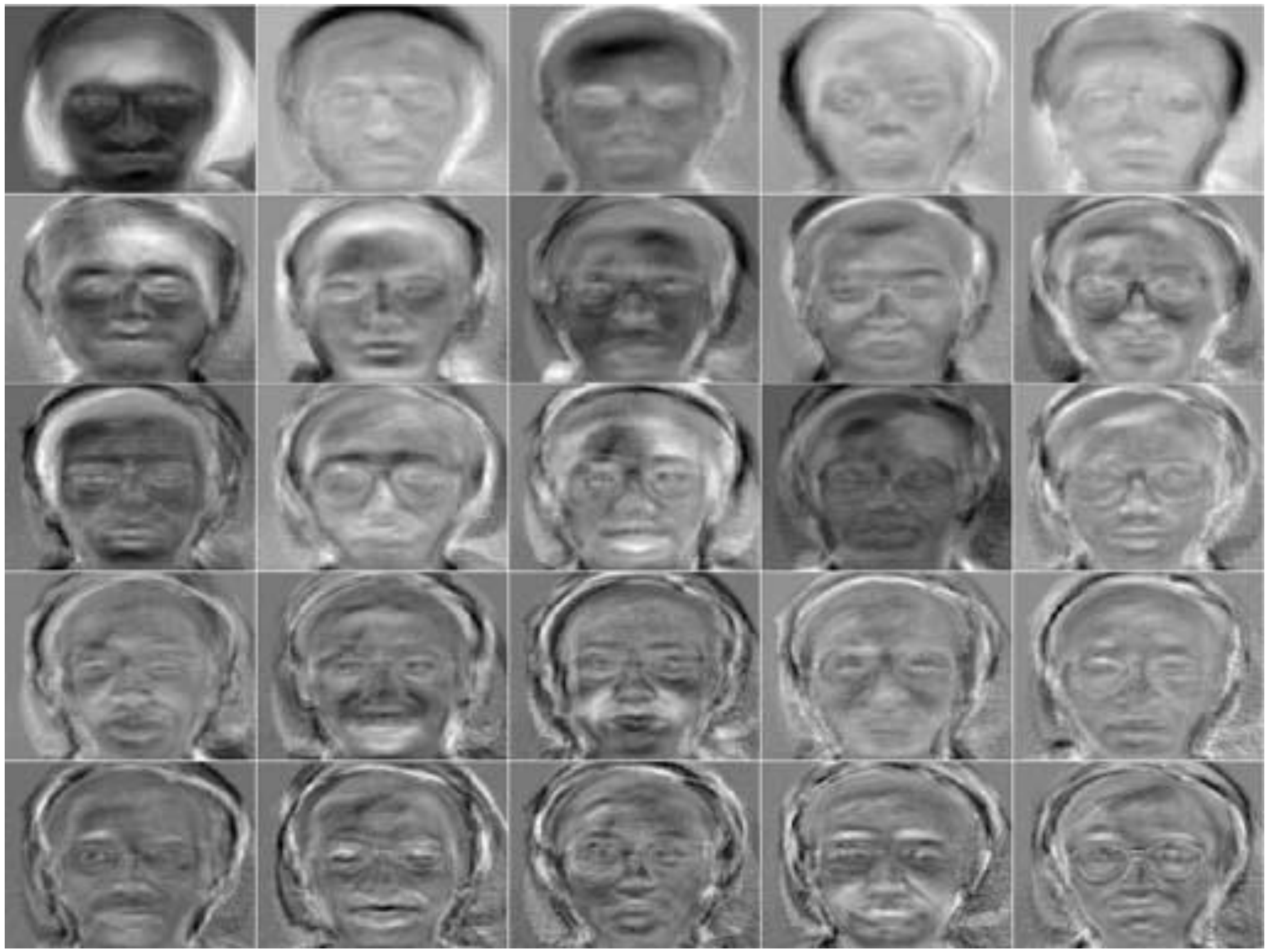
$$\mathbf{x} \rightarrow [\mathbf{u}_1^{\mathrm{T}}(\mathbf{x}-\mu), \ldots, \mathbf{u}_k^{\mathrm{T}}(\mathbf{x}-\mu)]$$
$$= \quad w_1, \ldots, w_k$$

- Reconstruction:

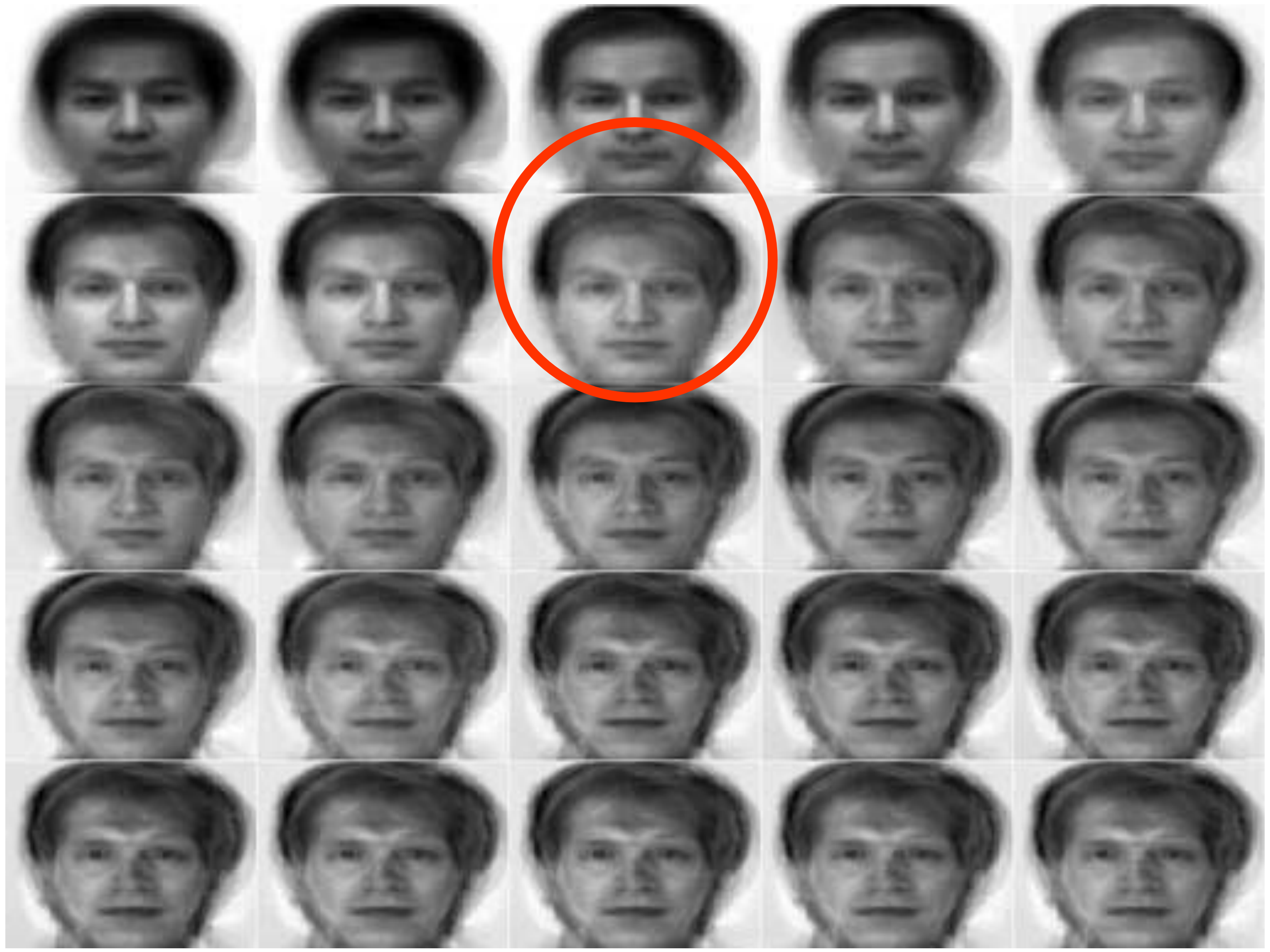


$\hat{x} = \mu + w_1u_1+w_2u_2+w_3u_3+w_4u_4+ \ldots$

Principle Components (Method B)



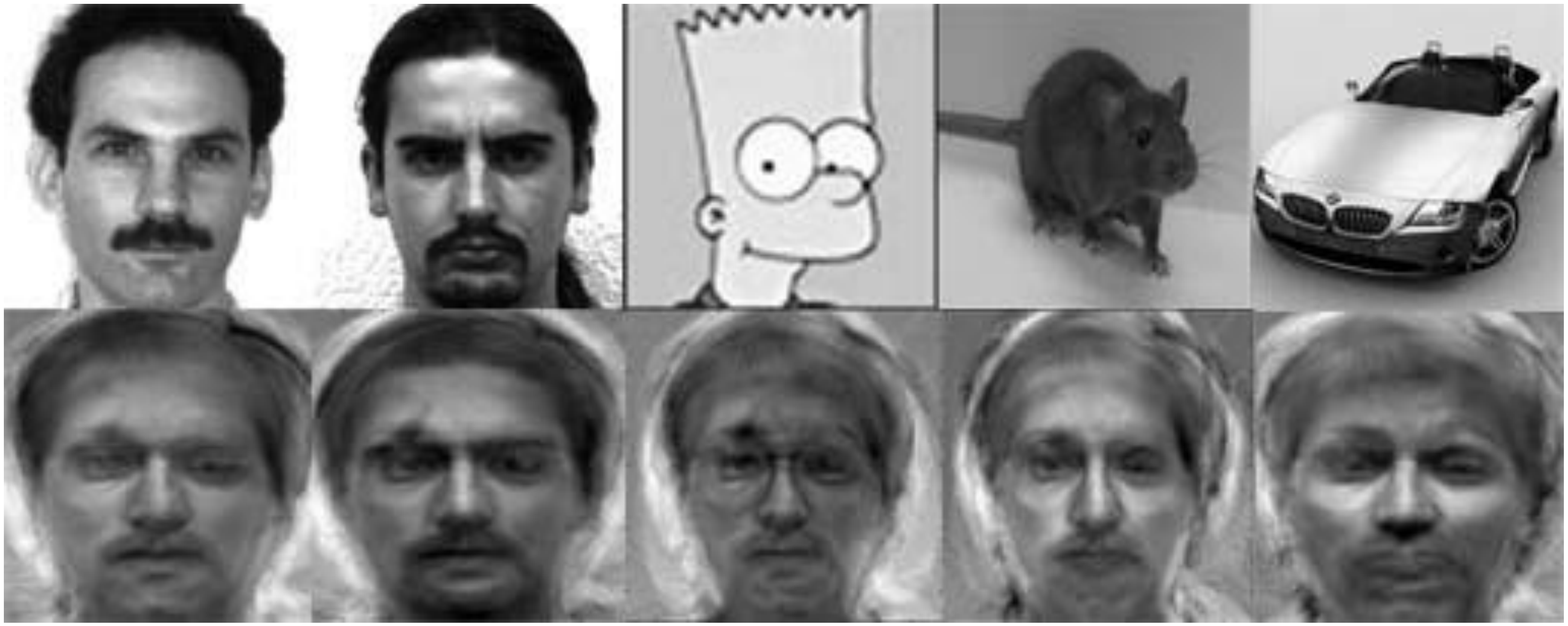
Principle Components (Method B)



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

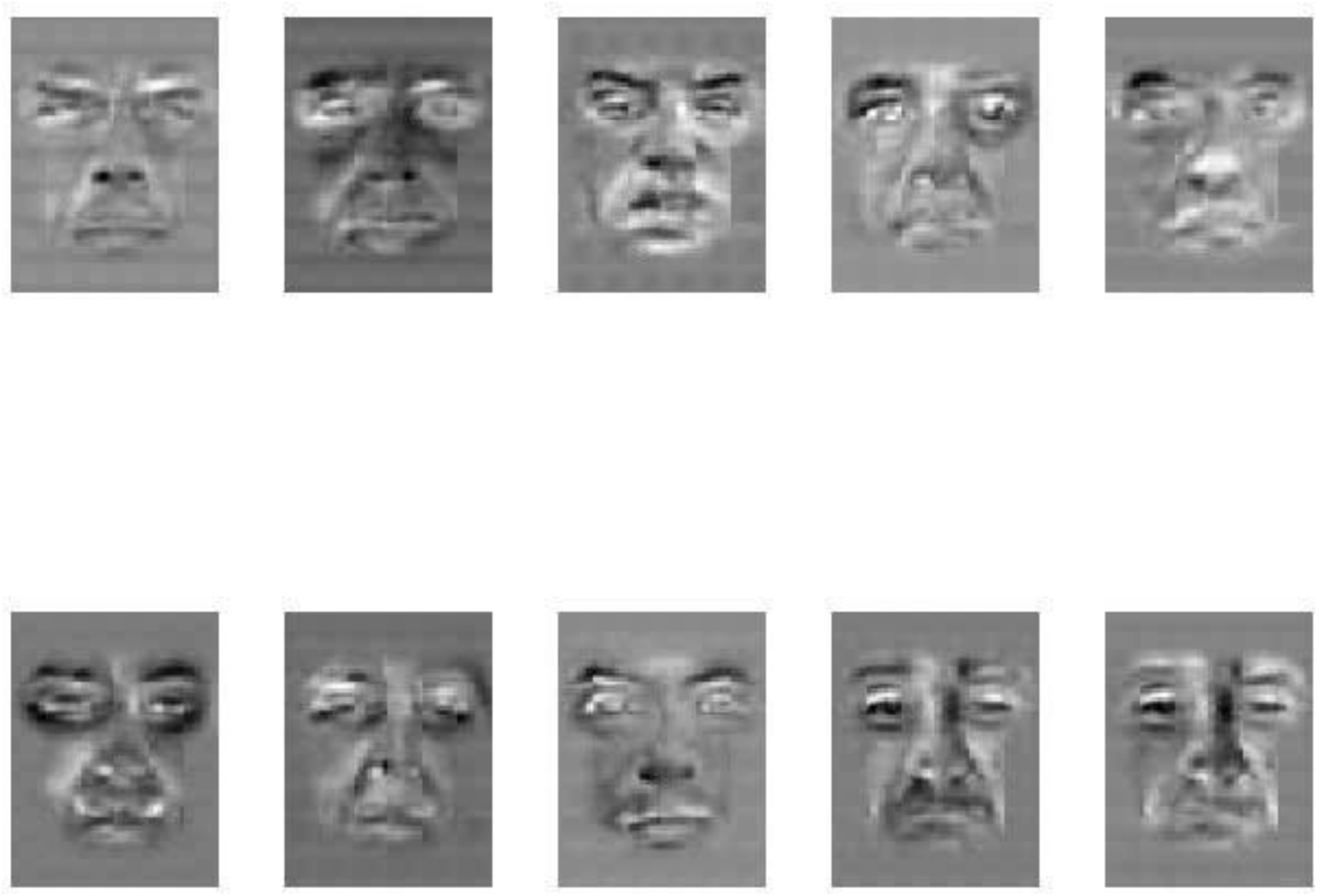
When projecting strange data

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

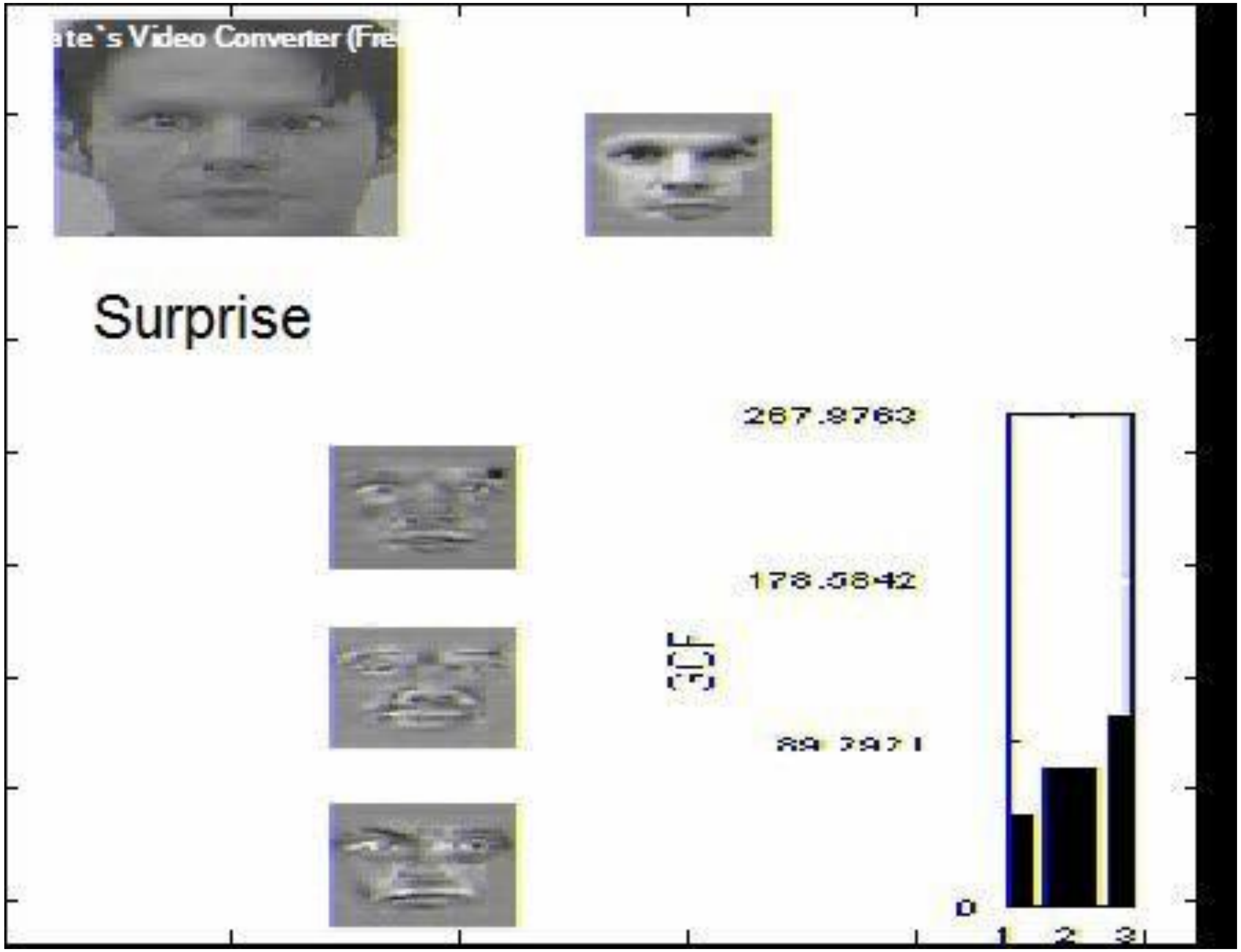


Happiness subspace (method A)

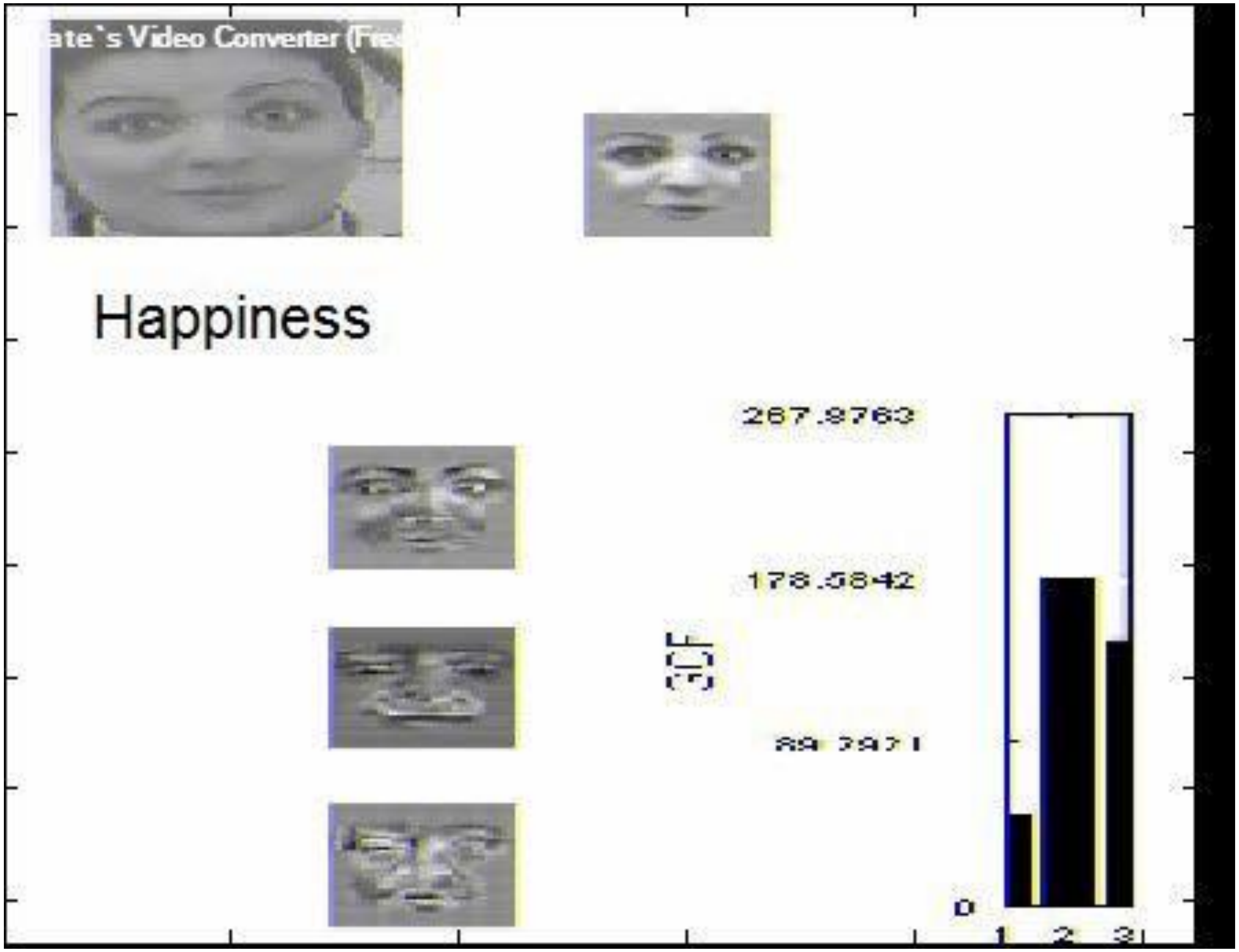
Disgust subspace (method A)



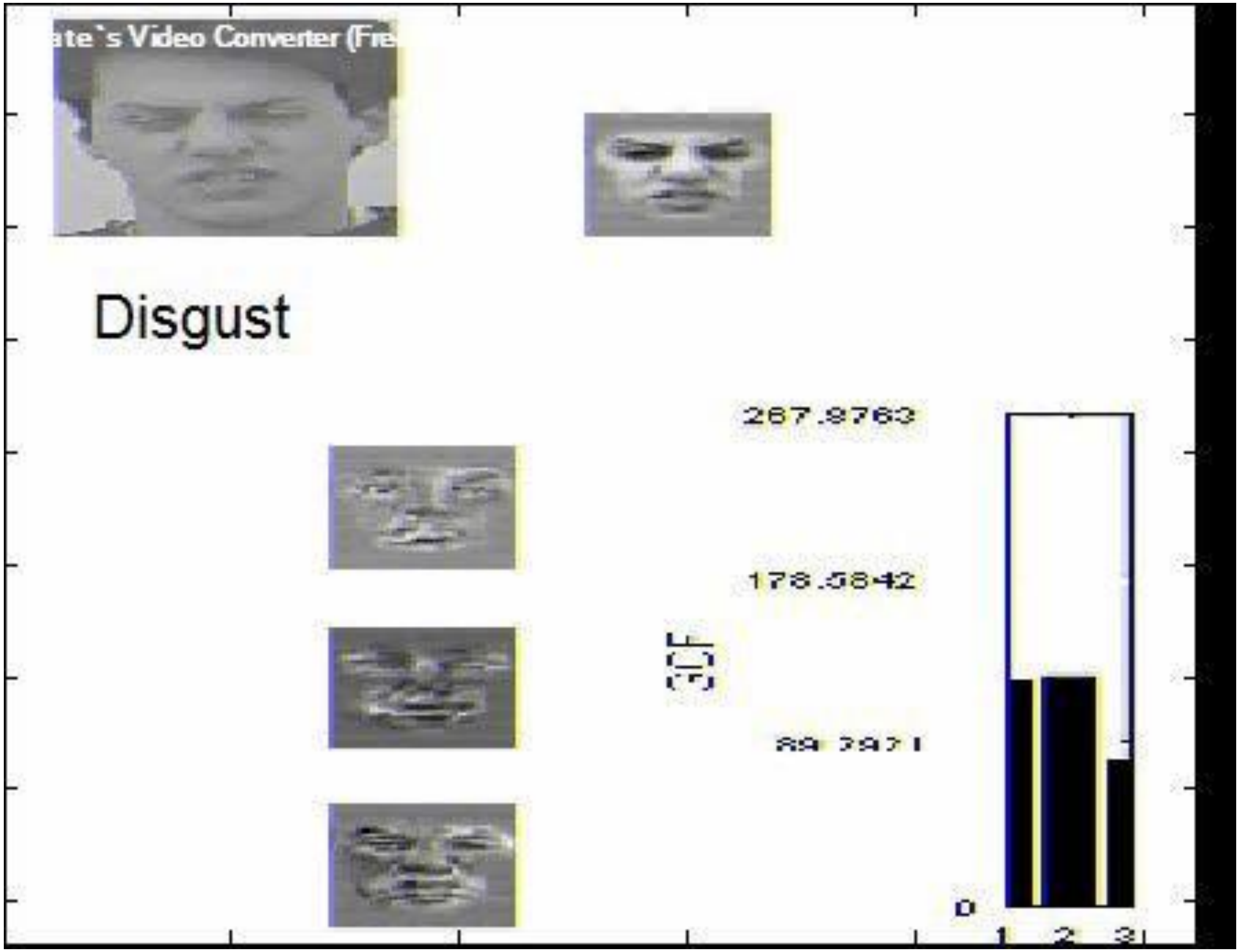
Facial Expression Recognition Movies



Facial Expression Recognition Movies



Facial Expression Recognition Movies



Shortcomings

- Requires carefully controlled data:
  - All faces centered in frame
  - Same size
  - Some sensitivity to angle

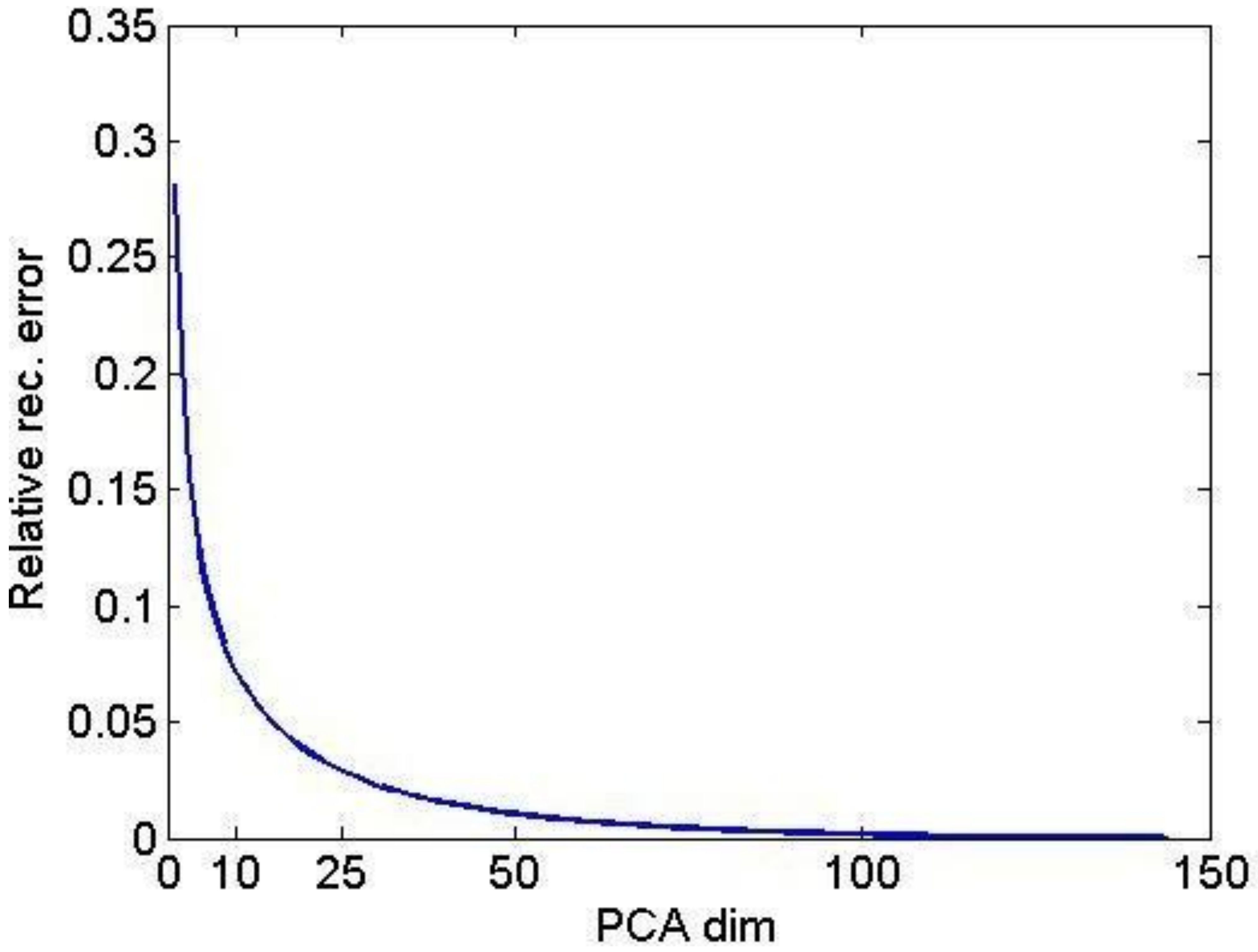
- Method is completely knowledge free
  - (sometimes this is good!)
  - Doesn’t know that faces are wrapped around 3D objects (heads)
  - Makes no effort to preserve class distinctions

Image Compression

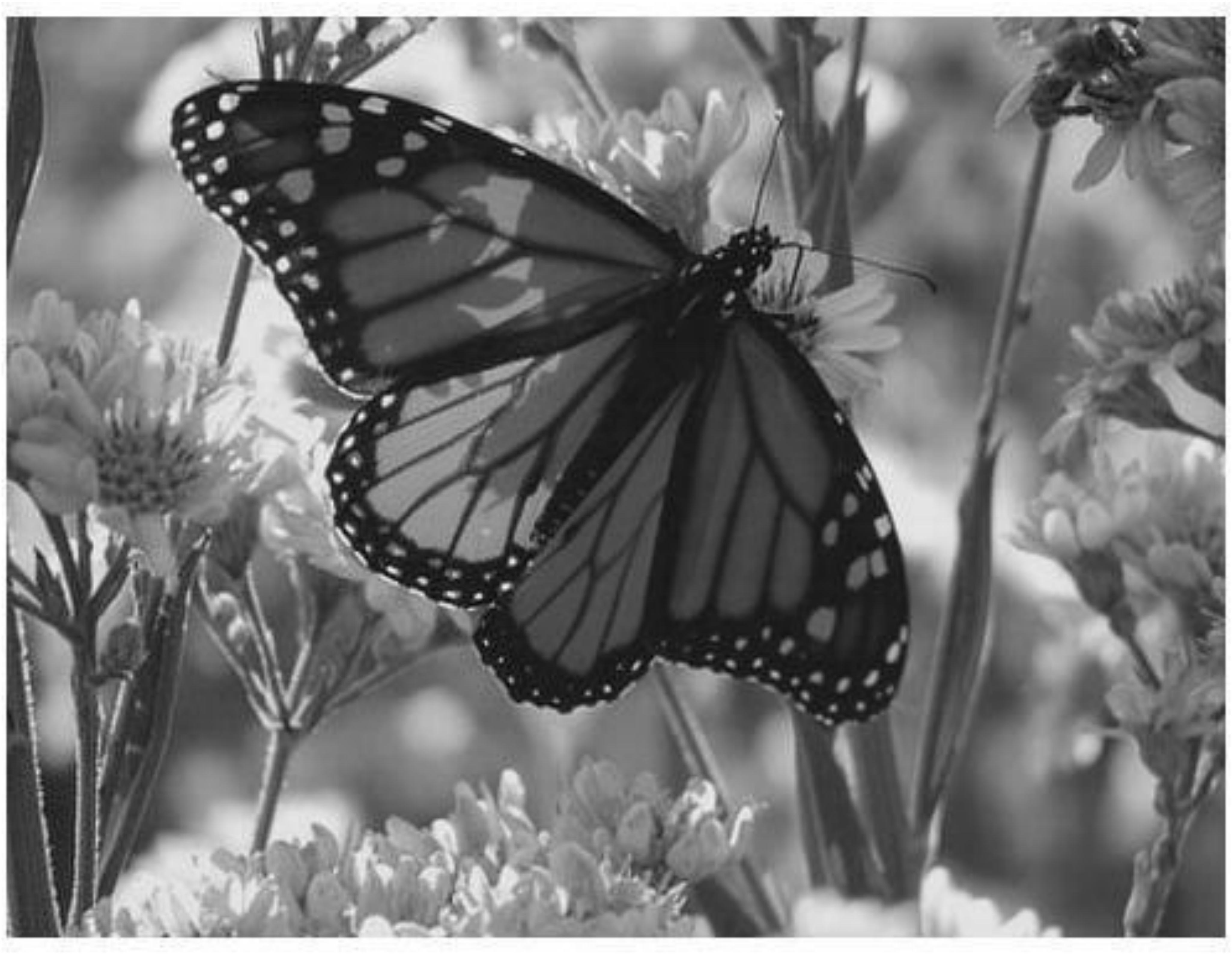
Original Image

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

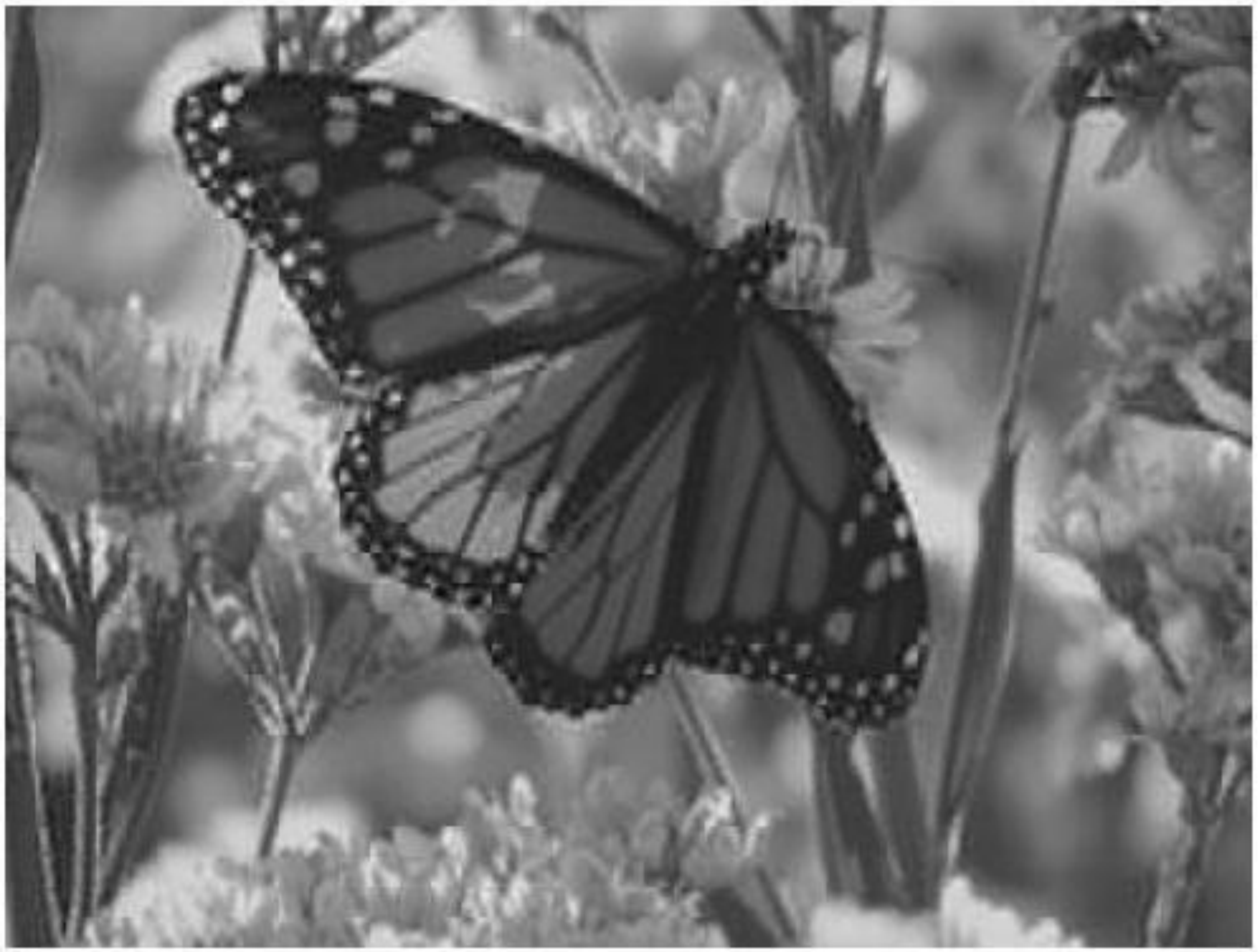
L_2 error and PCA dim



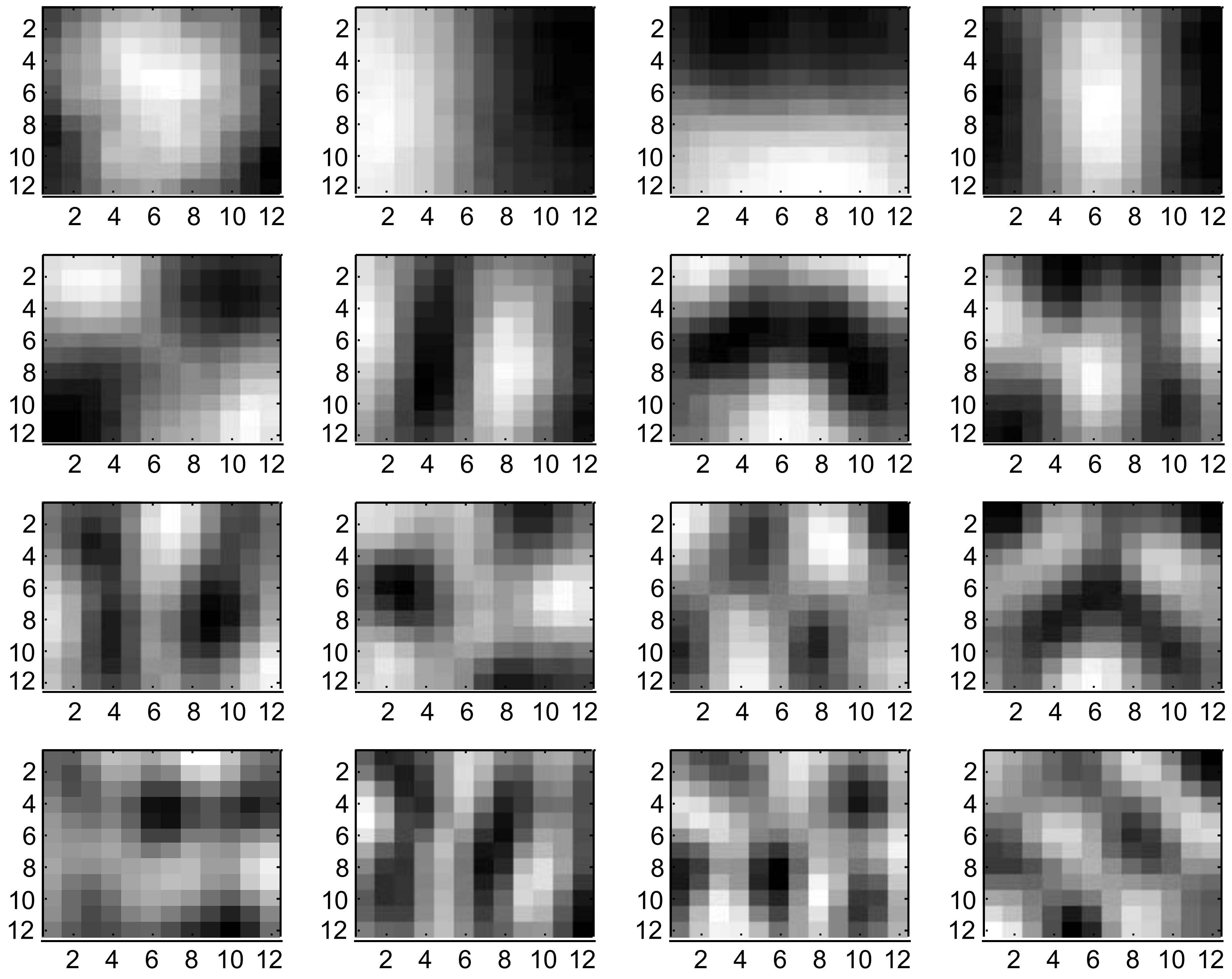
PCA compression: 144D => 60D



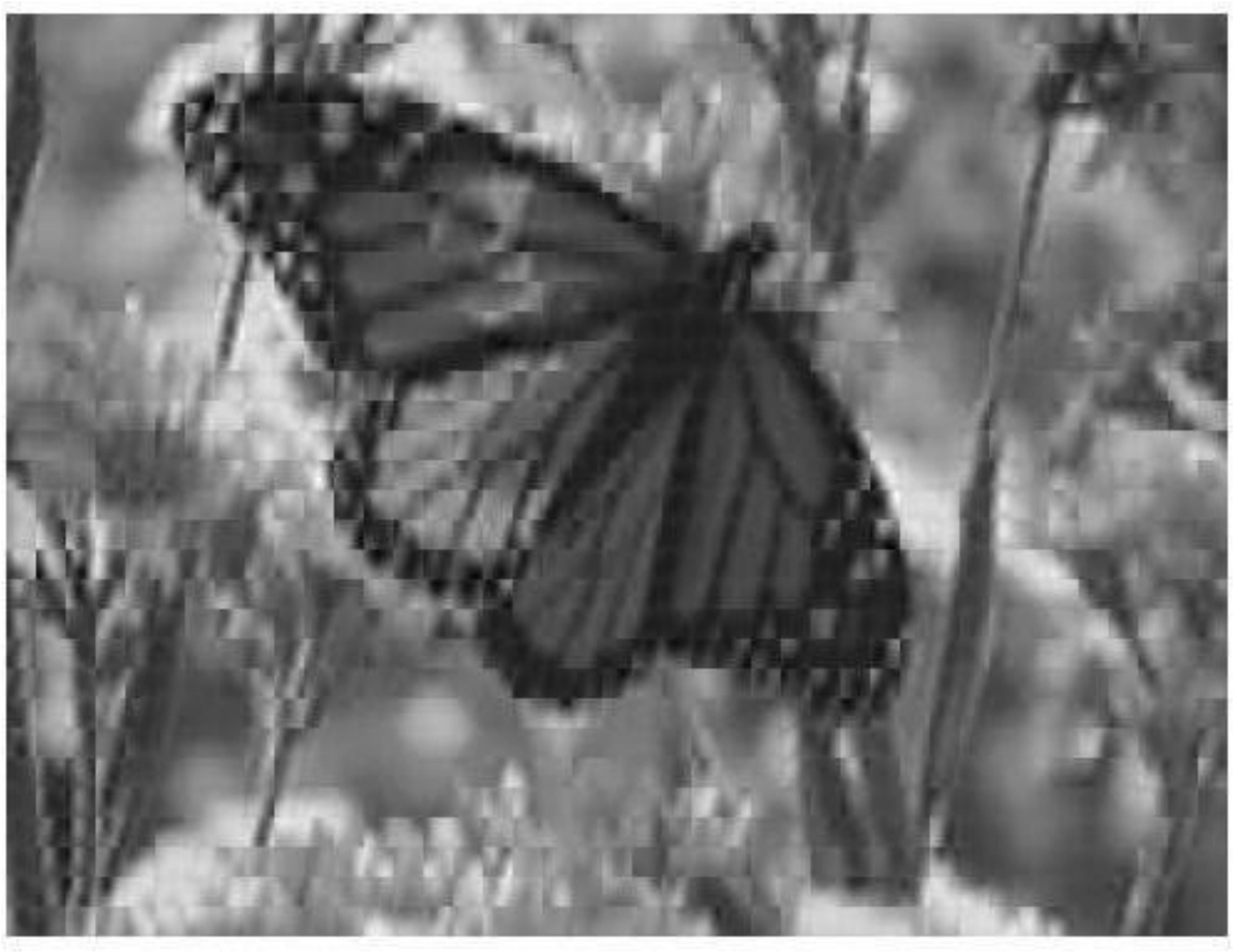
PCA compression: 144D => 16D



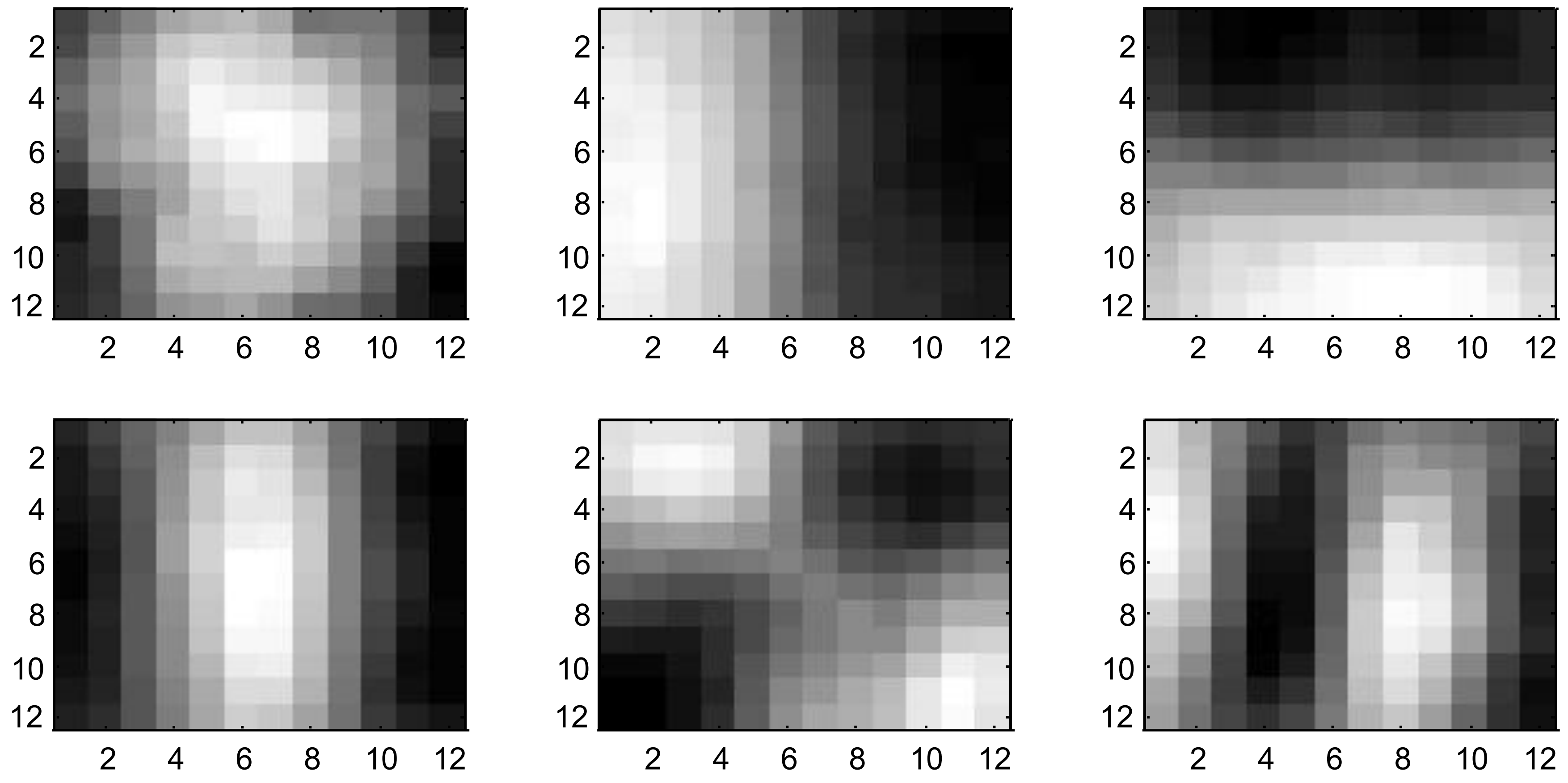
16 most important eigenvectors



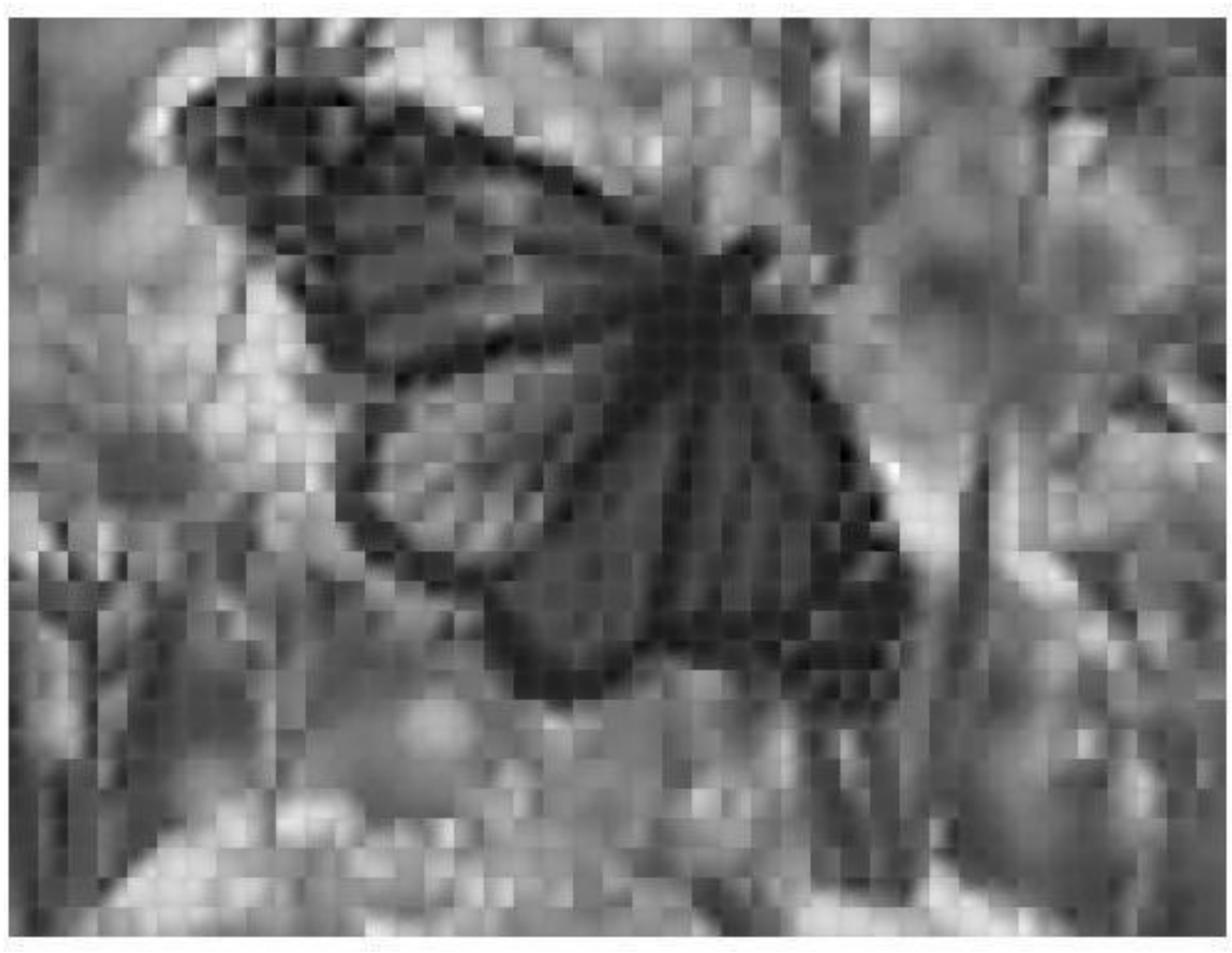
PCA compression: 144D => 6D



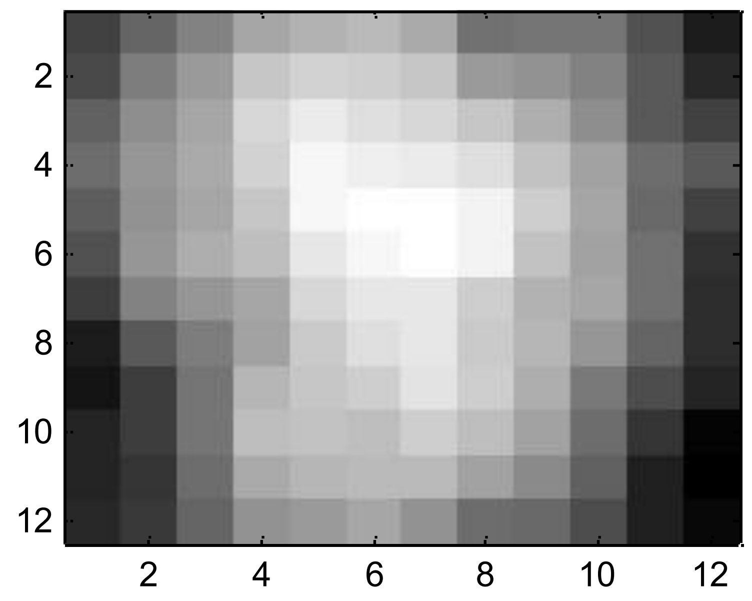
6 most important eigenvectors

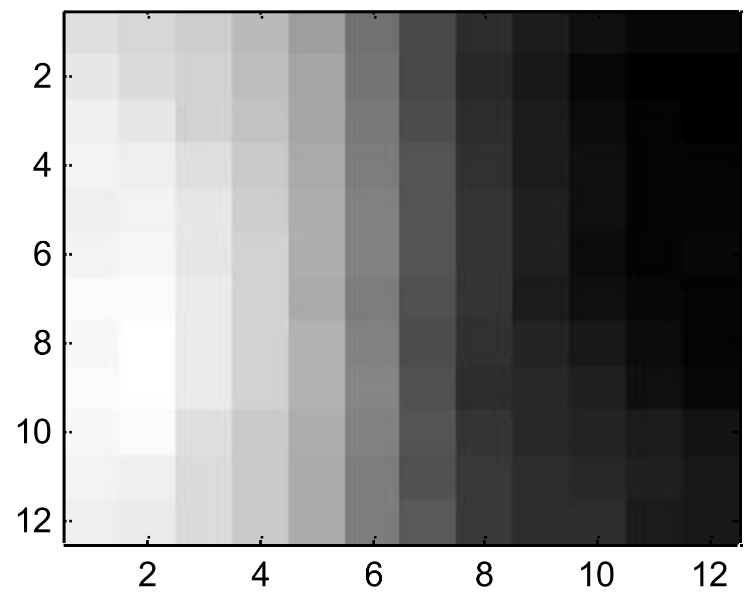


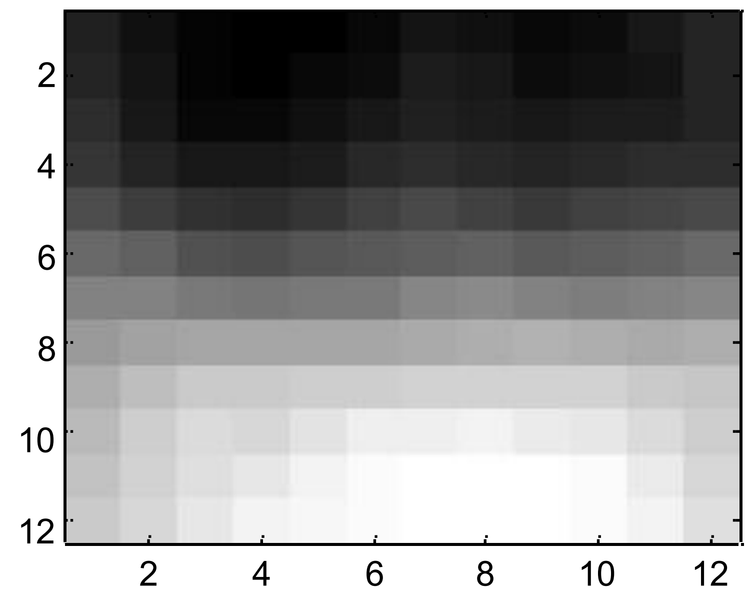
PCA compression: 144D => 3D



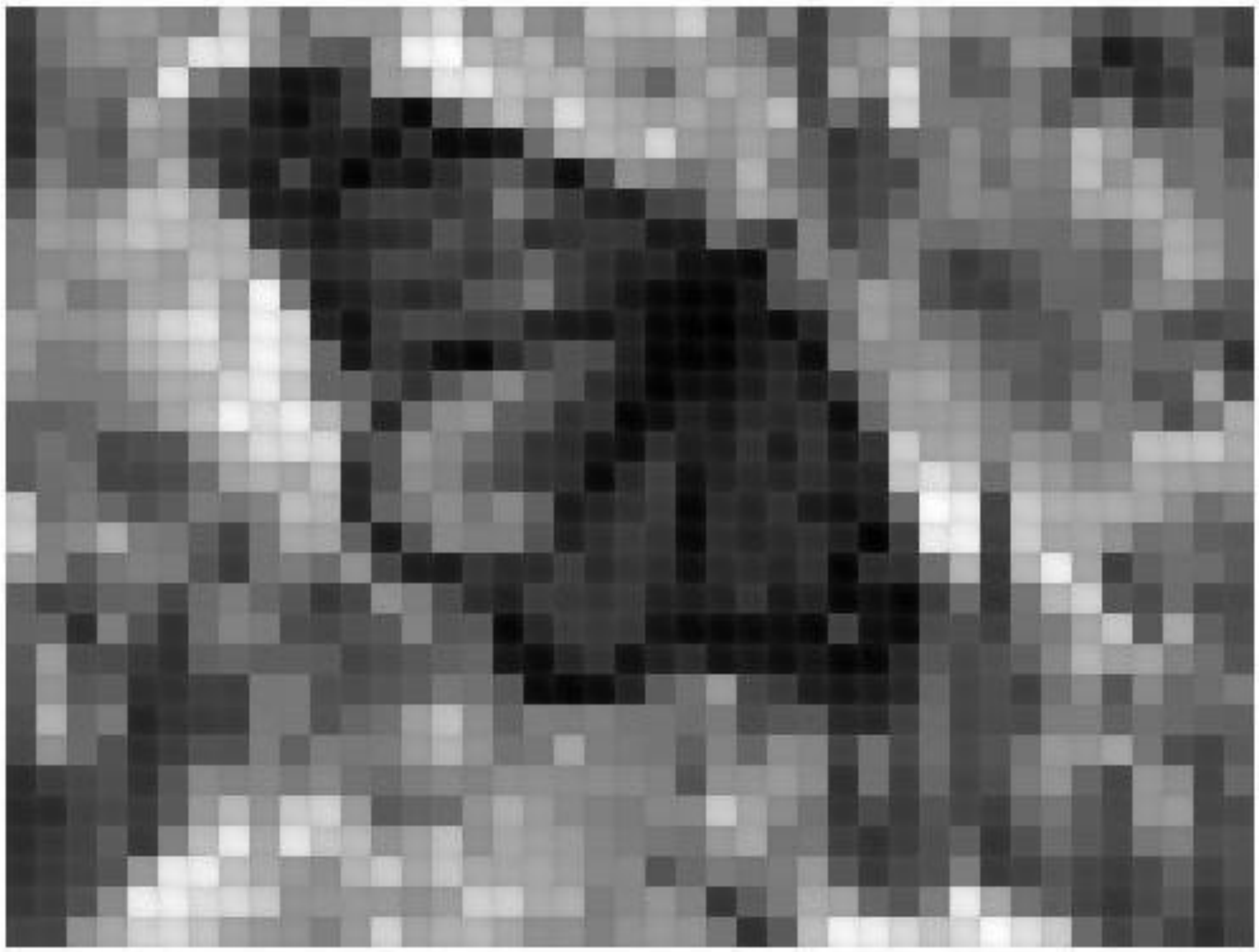
3 most important eigenvectors



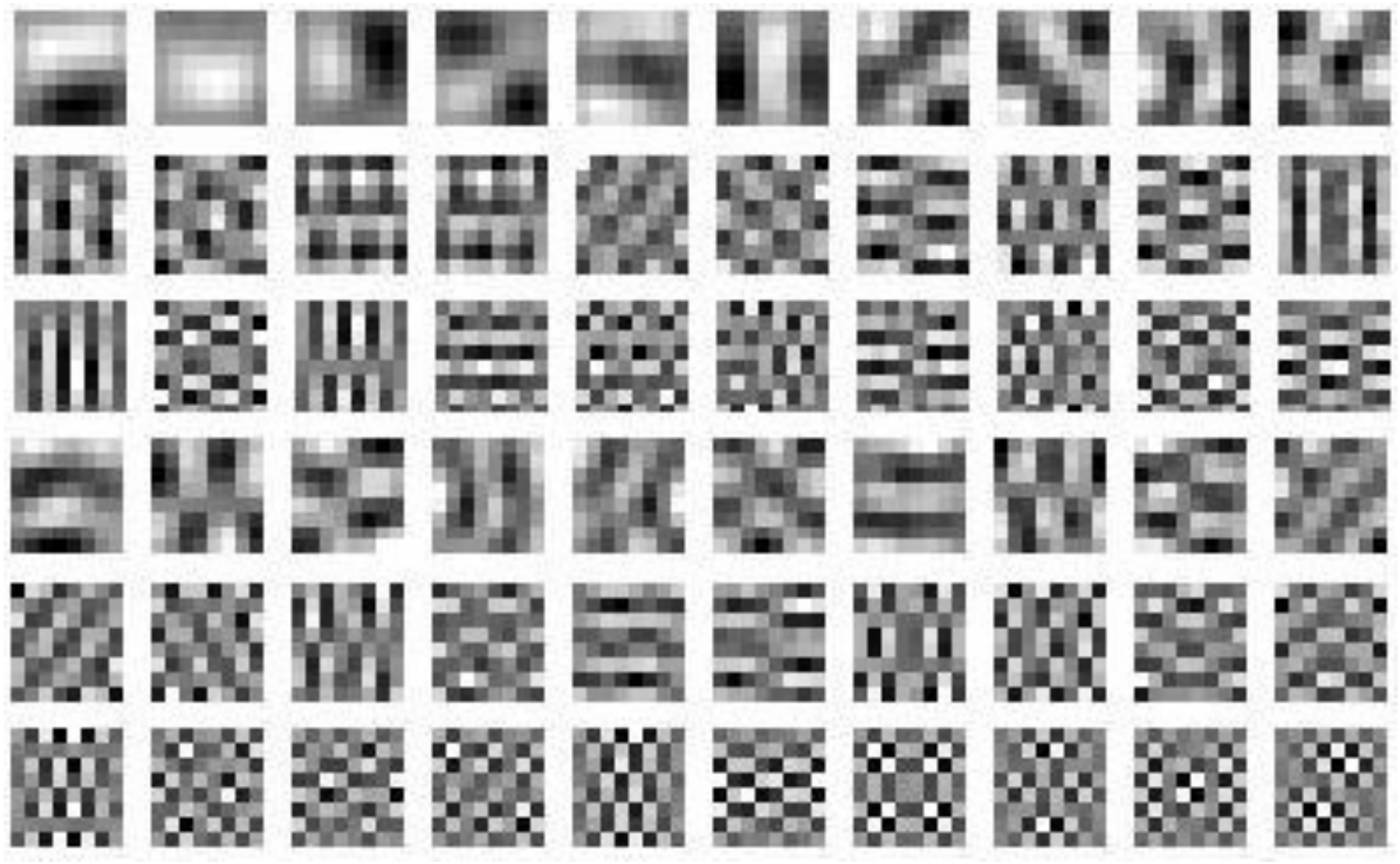




PCA compression: 144D => 1D

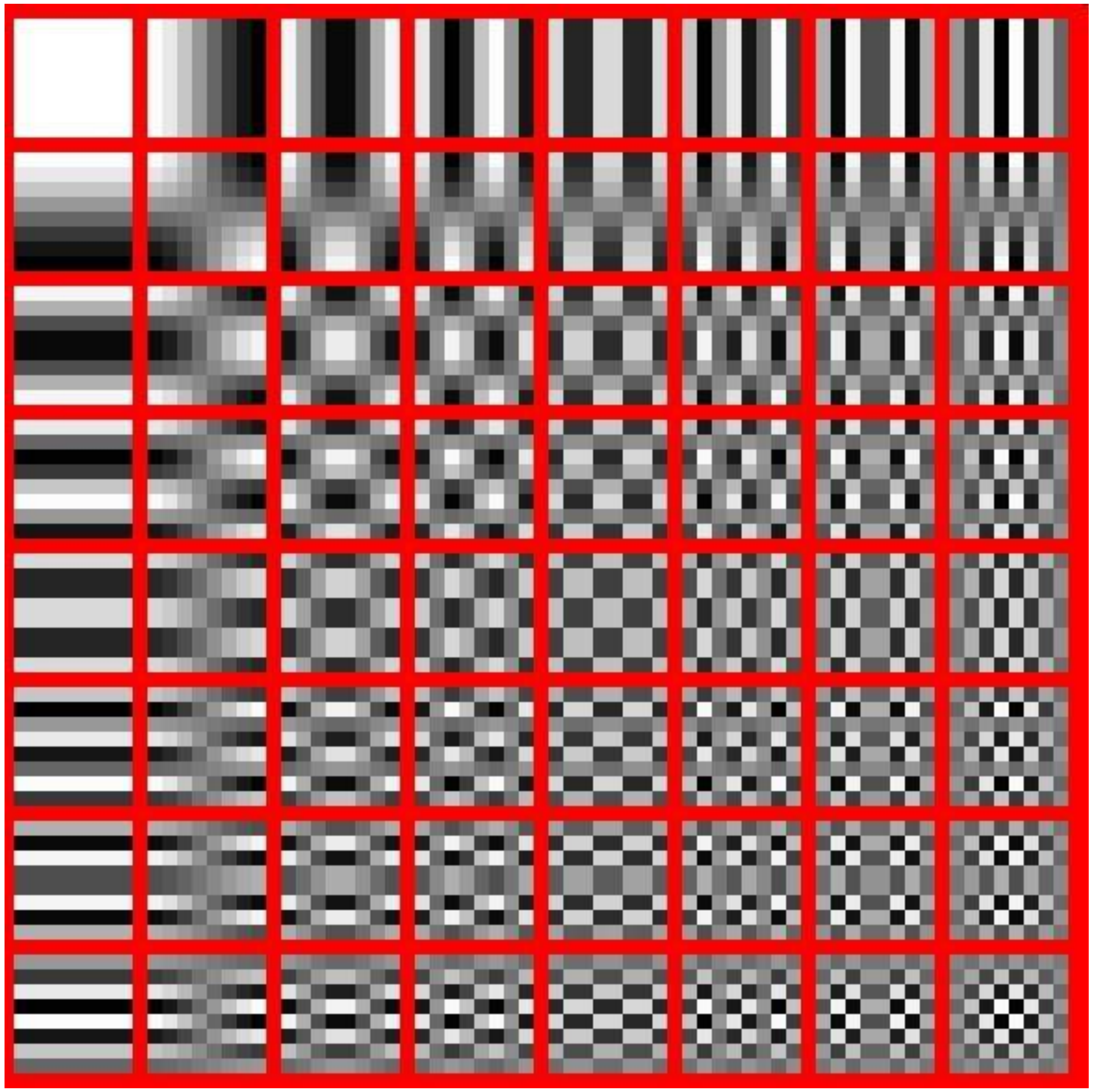


60 most important eigenvectors



- Looks like the discrete cosine bases of JPG!...

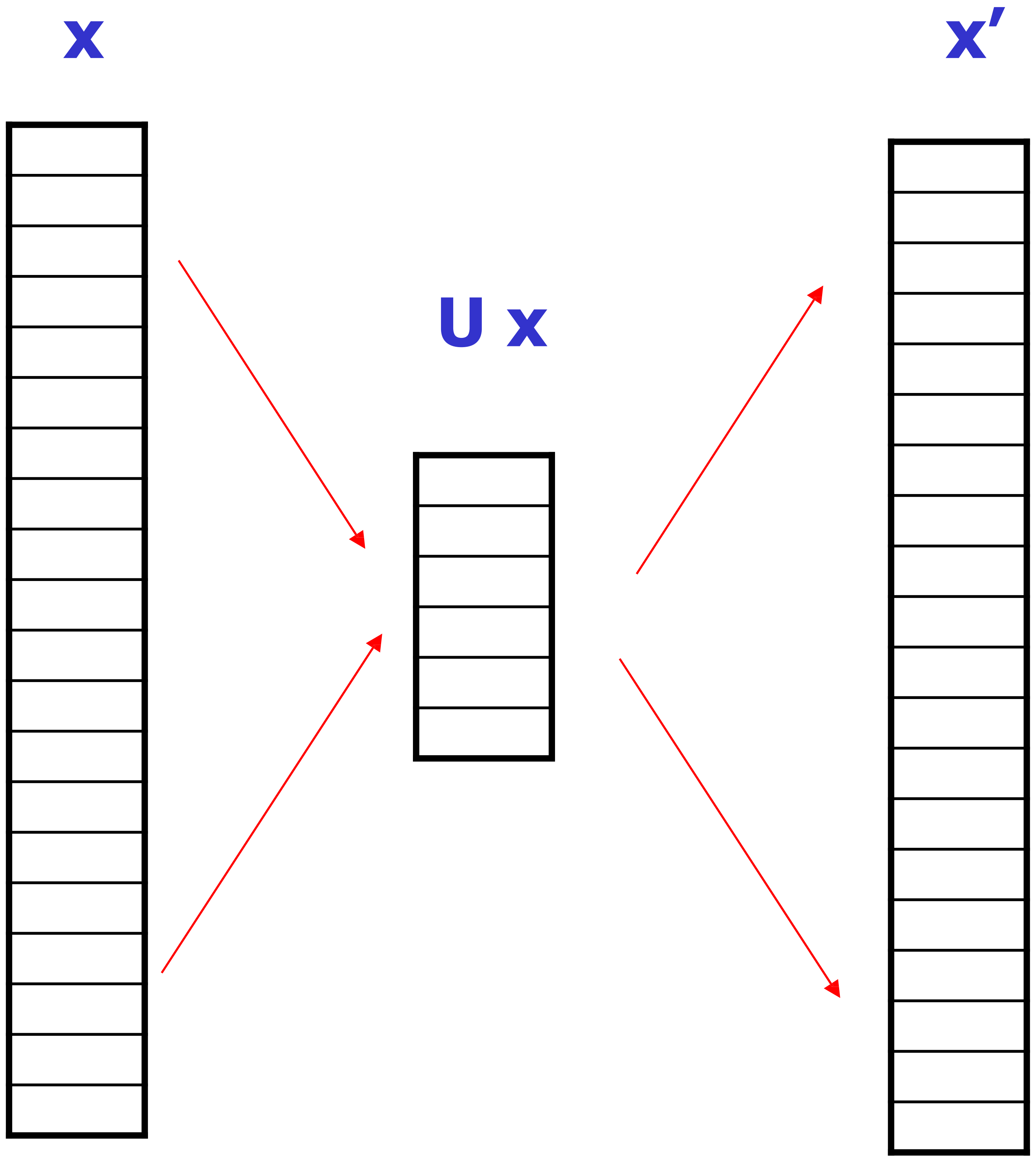
2D Discrete Cosine Basis



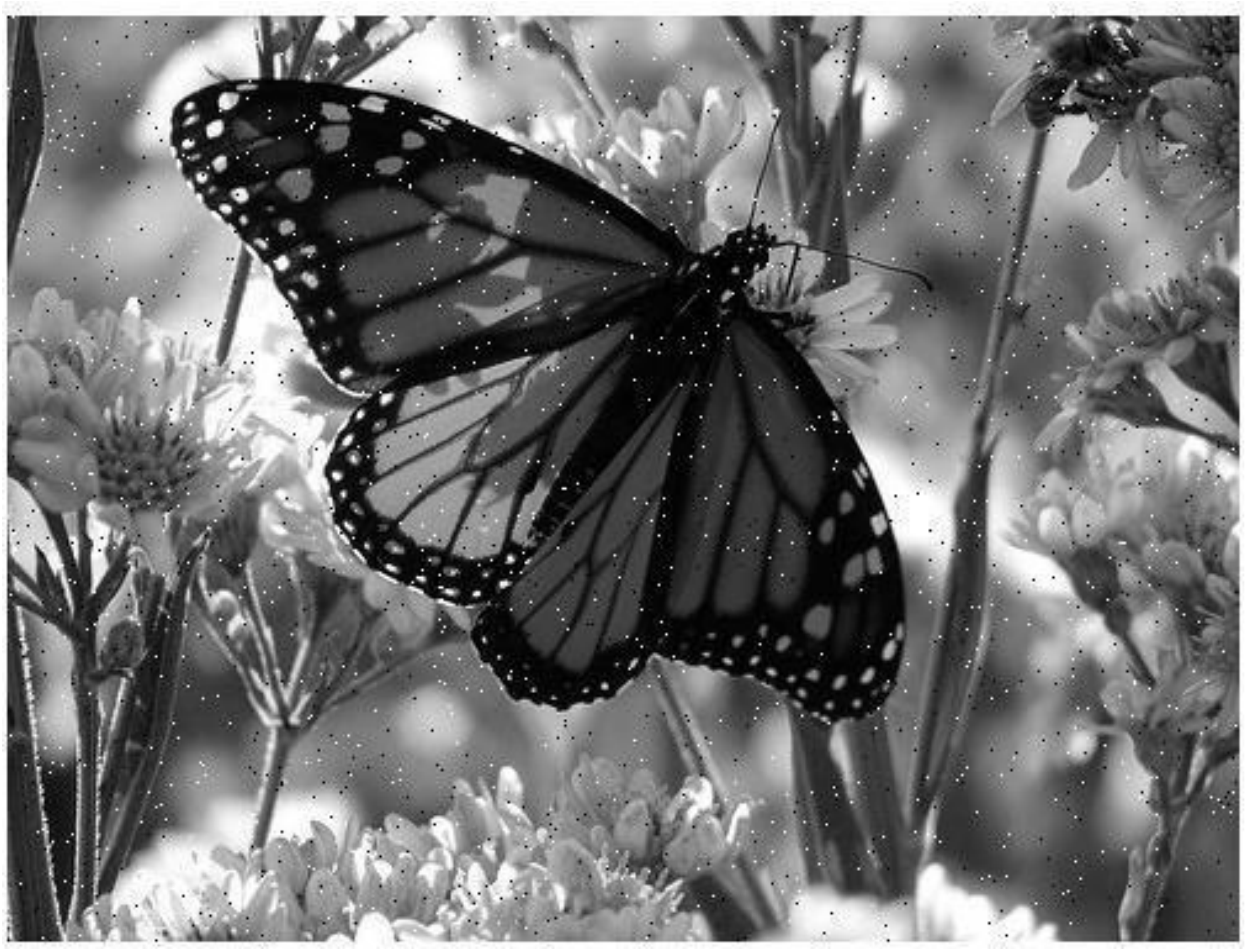
http://en.wikipedia.org/wiki/Discrete_cosine_transform

Noise Filtering

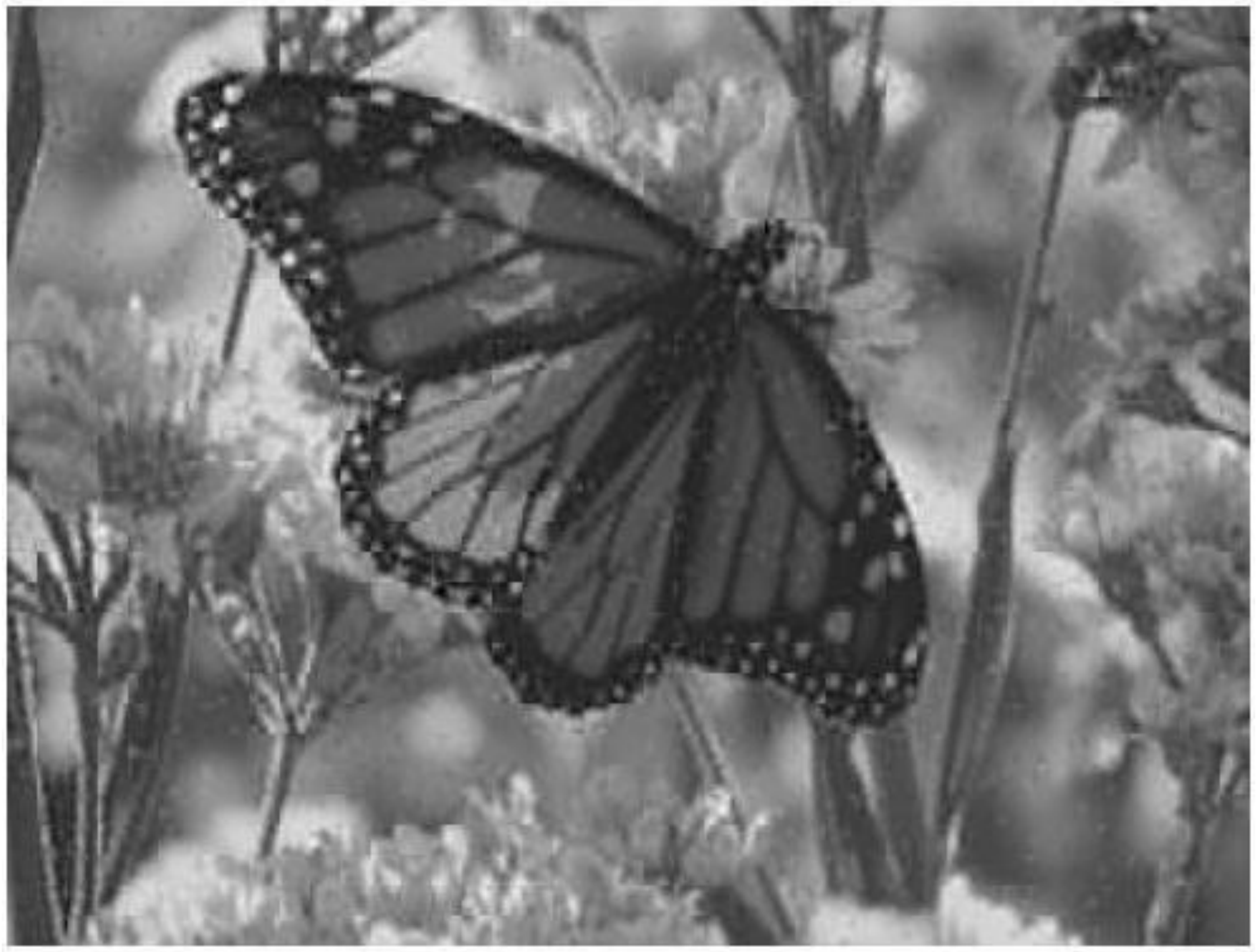
Noise Filtering



Noisy image



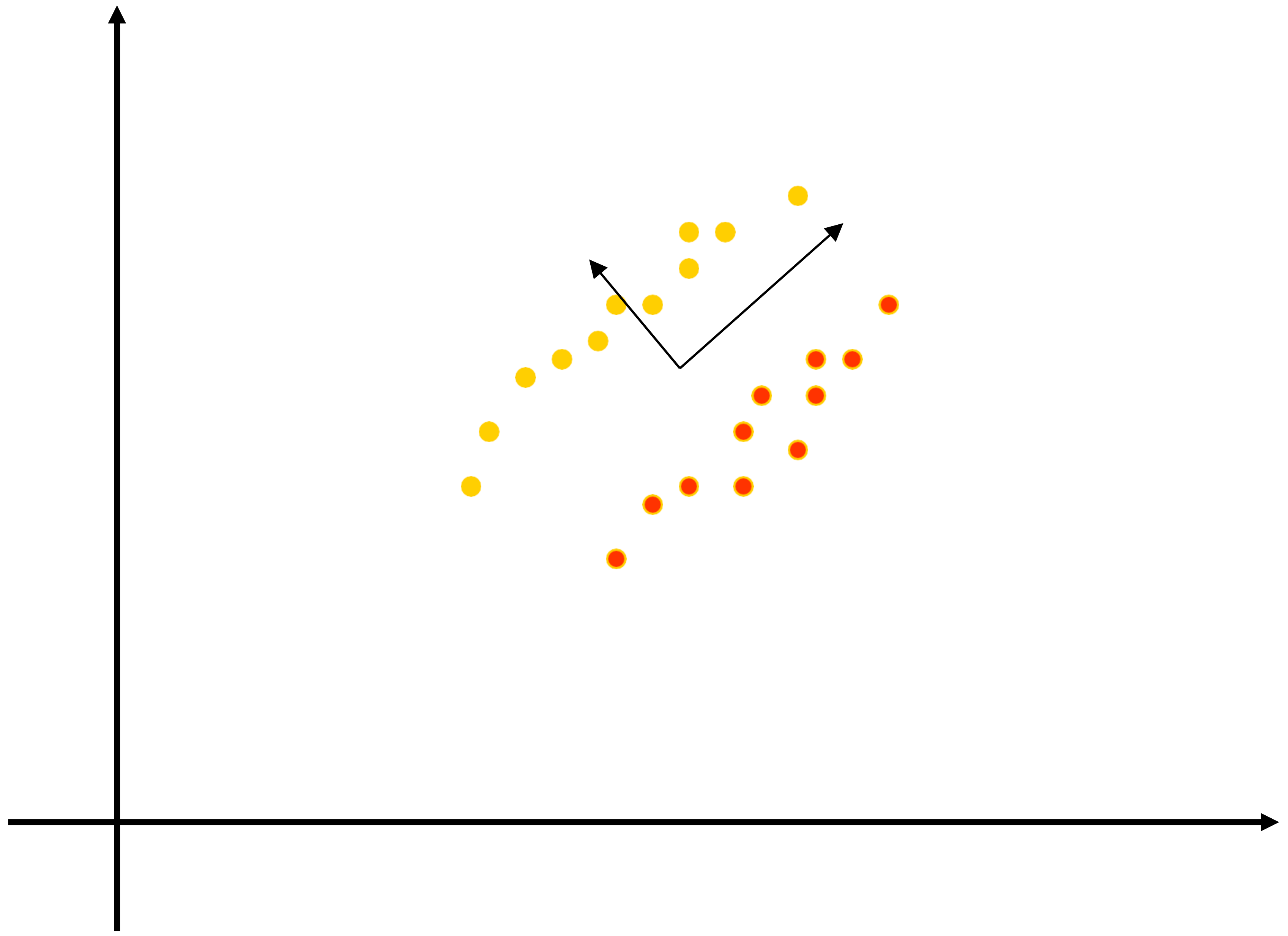
Denoised image using 15 PCA components



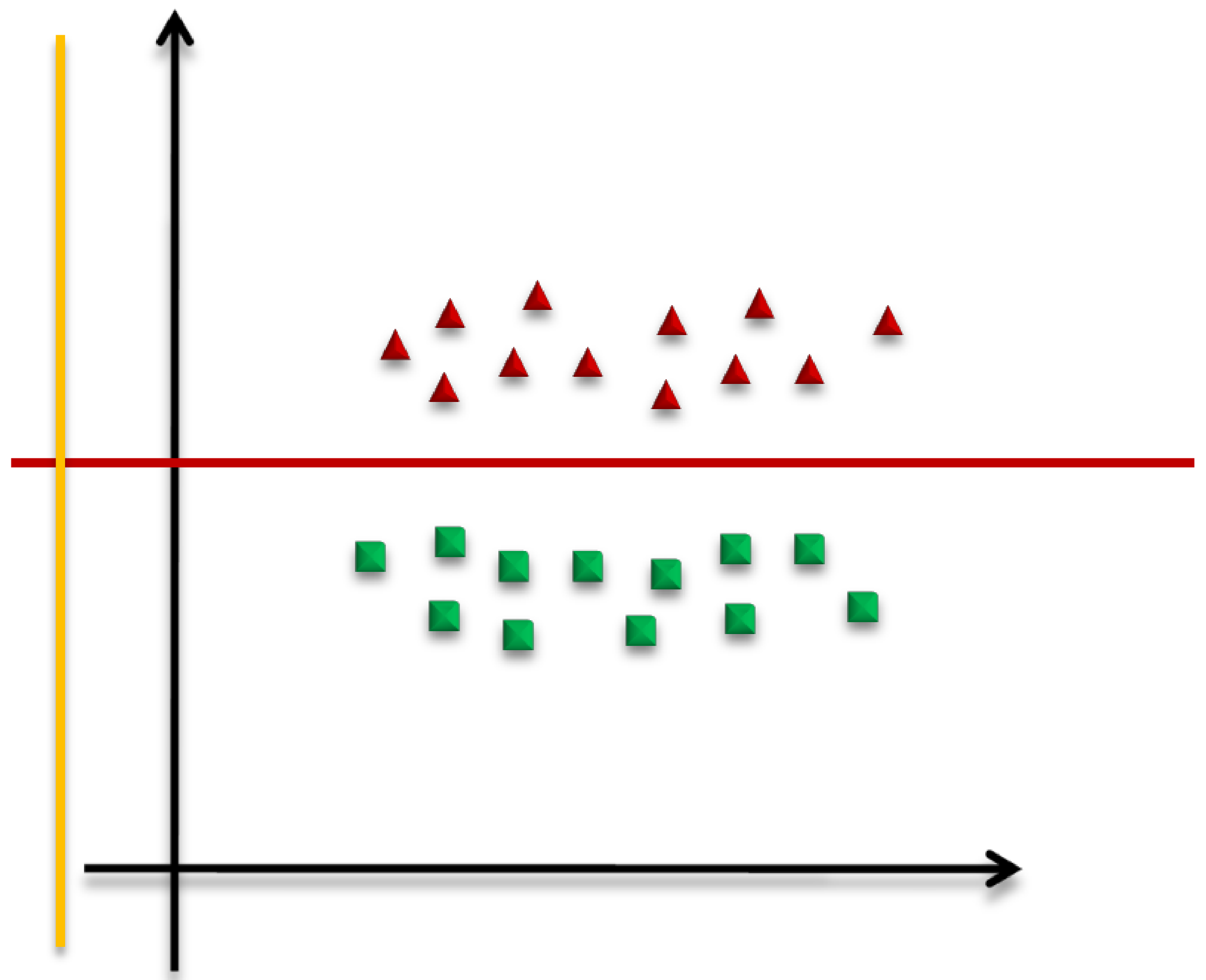
PCA Shortcomings

Problematic Data Set for PCA

- PCA doesn't know labels!

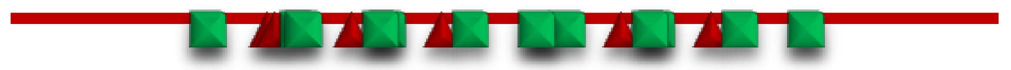


PCA vs. Fisher Linear Discriminant



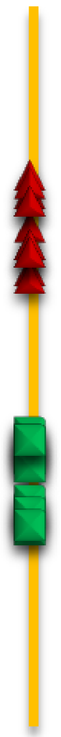
Principal Component Analysis

- higher variance
- bad for discriminability



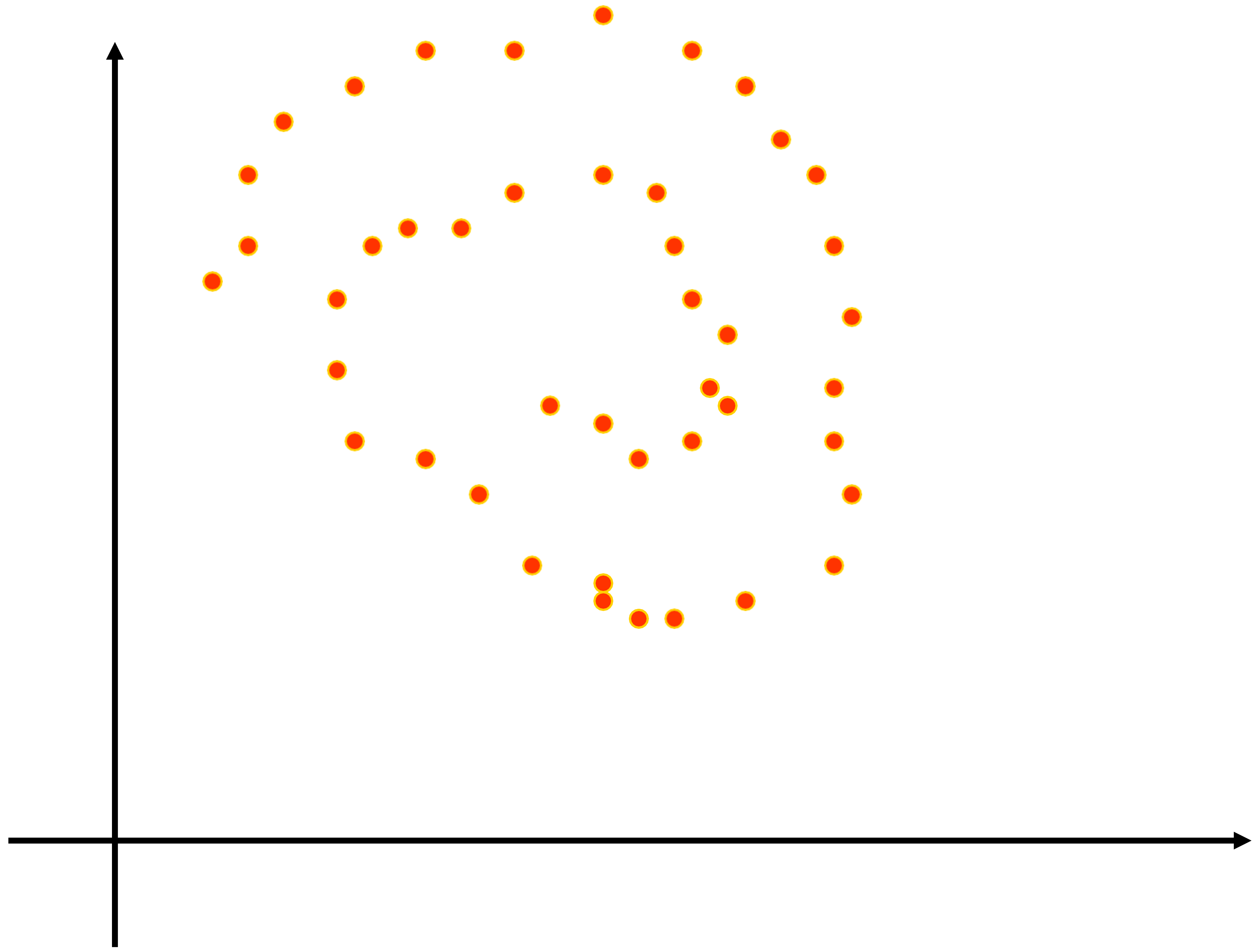
Fisher Linear Discriminant

- smaller variance
- good discriminability



Problematic Data Set for PCA

- PCA cannot capture NON-LINEAR structure!



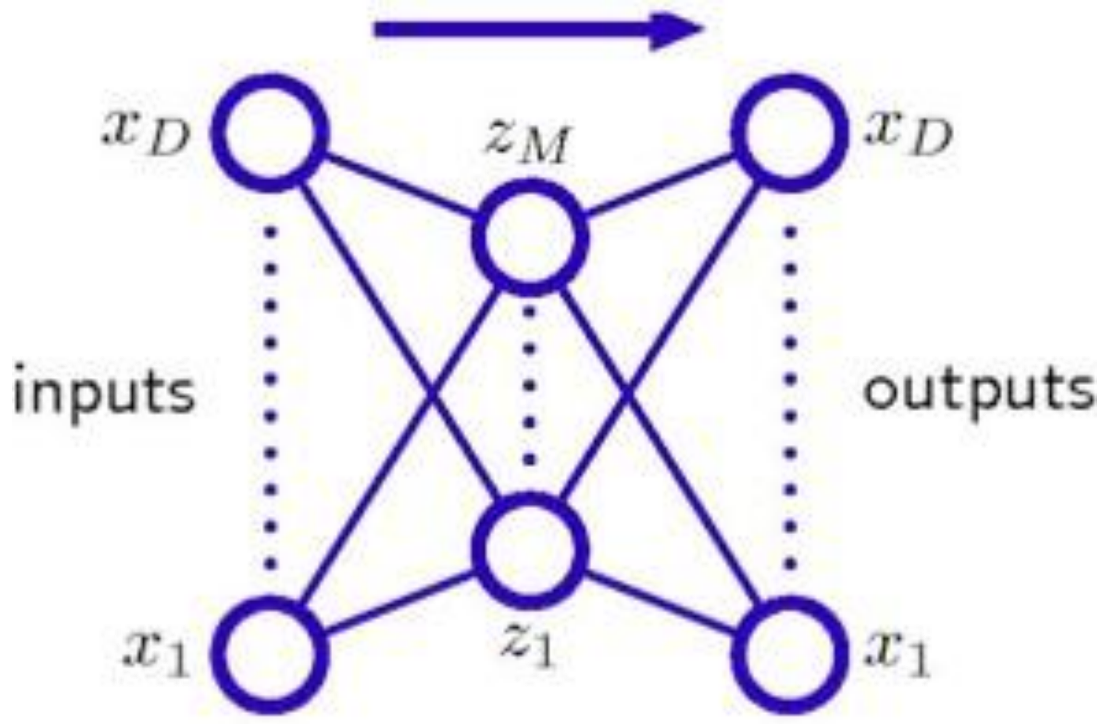
PCA Conclusions

- 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!

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

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

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

Auto encoders

- Define

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- If g and f are linear

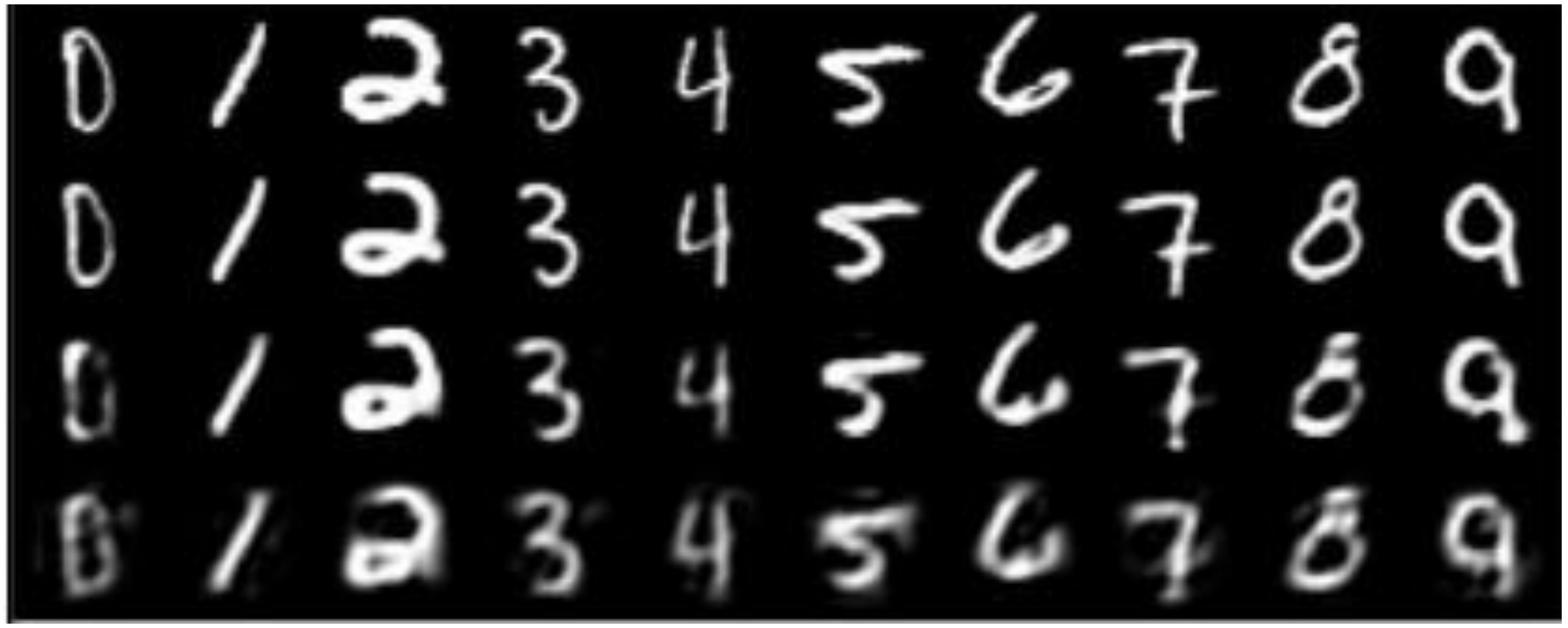
$$\min_{\mathbf{w},\mathbf{v}} \frac{1}{2N} \sum_{n=1}^{N} ||\mathbf{x}^{(n)} - VW\mathbf{x}^{(n)}||^2$$

- In other words, the optimal solution is PCA

Auto encoders: Nonlinear PCA

- What if *g*( ) is not linear?
- Then we are basically doing nonlinear PCA

Comparing Reconstructions



Real data

30-d deep autoencoder

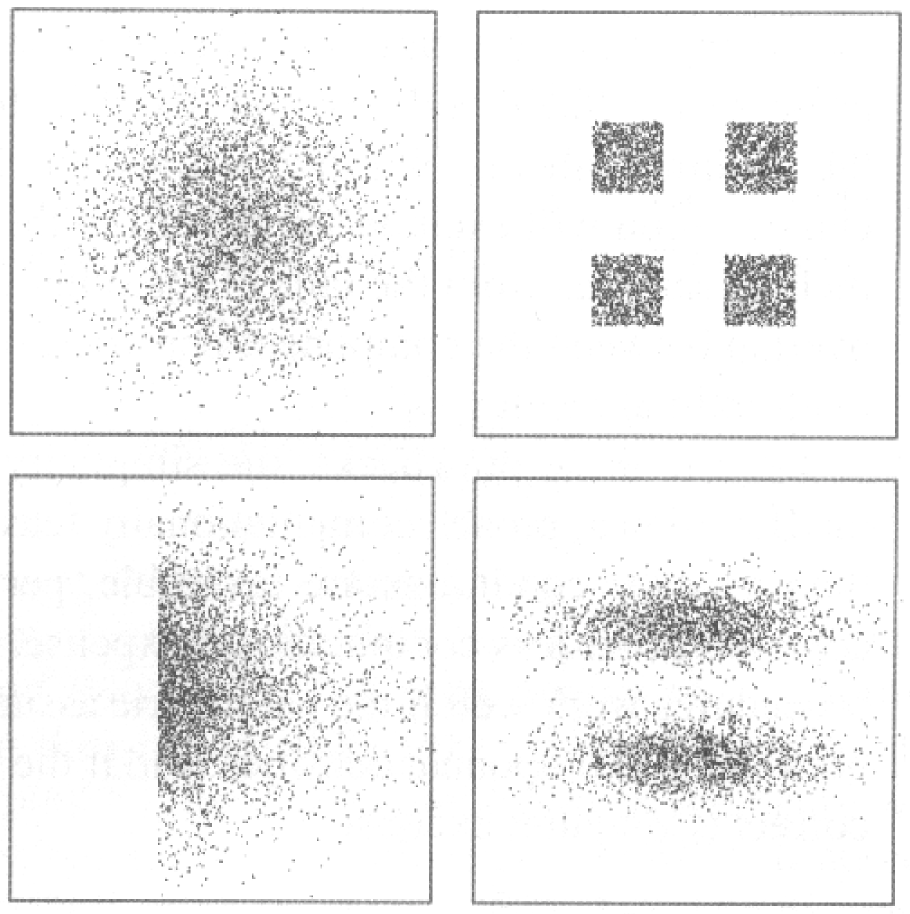
30-d logistic PCA

30-d PCA

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.

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.

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,

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

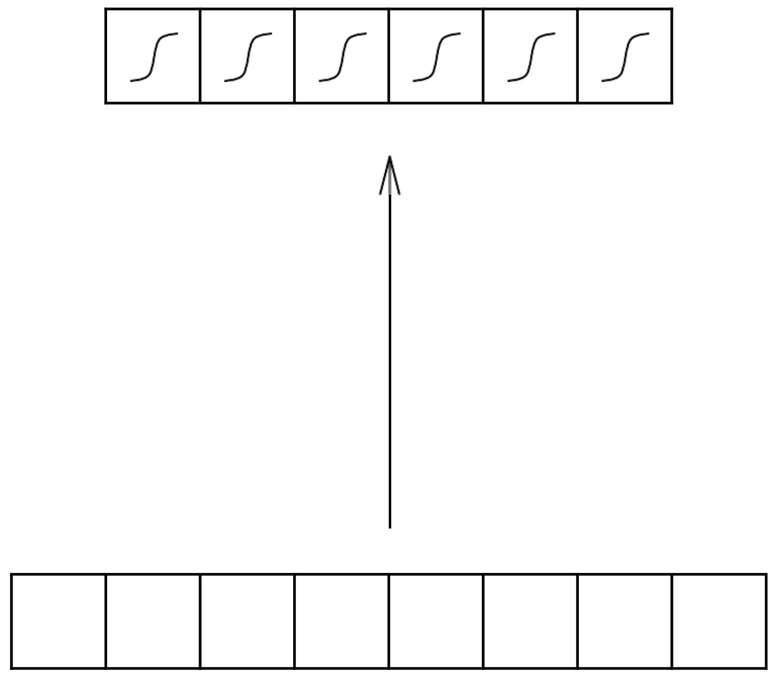
for any functions g_1 and g_2.

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.

Neural Network for ICA

- Single layer network:

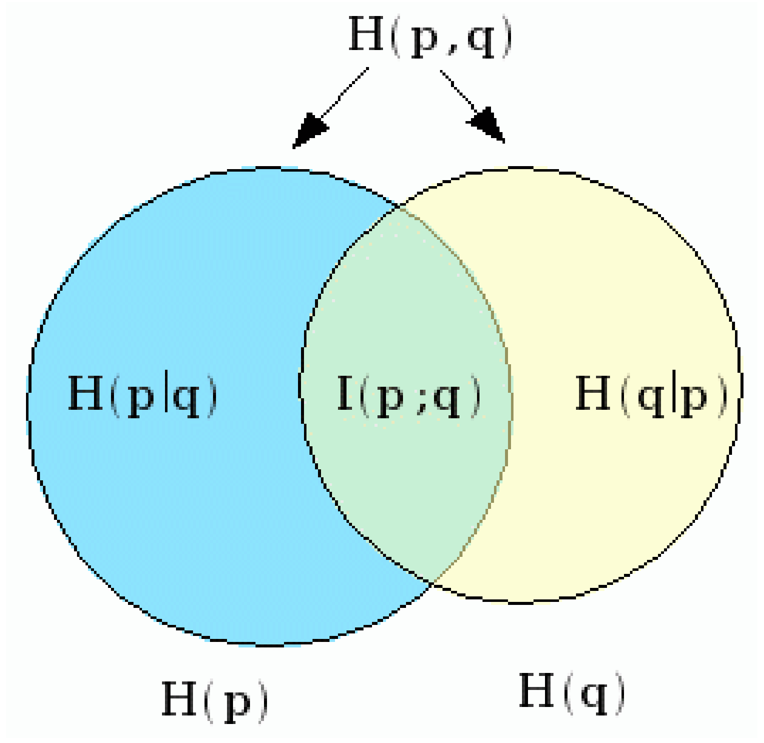


- Patterns $\{\xi\}$ are fed into the input layer.
- Inputs multiplied by weights in matrix **W**.
- Output logistic (vector notation here):

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

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).

Blind Source Separation (BSS)

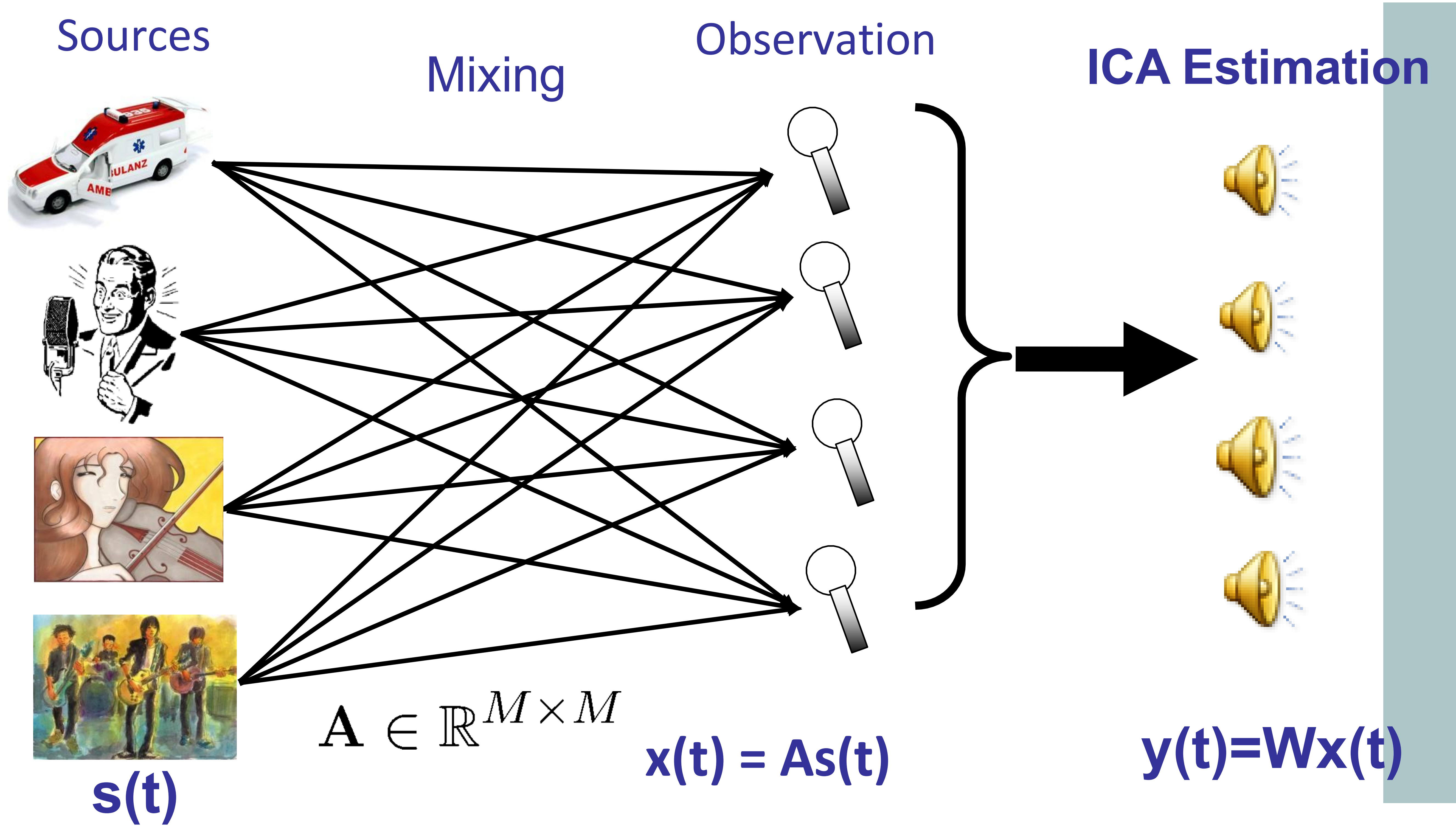
- The most famous application of ICA.
- Have K sources $\{s_k[t]\}$, and K signals $\{x_k[t]\}$. Both $\{s_k[t]\}$ and $\{x_k[t]\}$ are time series (t is a discrete time index).
- Each signal is a linear mixture of the sources

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

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 $s_k[n]$.

The Cocktail Party


Sources
Mixing
Observation
ICA Estimation
s(t)
$\mathbf{A} \in \mathbb{R}^{M \times M}$
x(t) = As(t)
y(t)=Wx(t)