Machine Learning

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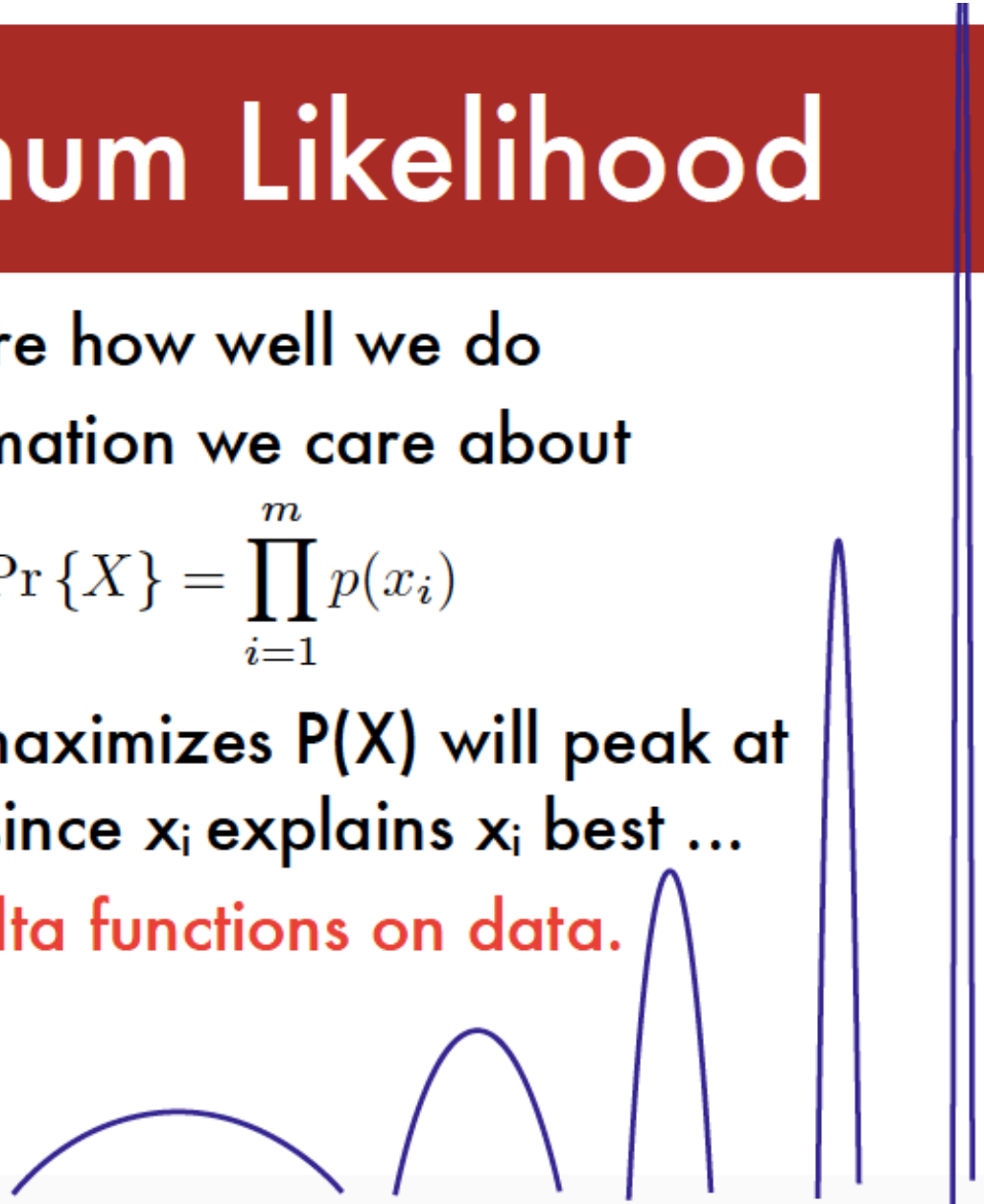
Model Selection

Maximum Likelihood

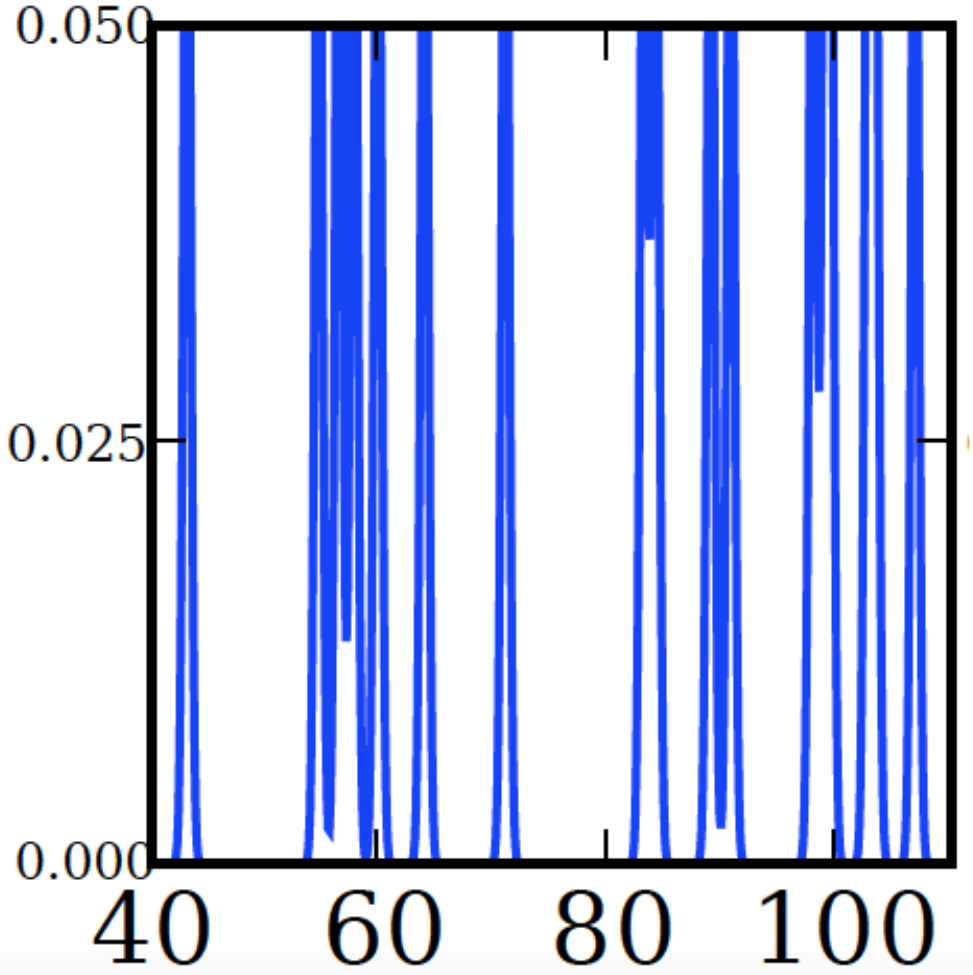
- Need to measure how well we do
- For density estimation we care about

$$\Pr\{X\} = \prod_{i=1}^{m} p(x_i)$$

- Finding a that maximizes P(X) will peak at all data points since x_i explains x_i best …
- Maxima are delta functions on data.
- Overfitting!



Overfitting



Likelihood on training set is much higher than typical.

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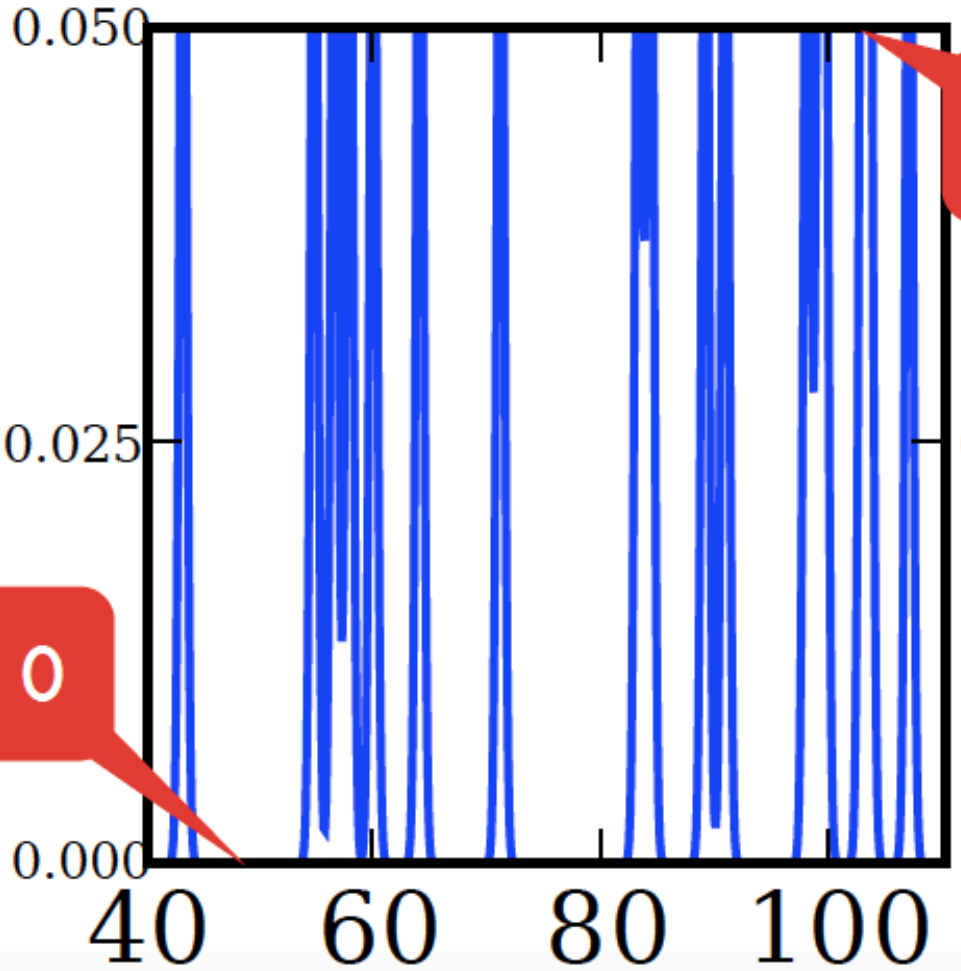
Overfitting



density » 0

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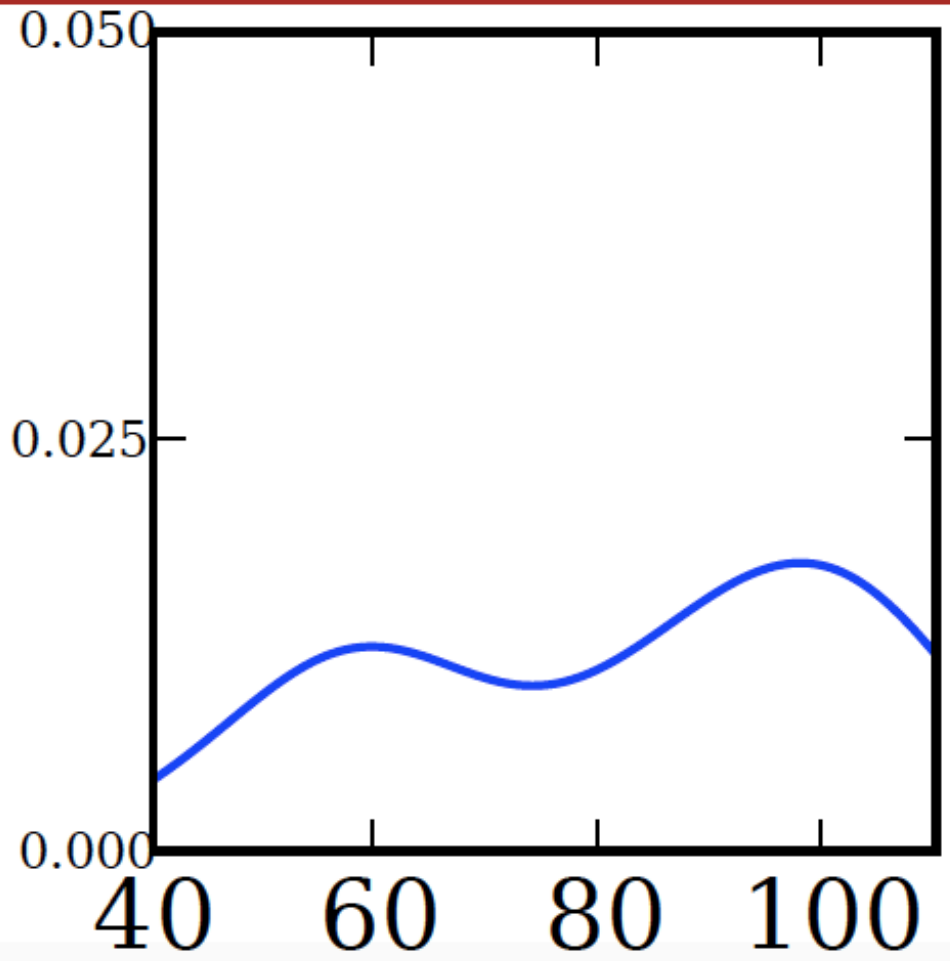
Underfitting



Likelihood on training set is very similar to typical one.

Too simple.

Model Selection

- Validation
  - Use some of the data to estimate density.
  - Use other part to evaluate how well it works
  - Pick the parameter that works best

$$\mathcal{L}(X'|X) := \frac{1}{n'} \sum_{i=1}^{n'} \log \hat{p}(x'_i)$$

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  - Use data to build model
  - Measure complexity and use this to bound

$$\frac{1}{n} \sum_{i=1}^{n} \log \hat{p}(x_i) - \mathbf{E}_x \left[\log \hat{p}(x) \right]$$

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- Simple implementation

$$\frac{1}{n}\sum_{i=1}^{n} \log\left[\frac{n}{n-1}p(x_i) - \frac{1}{n-1}k(x_i, x_i)\right] \quad \text{where } p(x) = \frac{1}{n}\sum_{i=1}^{n} k(x_i, x)$$

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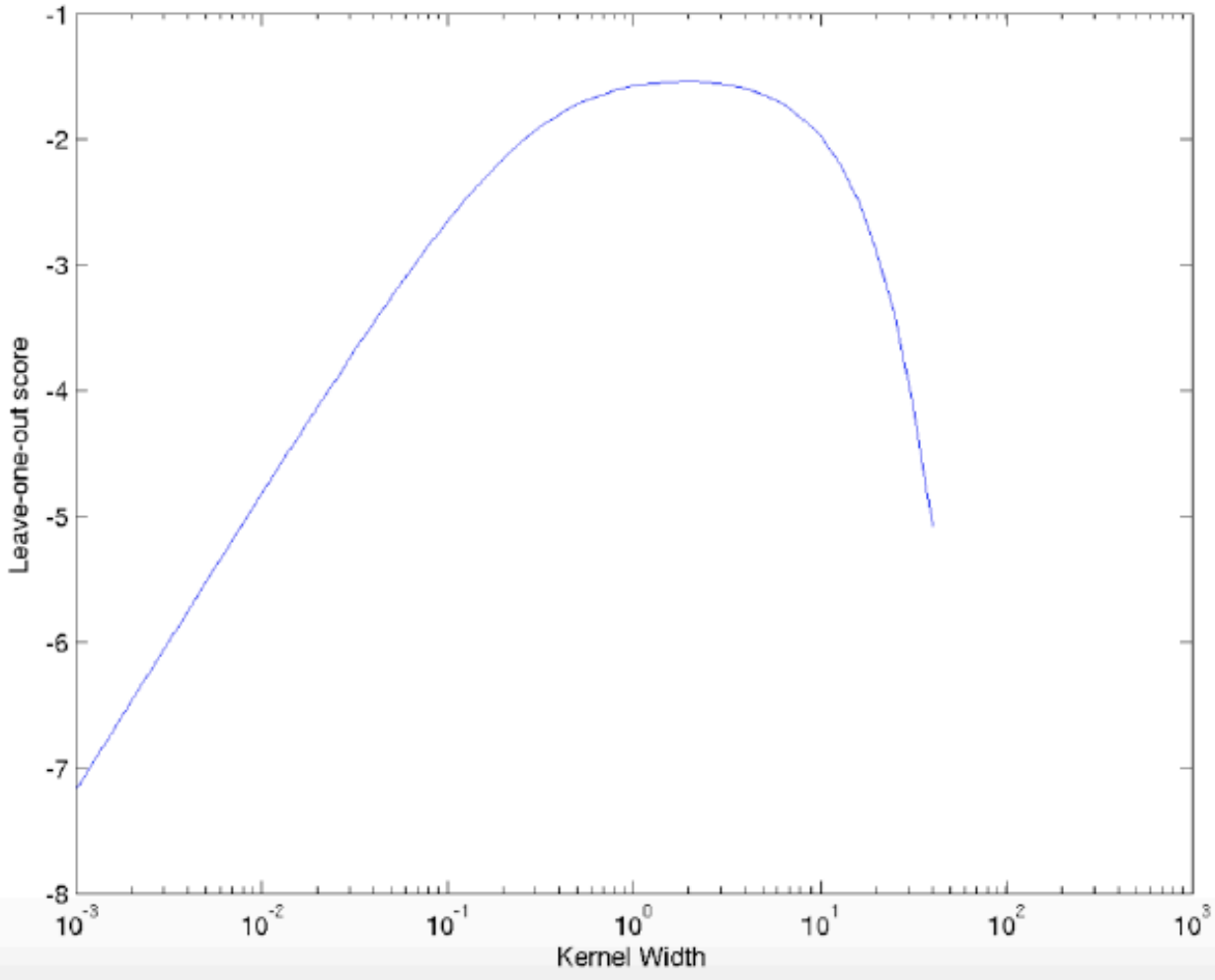
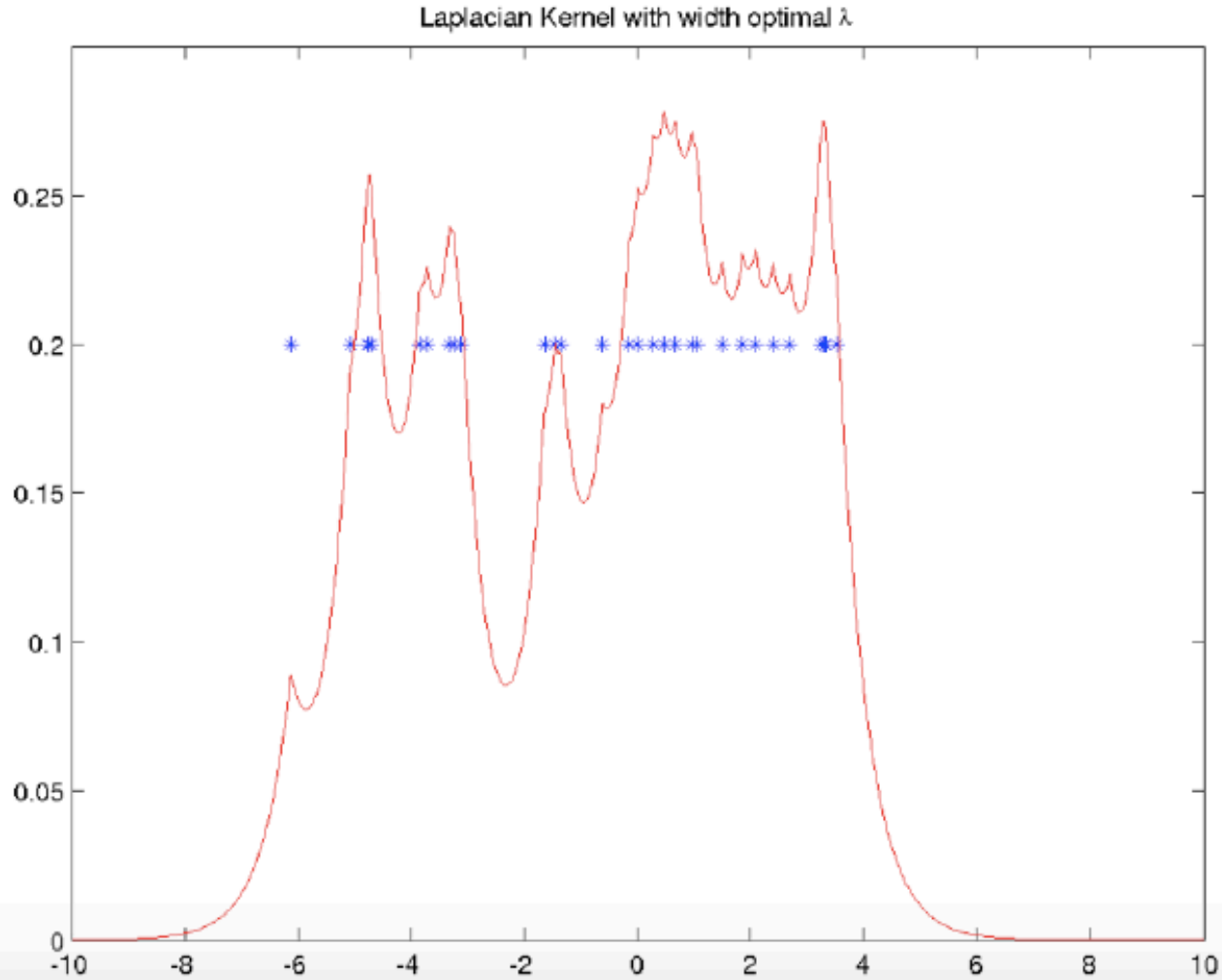
Leave-one out estimate



niversity

Optimal estimate



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- Almost unbiased (e.g. via Luntz and Brailovski, 1969) (error is for (k-1)/k sized set)

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- Pick best parameter

Contents

- ❑ Motivation
- ❑ PCA algorithms
- ❑ Applications

Some of these slides are taken from

- Karl Booksh Research group
- Tom Mitchell
- Ron Parr

Motivation

PCA Applications

- Data Visualization
- Data Compression
- Noise Reduction

Data Visualization

Example:

- Given 53 blood and urine samples (features) from 65 people.

- How can we visualize the measurements?

Data Visualization

- Matrix format (65x53)

	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

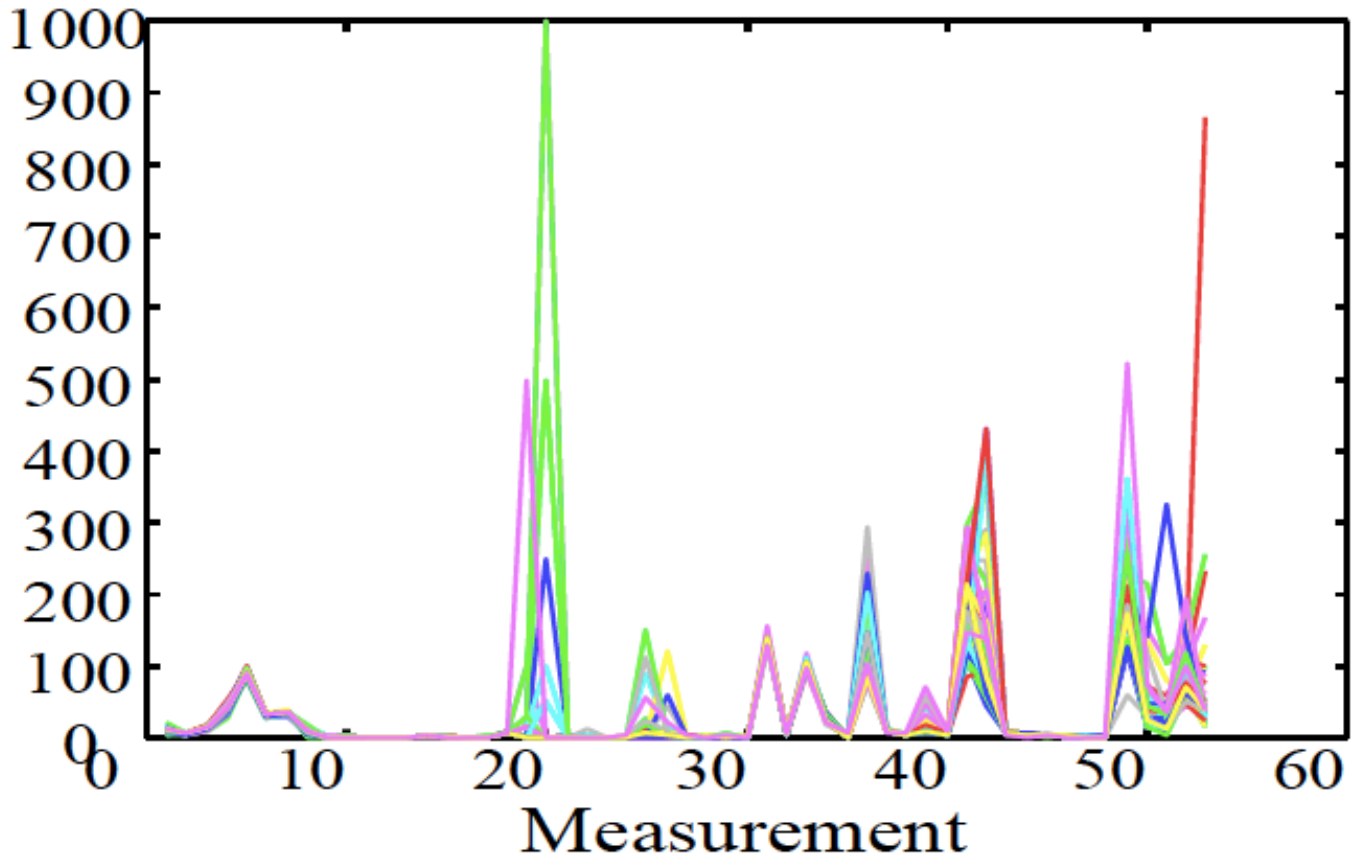
Instances

Features

Difficult to see the correlations between the features...

Data Visualization

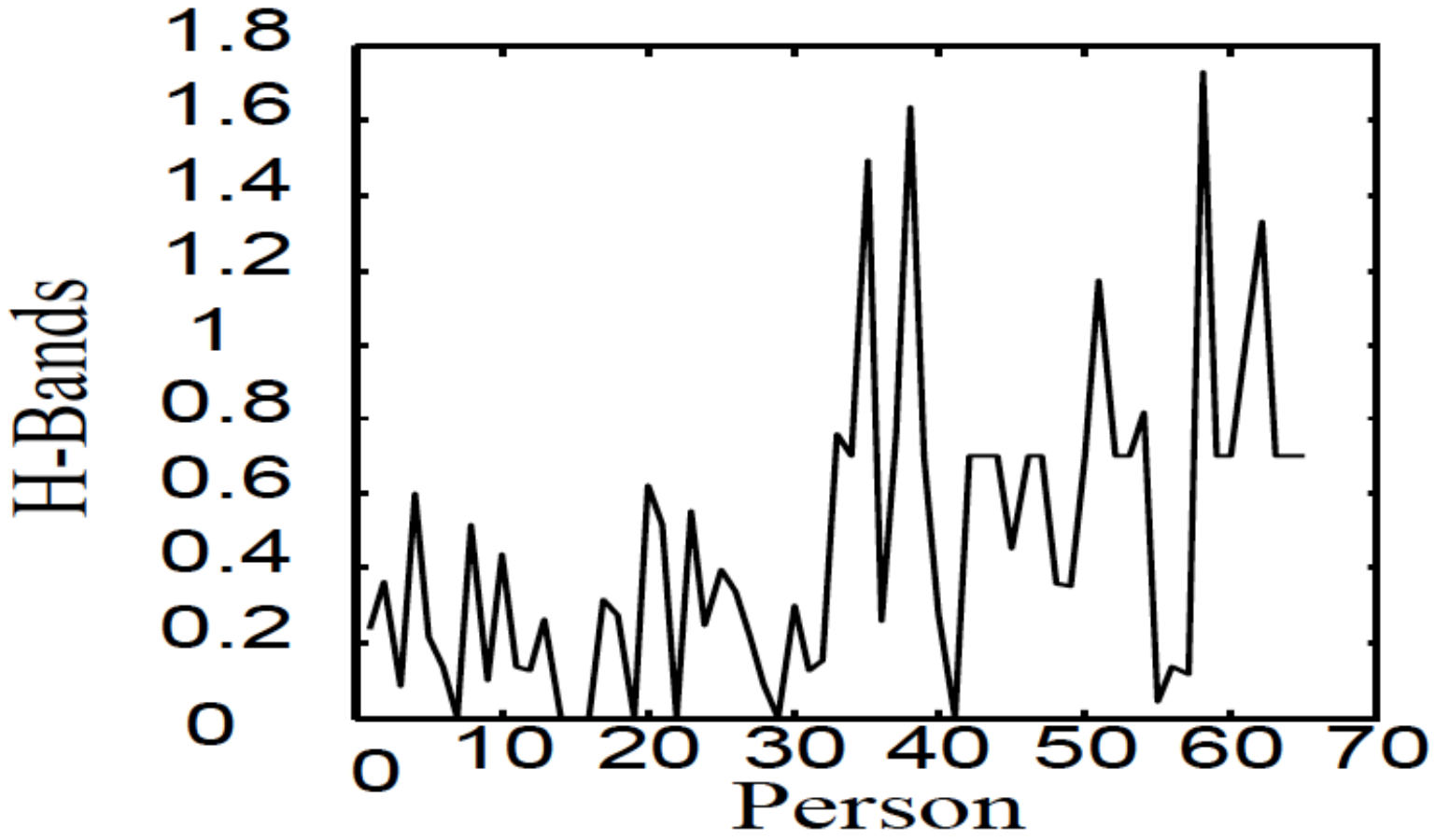
- Spectral format (65 curves, one for each person)



Difficult to compare the different patients...

Data Visualization

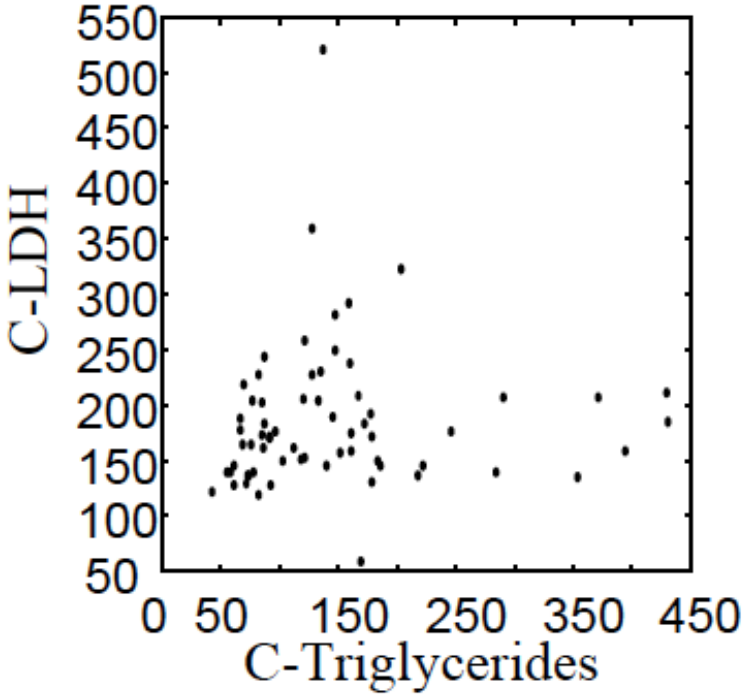
- Spectral format (53 pictures, one for each feature)



Difficult to see the correlations between the features...

Data Visualization

Bi-variate



Data Visualization

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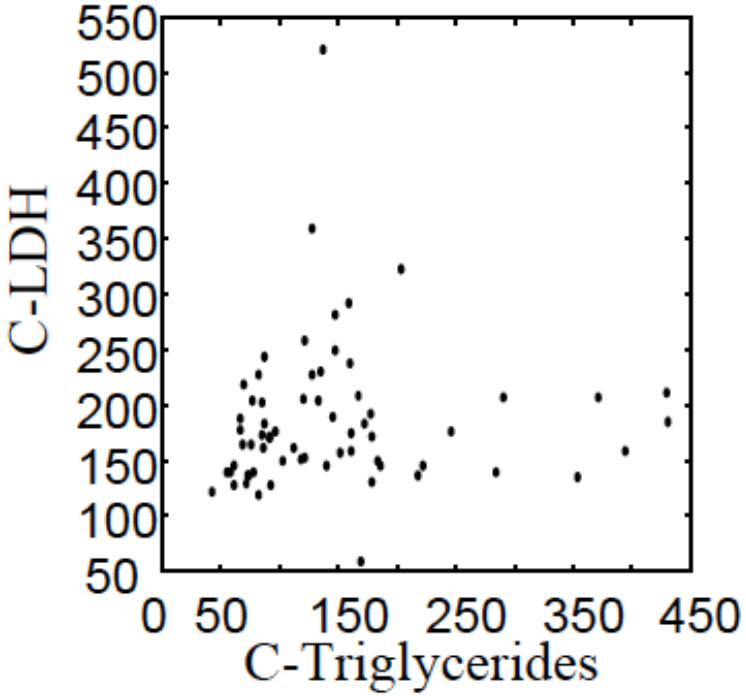
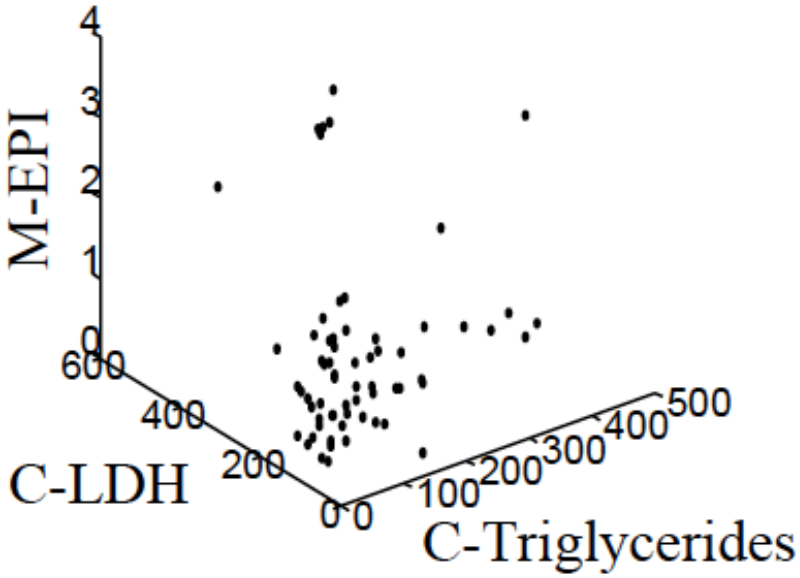


Tri-variate



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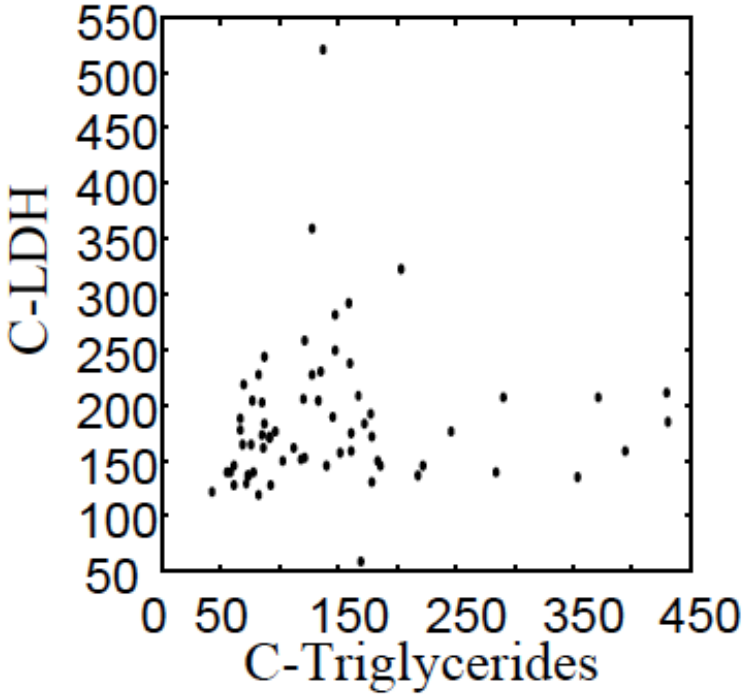

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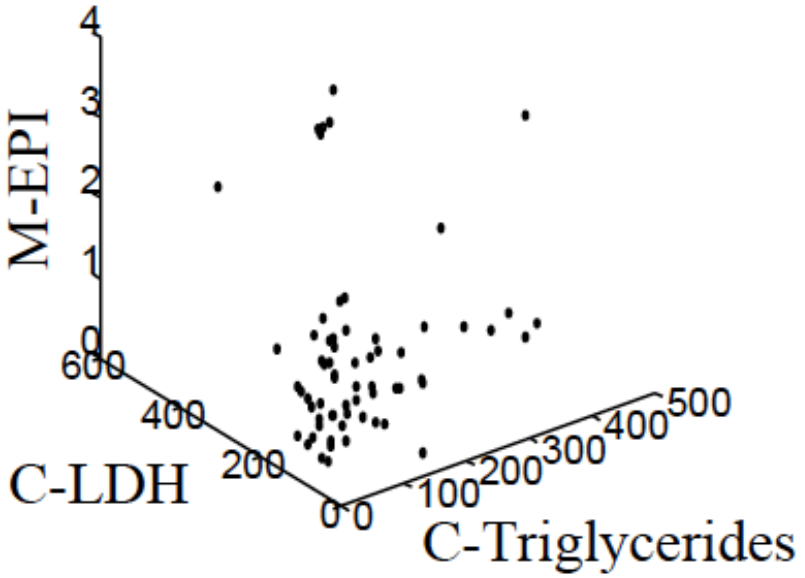

How can we visualize the other variables???

… difficult to see in 4 or higher dimensional spaces…

Data Visualization

- Is there a representation better than the coordinate axes?

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  - … what if there are strong correlations between the features?

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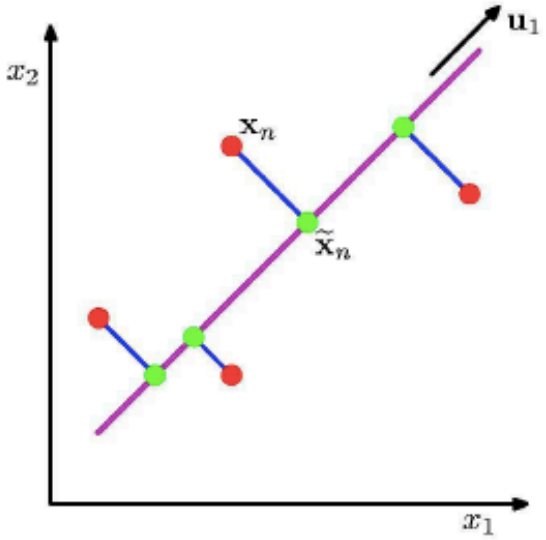
- A solution: **Principal Component Analysis**

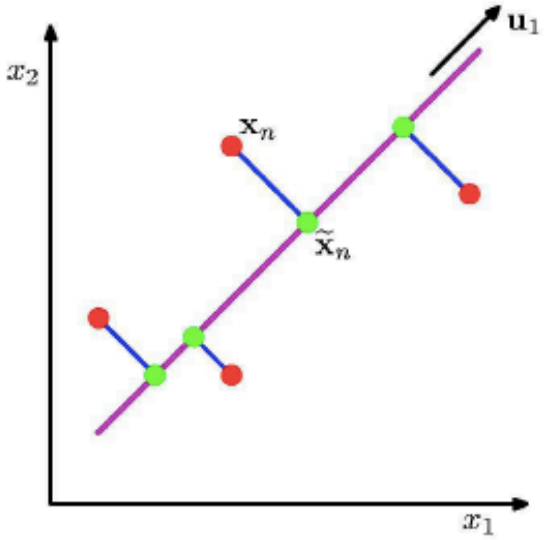
PCA Algorithms

Principal Component Analysis

PCA:



Principal Component Analysis



PCA:

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

- ❑maximizes variance of projected data (purple line)

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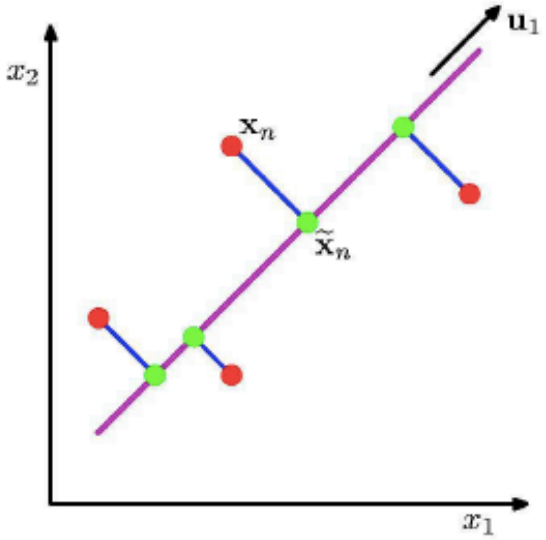

PCA:

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

Idea:

- Given data points in a d-dimensional space, project them into a lower dimensional space while preserving as much information as possible.
  - Find best planar approximation to 3D data
  - Find best 12-D approximation to 10^4-D data

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- In particular, choose projection that minimizes *squared error* in reconstructing the original data.

Principal Component Analysis

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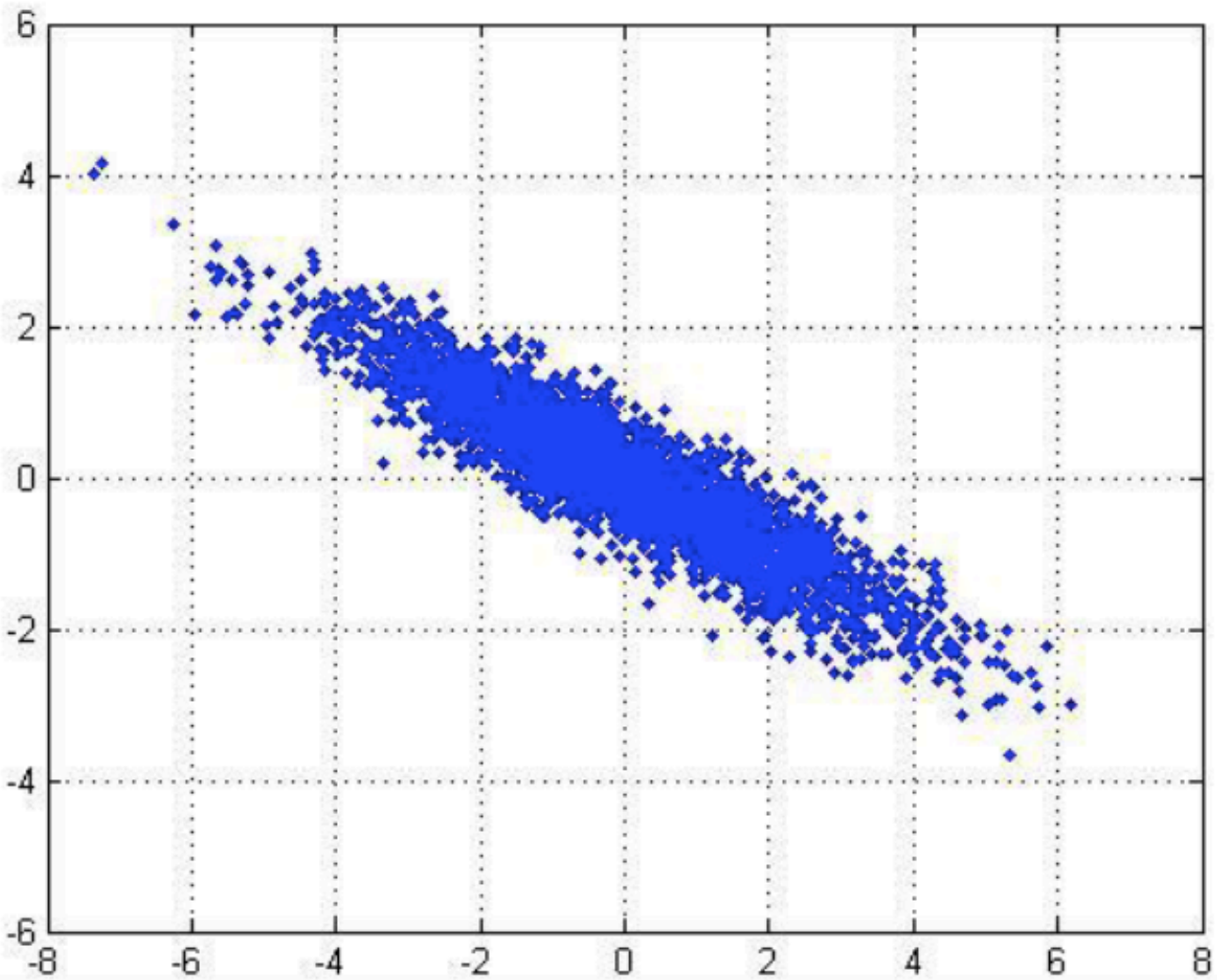
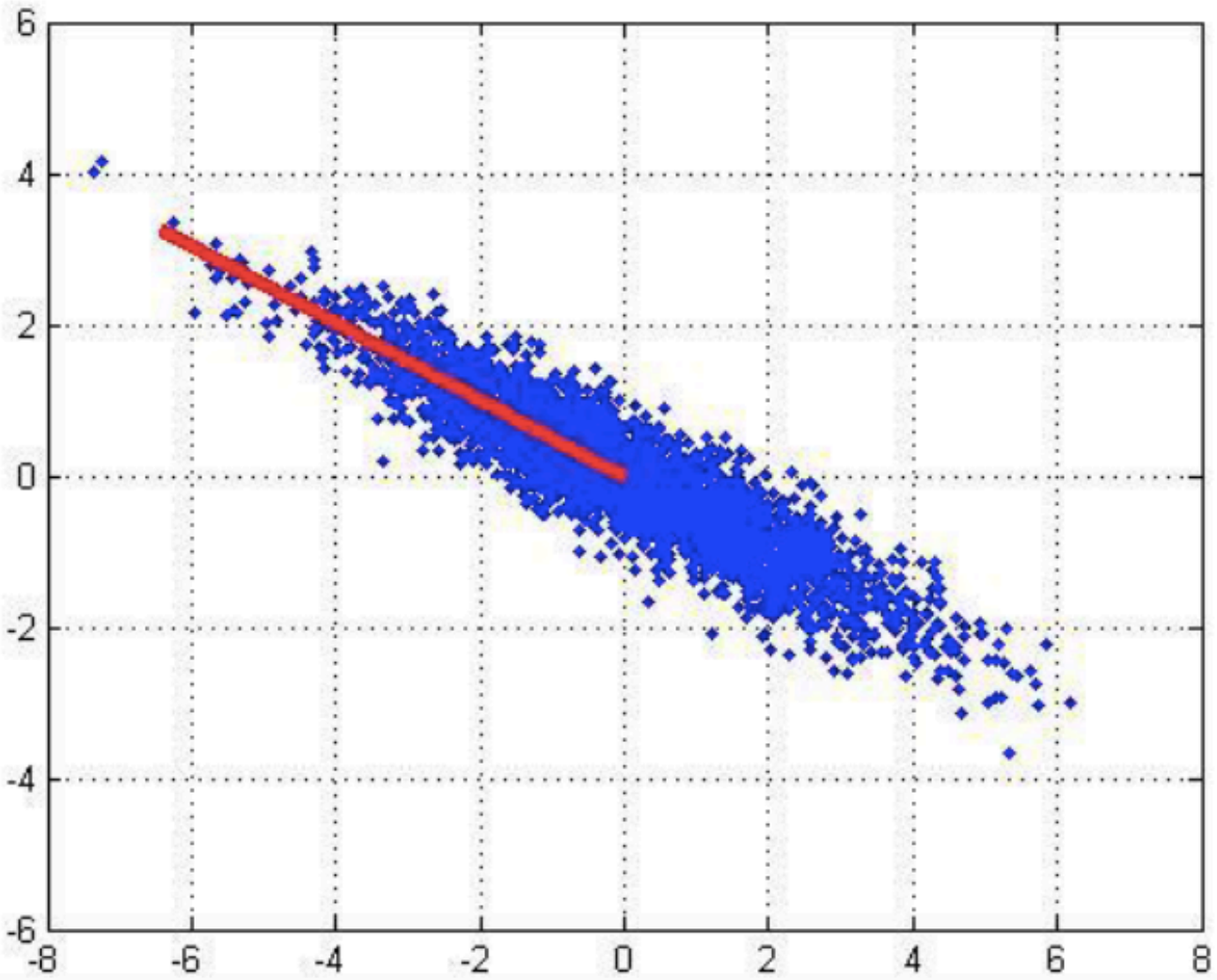
- Each subsequent principal component
  - is **orthogonal** to the previous ones, and
  - points in the directions of the **largest variance of the residual subspace**

2D Gaussian dataset



1st PCA axis



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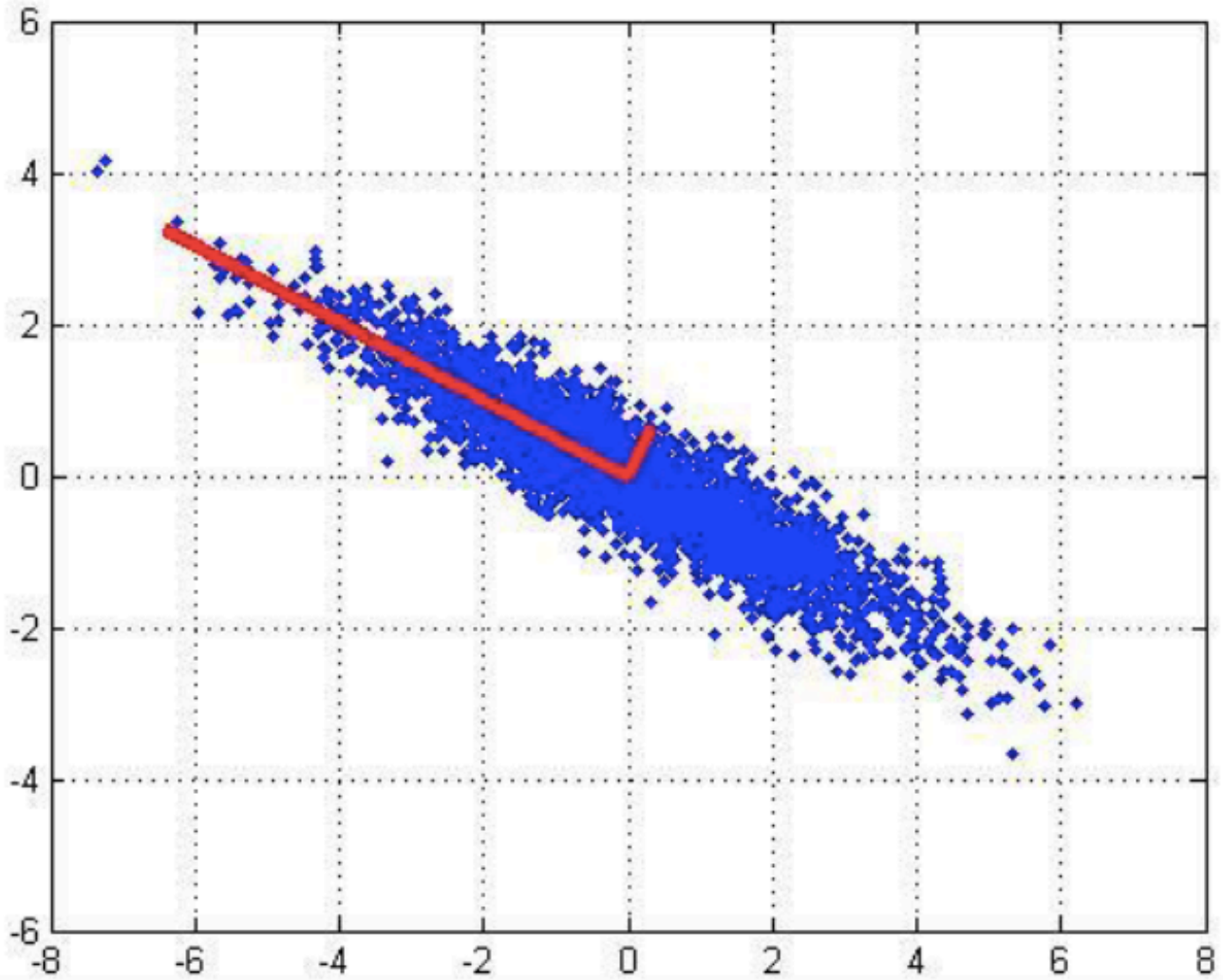
2nd PCA axis



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PCA algorithm I (sequential)

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$$\mathbf{w}_2 = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m} \sum_{i=1}^{m} \{[\mathbf{w}^T (\mathbf{x}_i - \underbrace{\mathbf{w}_1 \mathbf{w}_1^T \mathbf{x}_i}_{\mathbf{x}' \text{ PCA reconstruction}})]^2\}$$ k^{th} PCA vector

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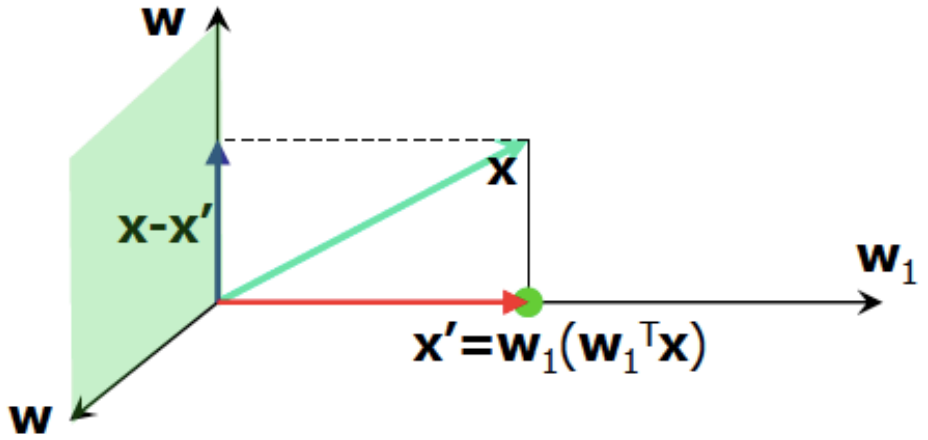

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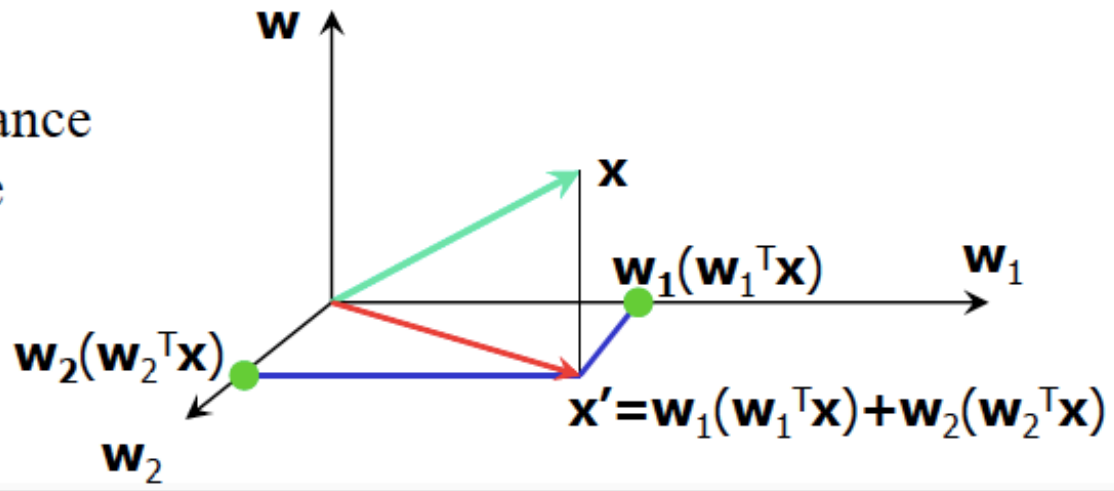

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PCA algorithm II (sample covariance matrix)

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

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

where

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

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

- Larger eigenvalue $\Rightarrow$ more important eigenvectors

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PCA algorithm II (sample covariance matrix)

PCA algorithm(**X**, *k*): top *k* eigenvalues/eigenvectors

% $\underline{\mathbf{X}}$ = N × m data matrix,
% … each data point $\mathbf{x}_i$ = column vector, i=1..m

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PCA algorithm II (sample covariance matrix)

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  … $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$
- Return $\{ \lambda_i, \mathbf{u}_i \}_{i=1..k}$
  % top k PCA components

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PCA algorithm III
(SVD of the data matrix)

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

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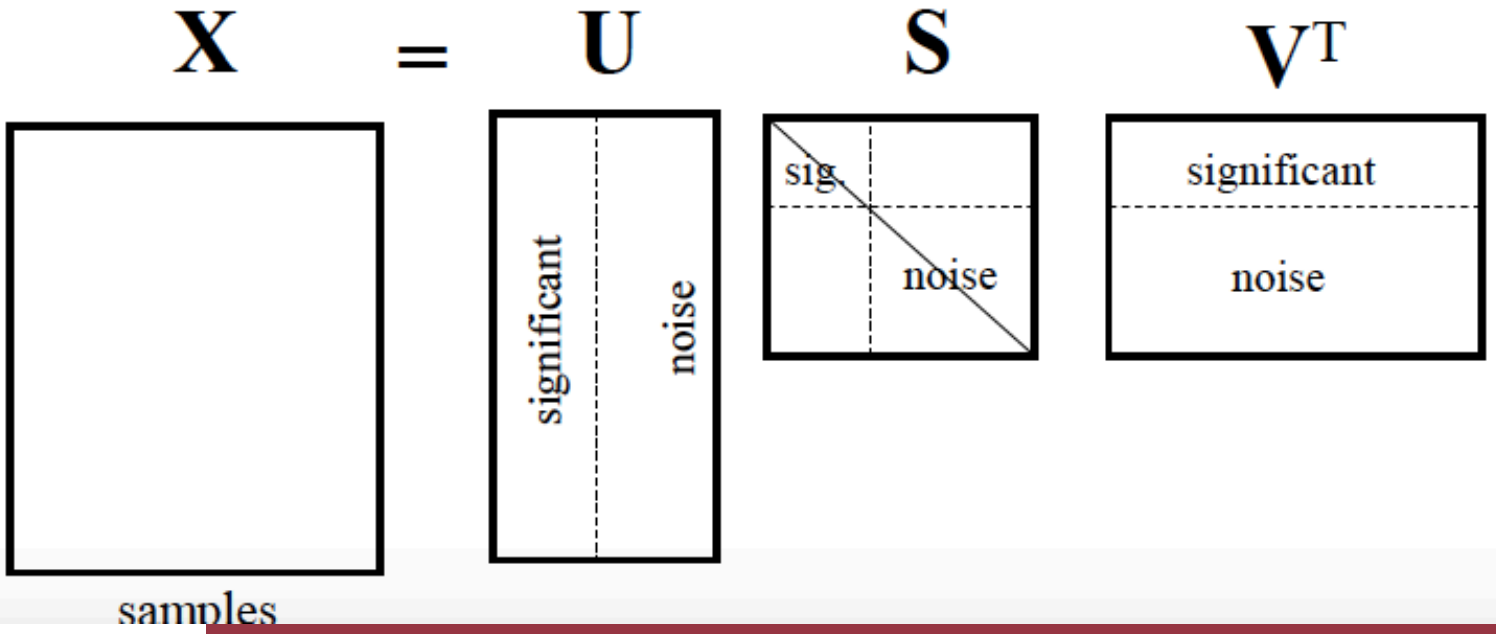

PCA algorithm III

- **Columns of U**
  - the principal vectors, $\{ \mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(k)} \}$
  - orthogonal and has unit norm – so $U^T U = I$
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- **Matrix S**
  - Diagonal
  - Shows importance of each eigenvector

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

5 minutes break

Applications

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

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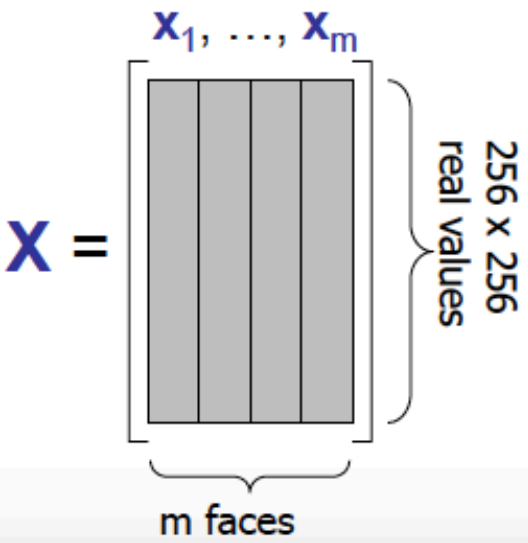
    [Turk & Pentland], [Sirovich & Kirby]
- Each face **x** is ...
  - 256 × 256 values (luminance at location)
  - **x** in $\Re^{256\times256}$ (view as 64K dim vector)
- Form $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_m]$ **centered** data mtx
- Compute $\Sigma = \mathbf{X}\mathbf{X}^T$
- Problem: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



Computational Complexity

- Suppose m instances, each of size N
  - Eigenfaces: m=500 faces, each of size N=64K

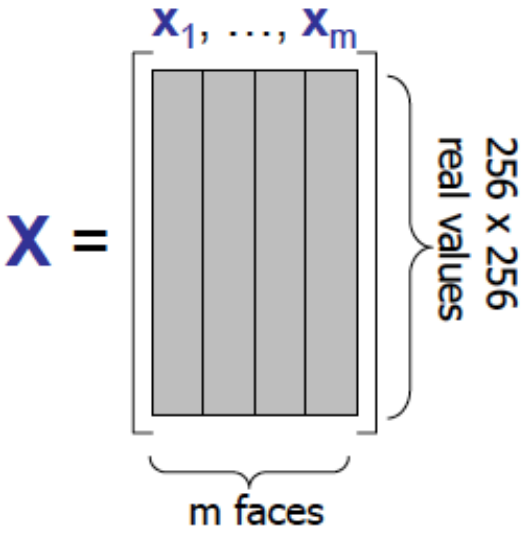
Computational Complexity

- Suppose m instances, each of size N
  - Eigenfaces: m=500 faces, each of size N=64K
- Given N×N covariance matrix Σ, can compute
  - all N eigenvectors/eigenvalues in $O(N^3)$
  - first k eigenvectors/eigenvalues in $O(k\ N^2)$

- But if N=64K, EXPENSIVE!

A Clever Workaround

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



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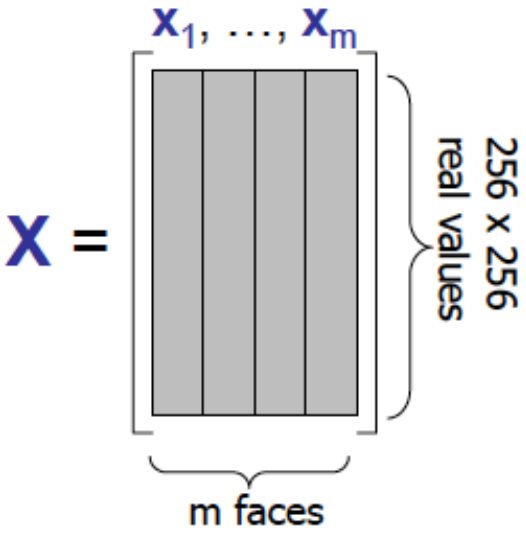
Proof: $L\ \mathbf{v} = \gamma\ \mathbf{v}$



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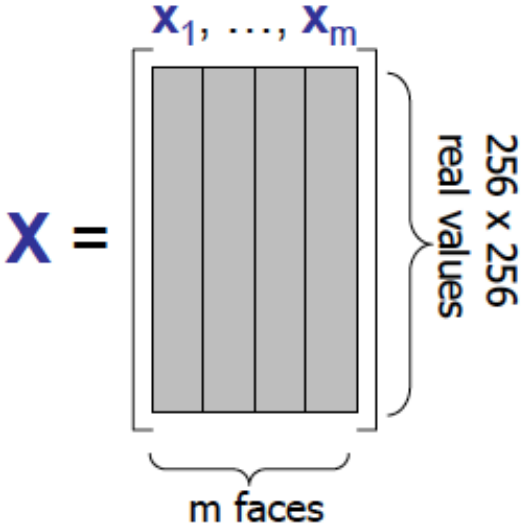

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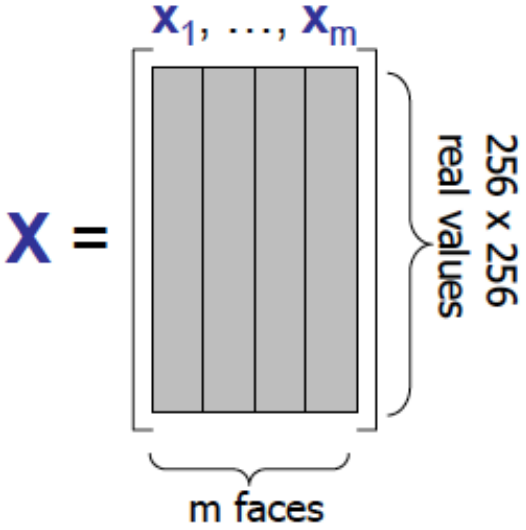

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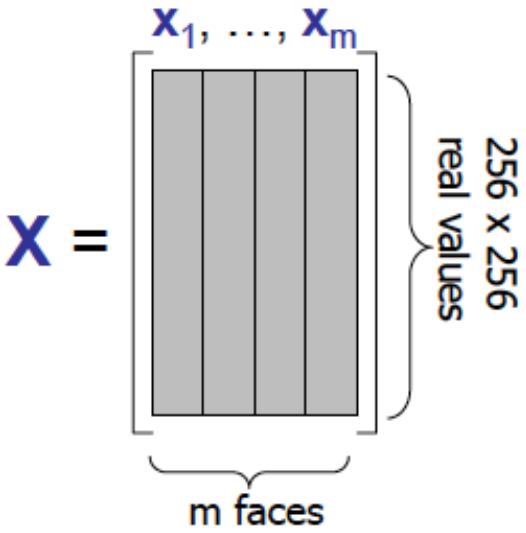

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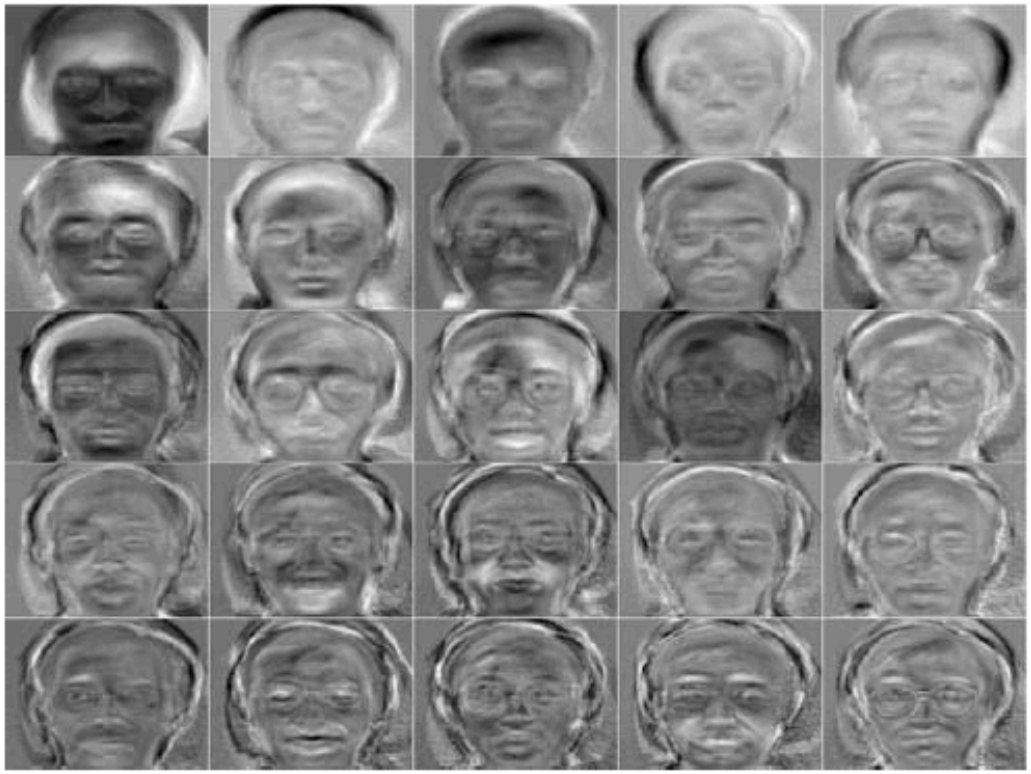
$$(XX^T)X\,v = \gamma\,(Xv)$$

$$\Sigma\,(Xv) = \gamma\,(Xv)$$

Principle Components (Method B)



Reconstructing… (Method B)

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

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Shortcomings

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

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

,50 in

Happiness subspace (method A)

Disgust subspace (method A)

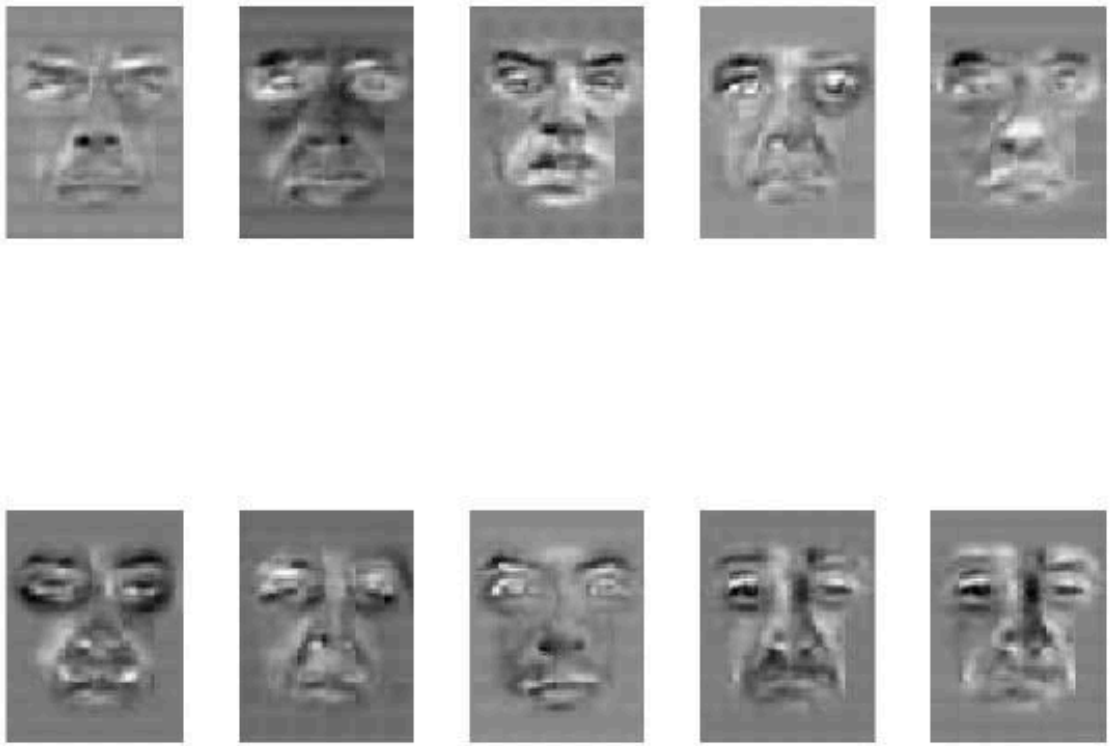

Image Compression

Original Image

- Divide the original 372x492 image into patches:
  - Each patch is an instance that contains 12x12 pixels on a grid
- View each as a 144-D vector

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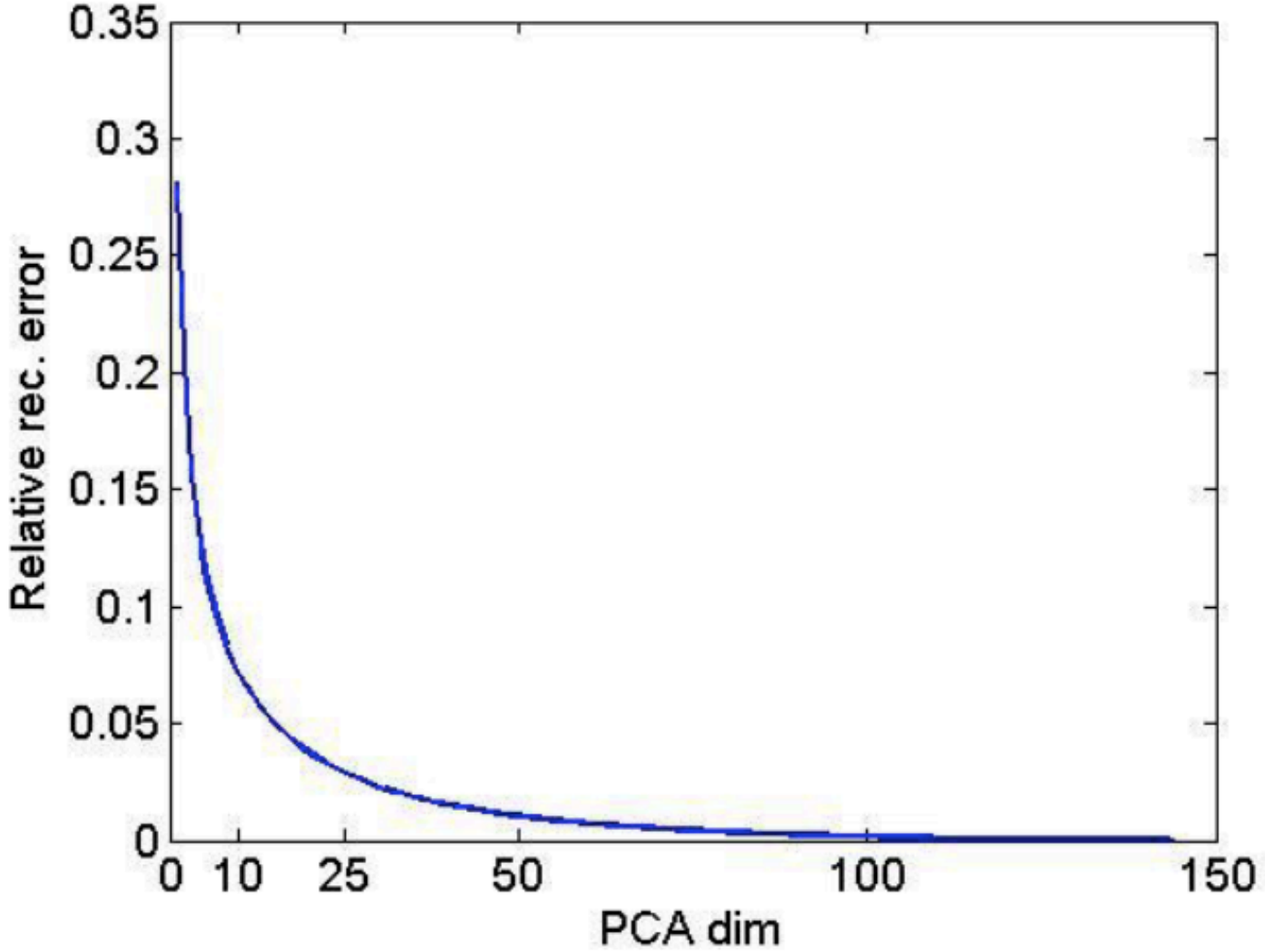
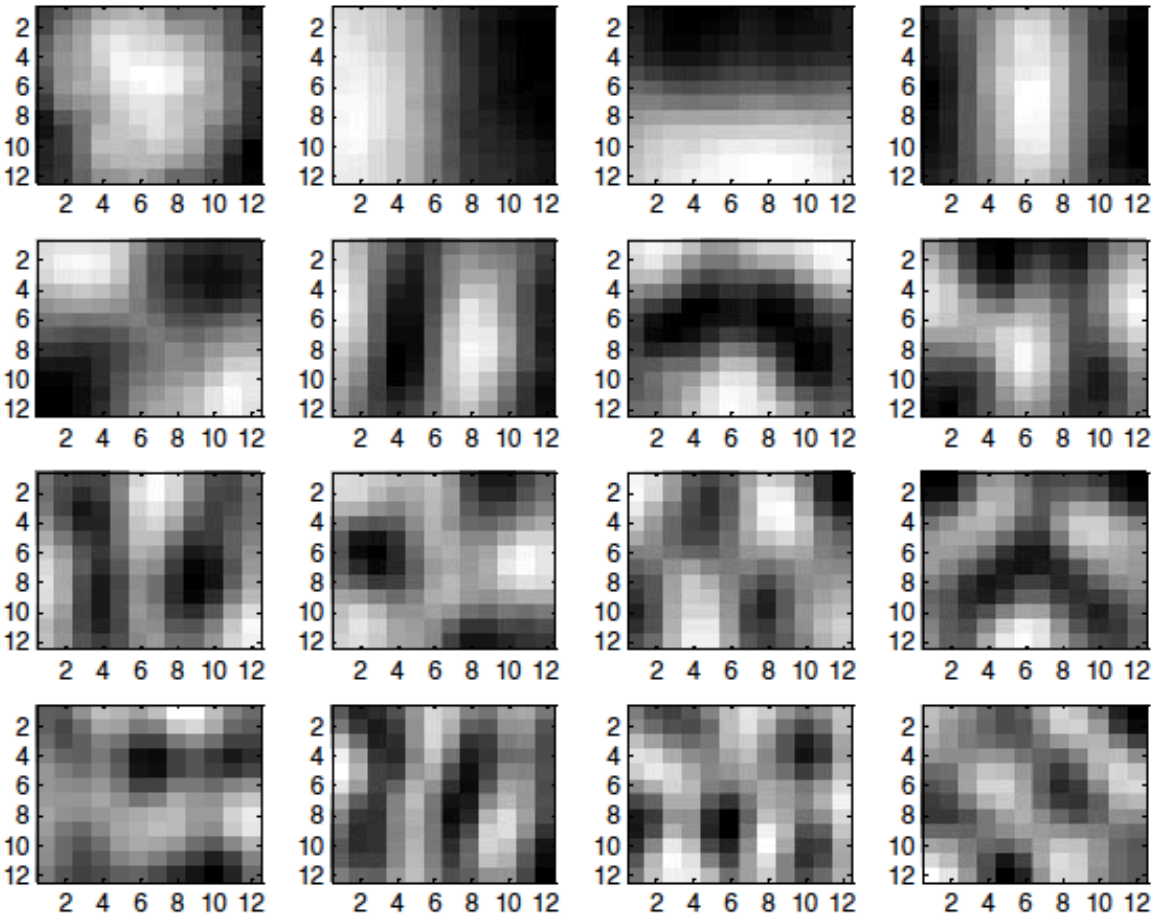
L_2 error and PCA dim



PCA compression: 144D ⇒ 60D

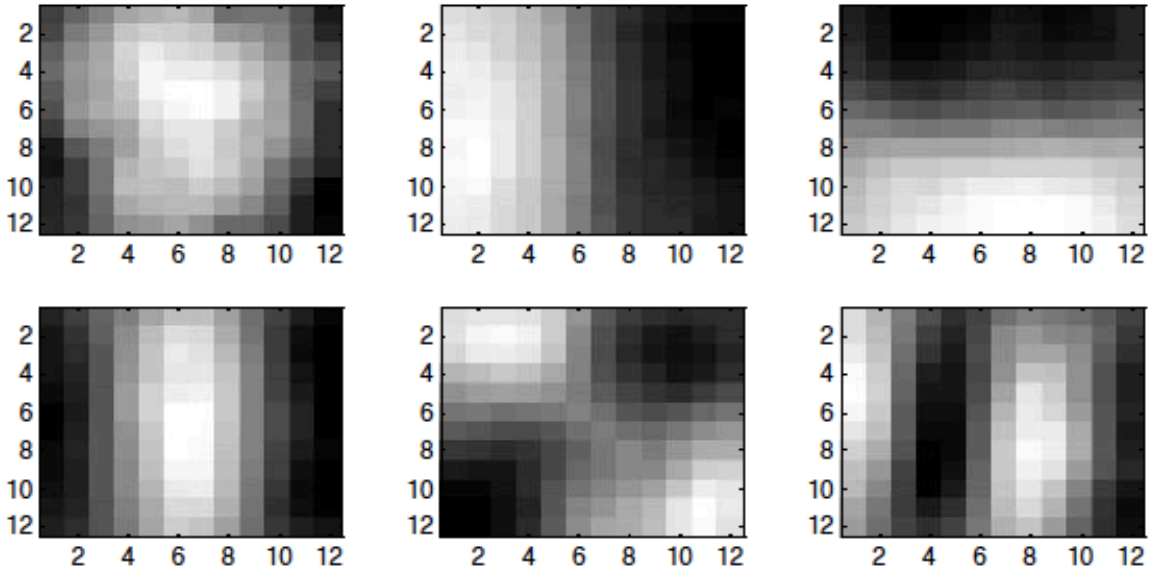
PCA compression: 144D ⇒ 16D

16 most important eigenvectors



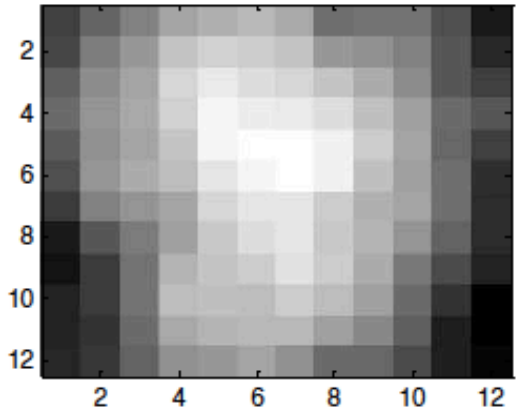
PCA compression: 144D ⇒ 6D

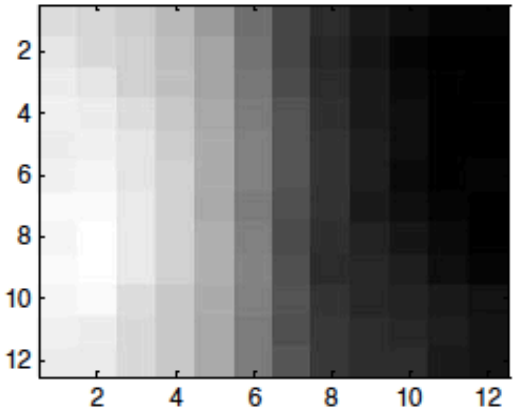
6 most important eigenvectors

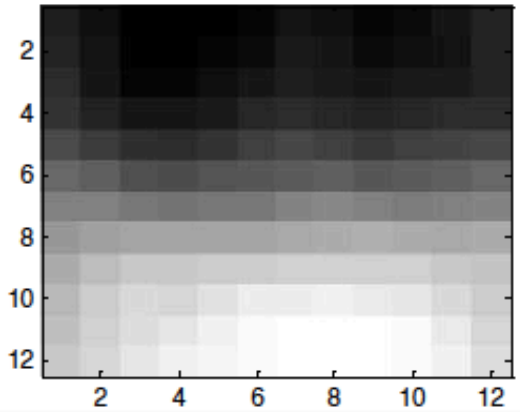


PCA compression: 144D ⇒ 3D

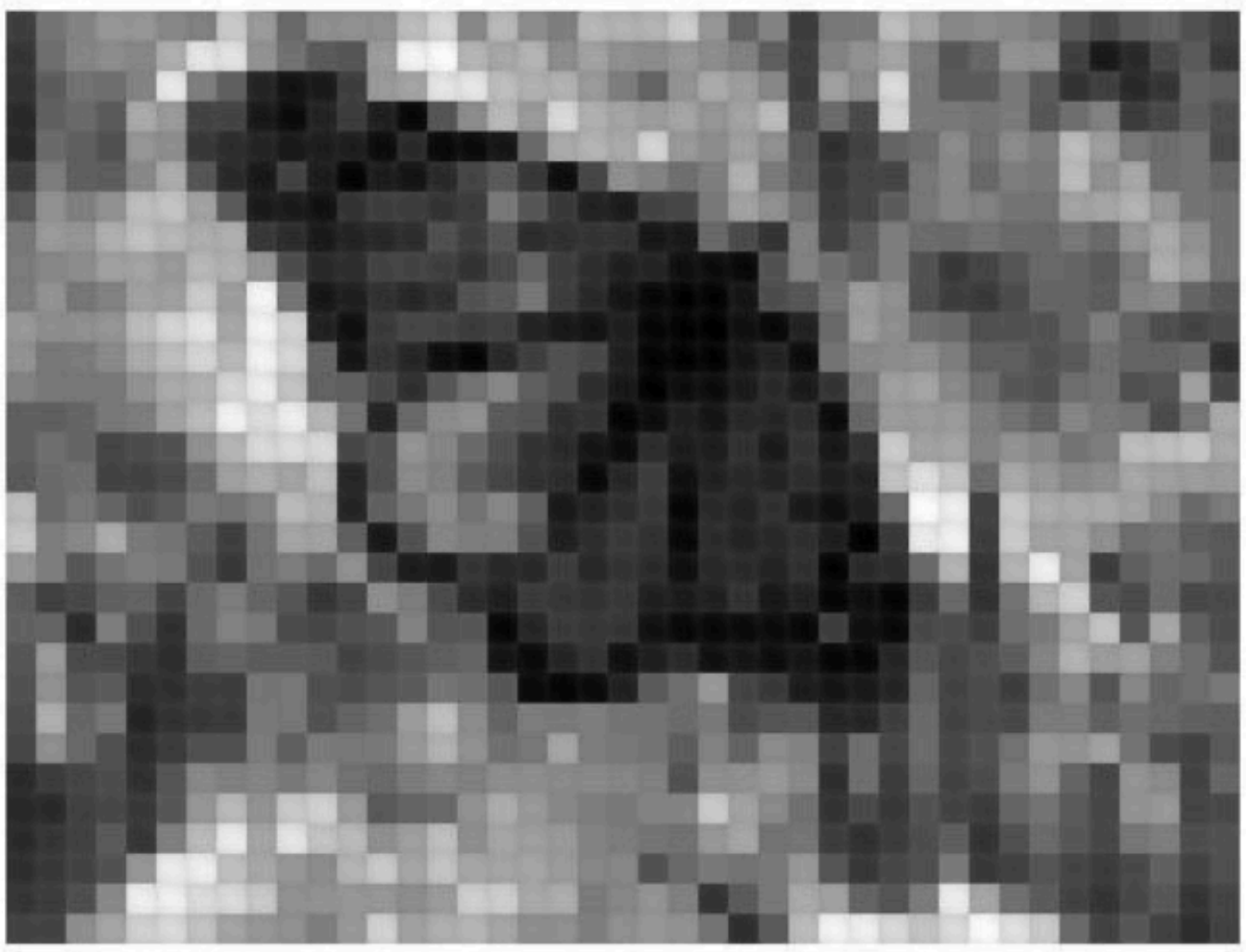
3 most important eigenvectors



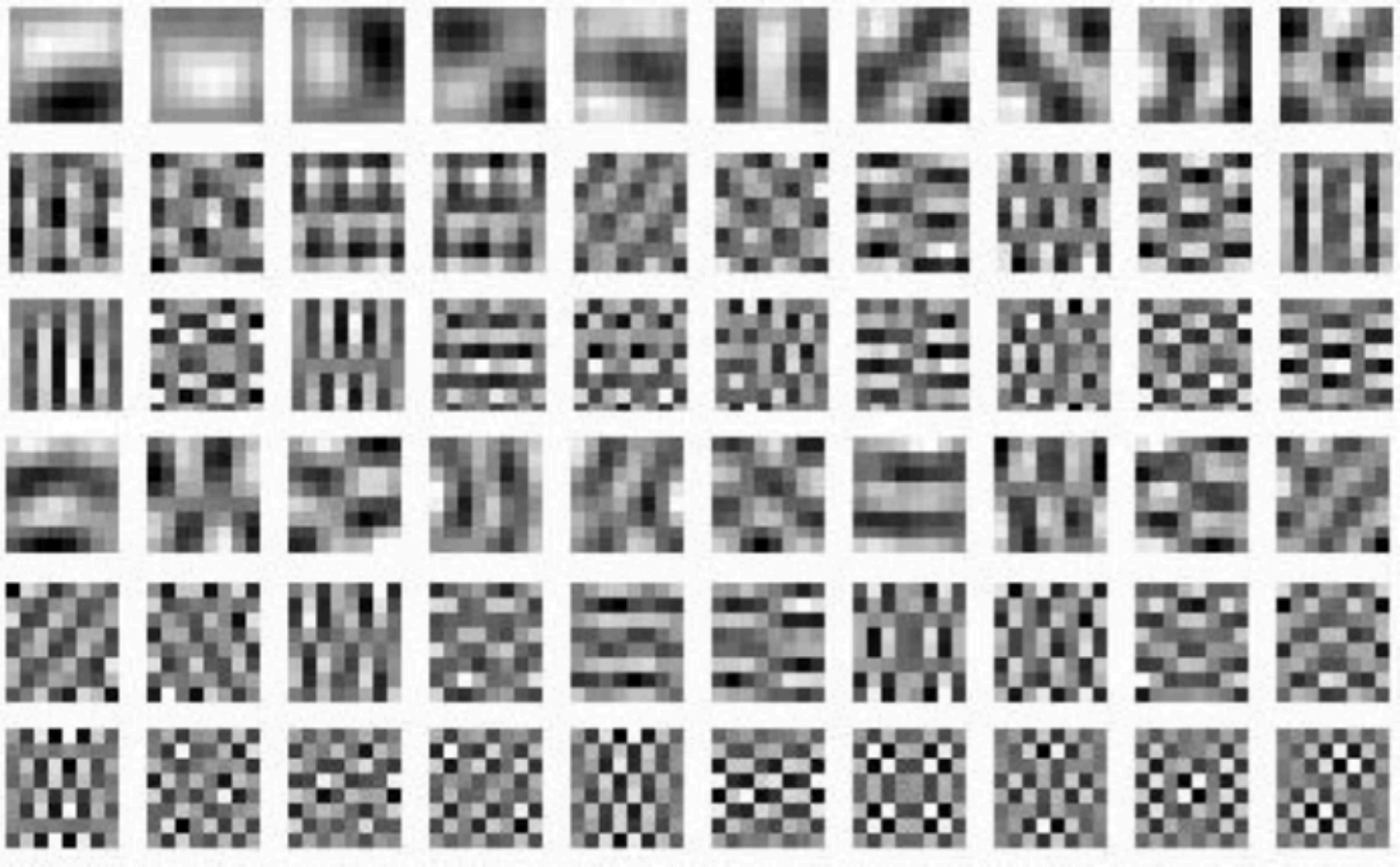




PCA compression: 144D ⇒ 1D

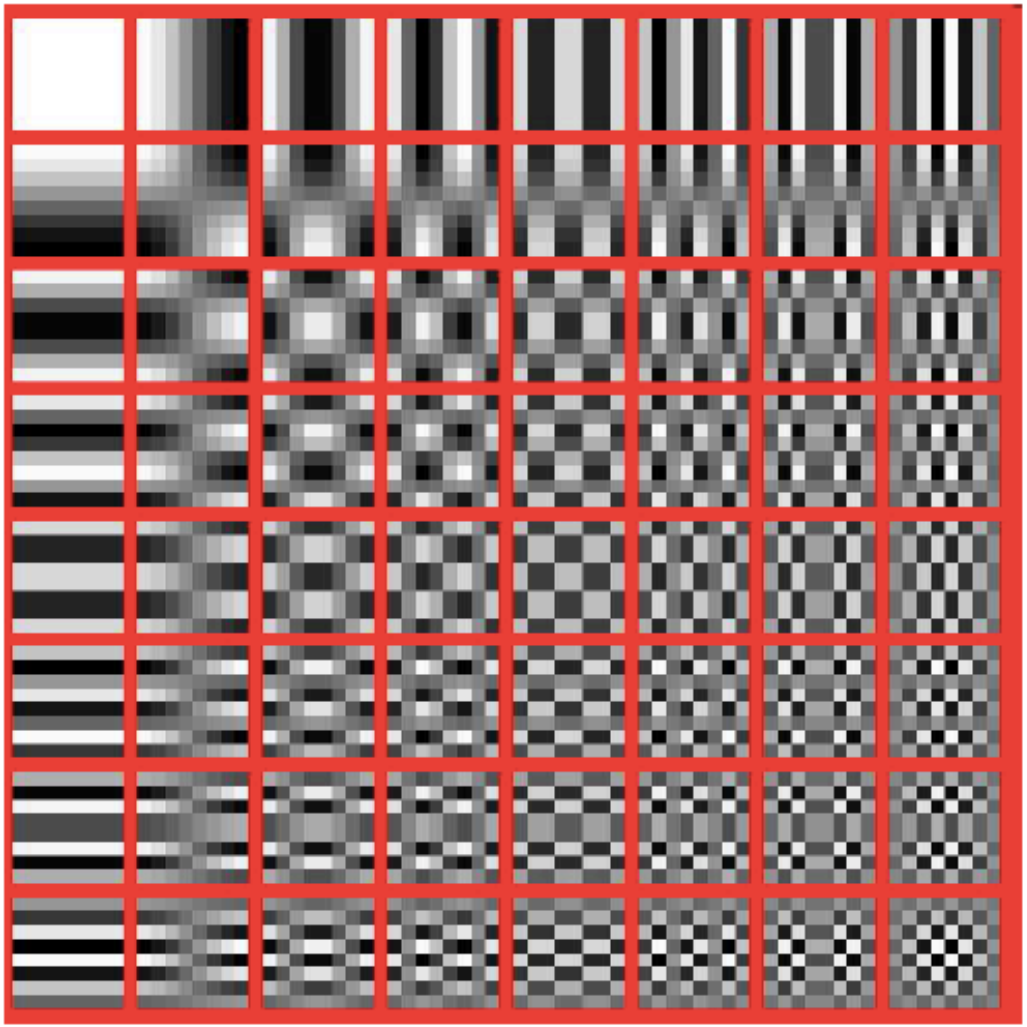


60 most important eigenvectors



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

2D Discrete Cosine Basis



http://en.wikipedia.org/wiki/Discrete_cosine_transform 50

Noise Filtering

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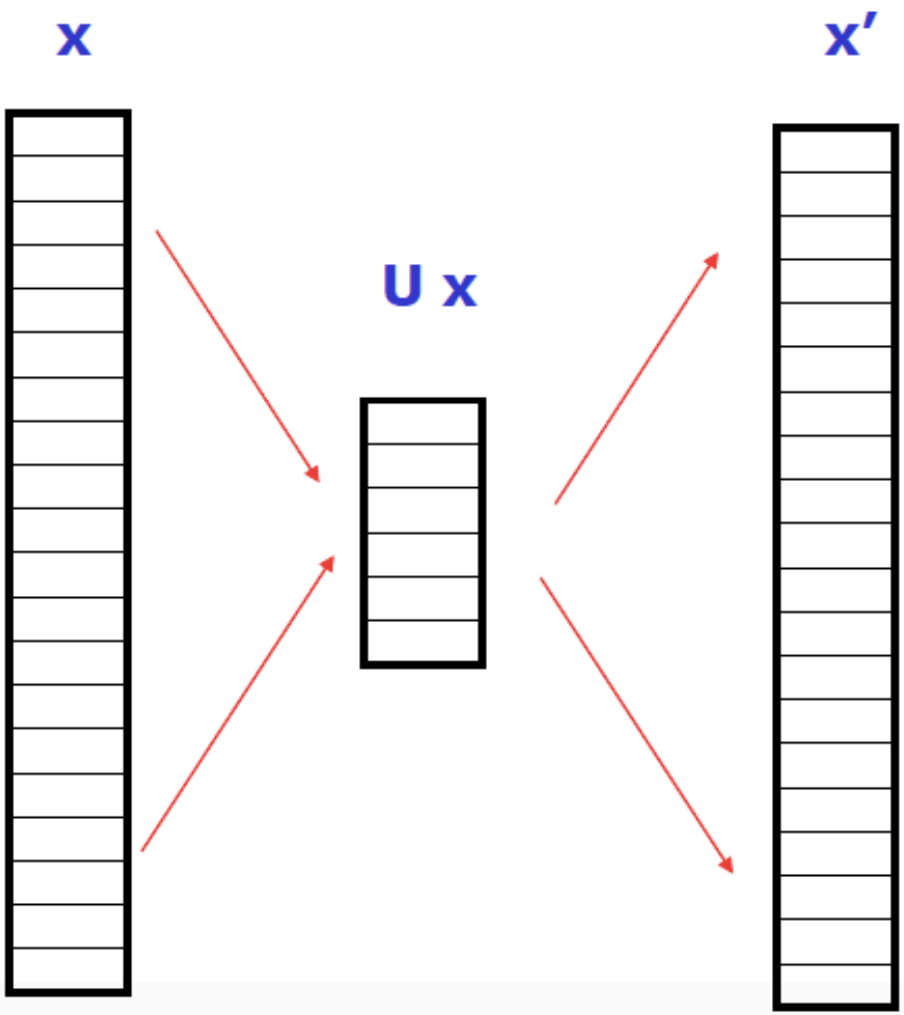

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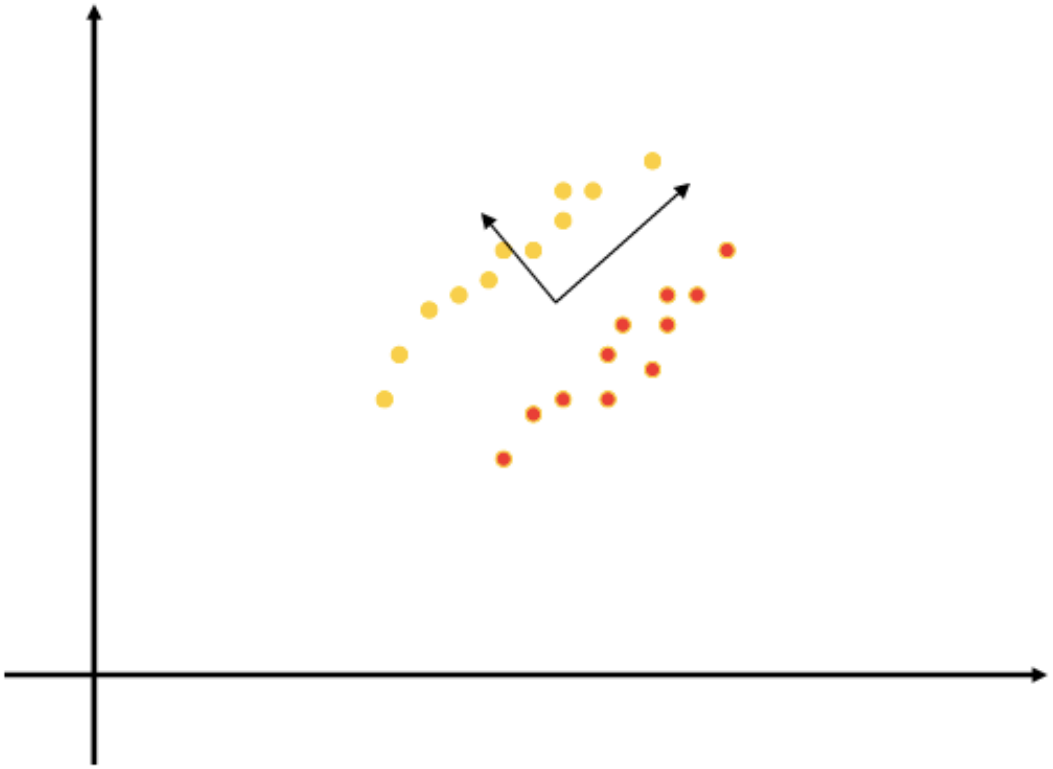
Noisy image

Denoised image using 15 PCA components

PCA Shortcomings

Problematic Data Set for PCA



PCA doesn't know labels!

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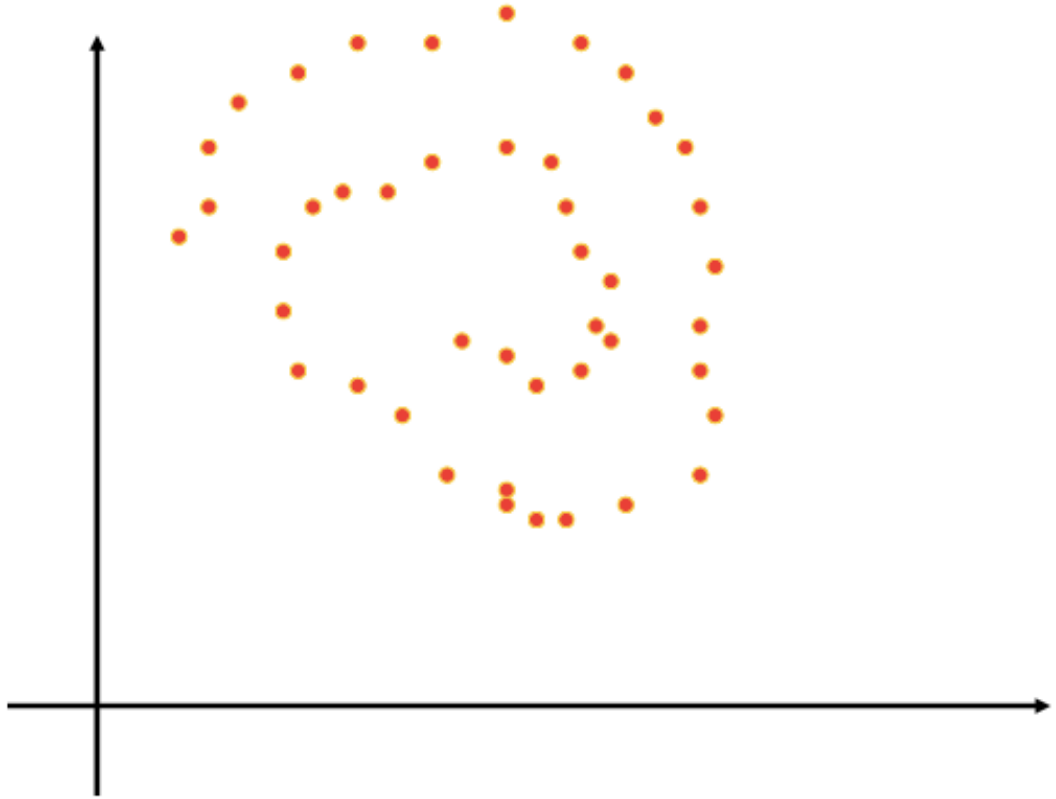

PCA cannot capture NON-LINEAR structure!

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!

That’s all!