# Principal Component Analysis (PCA)
# Learning Representations.
# Dimensionality Reduction.

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# Big & High-Dimensional Data

- High-Dimensions = Lot of Features


Document classification

Features per document =

thousands of words/unigrams

millions of bigrams, contextual information

Surveys - Netflix

480189 users x 17770 movies

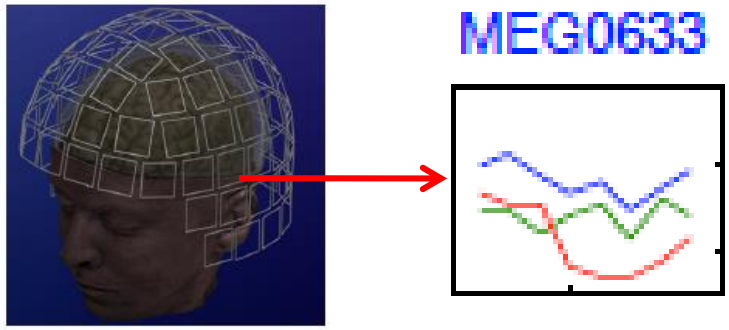
| | movie 1 | movie 2 | movie 3 | movie 4 | movie 5 | movie 6 |
|---|---|---|---|---|---|---|
| Tom | 5 | ? | ? | 1 | 3 | ? |
| George | ? | ? | 3 | 1 | 2 | 5 |
| Susan | 4 | 3 | 1 | ? | 5 | 1 |
| Beth | 4 | 3 | ? | 2 | 4 | 2 |

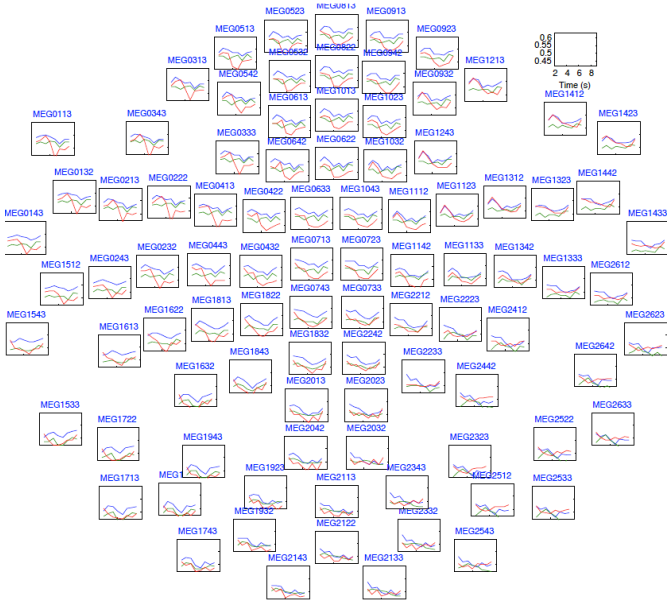
# Big & High-Dimensional Data

- High-Dimensions = Lot of Features

MEG Brain Imaging

120 locations x 500 time points
x 20 objects



Or any high-dimensional image data

- Big & High-Dimensional Data.

- Useful to learn lower dimensional representations of the data.

# Learning Representations

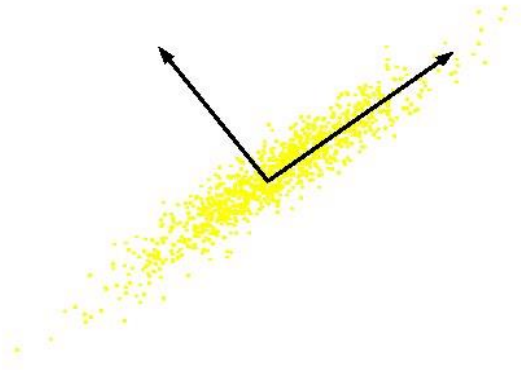
PCA, Kernel PCA, ICA: Powerful unsupervised learning techniques for extracting hidden (potentially lower dimensional) structure from high dimensional datasets.

**Useful for**:

- Visualization
- More efficient use of resources (e.g., time, memory, communication)
- Statistical: fewer dimensions → better generalization
- Noise removal (improving data quality)
- Further processing by machine learning algorithms

# Principal Component Analysis (PCA)

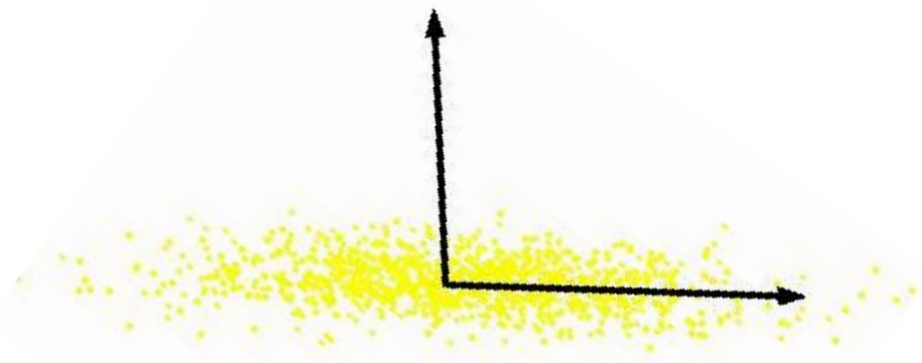
**What is PCA**: Unsupervised technique for extracting variance structure from high dimensional datasets.



- PCA is an orthogonal projection or transformation of the data into a (possibly lower dimensional) subspace so that the variance of the projected data is maximized.

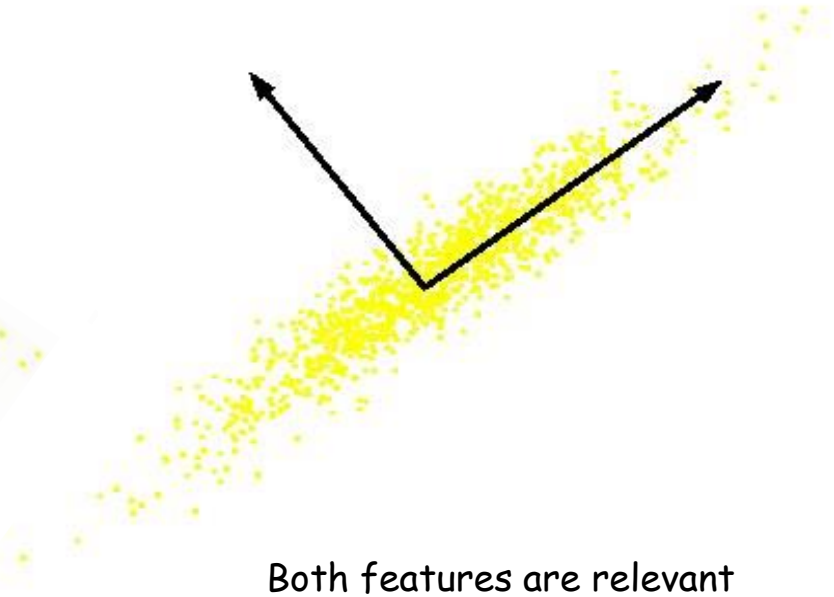
# Principal Component Analysis (PCA)

Intrinsically lower dimensional than the dimension of the ambient space.



Only one relevant feature

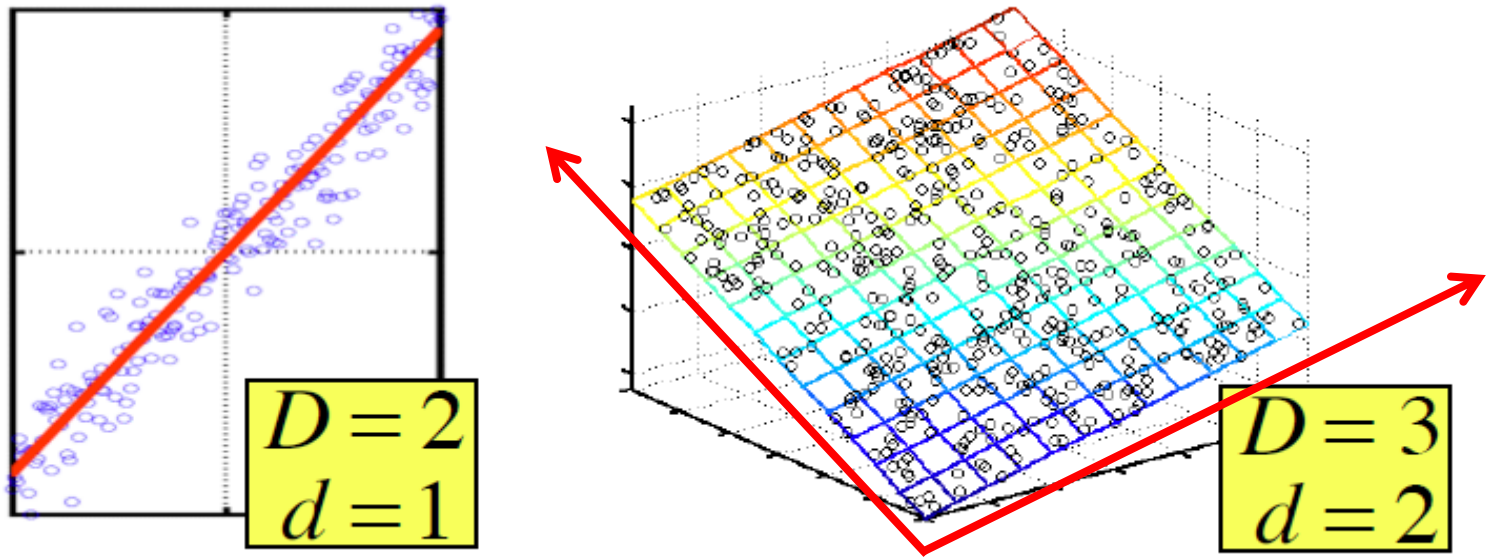
If we rotate data, again only one coordinate is more important.



Both features are relevant

Question: Can we transform the features so that we only need to preserve one latent feature?

# Principal Component Analysis (PCA)



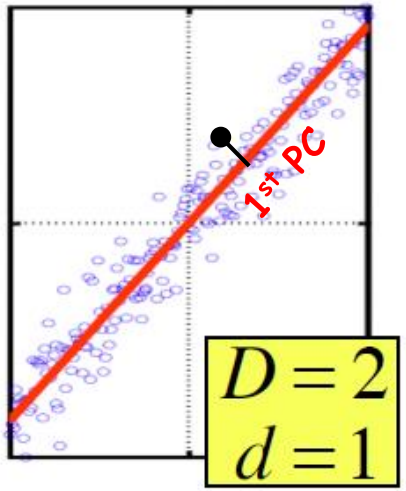

In case where data lies on or near a low d-dimensional linear subspace, axes of this subspace are an effective representation of the data.

Identifying the axes is known as Principal Components Analysis, and can be obtained by using classic matrix computation tools (Eigen or Singular Value Decomposition).

# Principal Component Analysis (PCA)

Principal Components (PC) are orthogonal directions that capture most of the variance in the data.

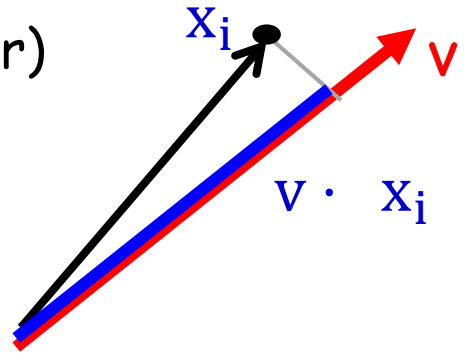
- First PC – direction of greatest variability in data.
- Projection of data points along first PC discriminates data most along any one direction
  (pts are the most spread out when we project the data on that direction compared to any other directions).




Quick reminder:

||v||=1, Point $x_i$ (D-dimensional vector)

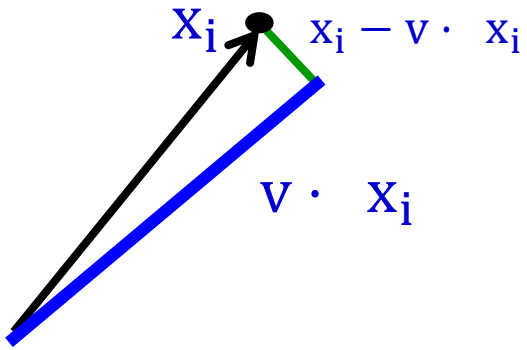
Projection of $x_i$ onto v is $v \cdot x_i$

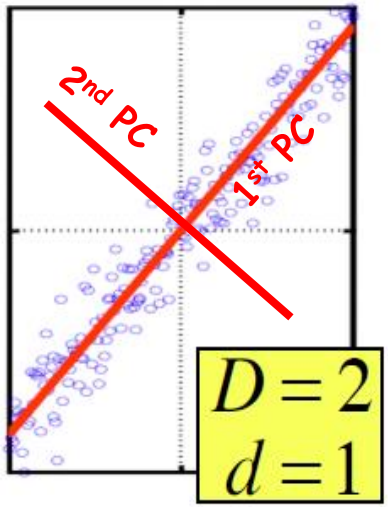


# Principal Component Analysis (PCA)

Principal Components (PC) are orthogonal directions that capture most of the variance in the data.

- 1st PC – direction of greatest variability in data.




- 2nd PC – Next orthogonal (uncorrelated) direction of greatest variability

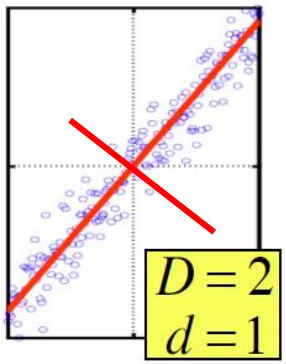
  (remove all variability in first direction, then find next direction of greatest variability)

- And so on …

# Principal Component Analysis (PCA)

Let $v_1, v_2, \ldots, v_d$ denote the d principal components.

$v_i \cdot v_j = 0, i \neq j$ and $v_i \cdot v_i = 1, \quad i = j$




Assume data is centered (we extracted the sample mean).

Let $X = [x_1, x_2, \ldots, x_n]$ (columns are the datapoints)

Find vector that maximizes sample variance of projected data

$$\frac{1}{n}\sum_{i=1}^{n}(\mathbf{v}^T\mathbf{x}_i)^2 = \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v}$$

$$\max_{\mathbf{v}} \ \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} \quad \text{s.t.} \quad \mathbf{v}^T\mathbf{v} = 1$$

Lagrangian: $\max_{\mathbf{v}} \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} - \lambda\mathbf{v}^T\mathbf{v}$

Wrap constraints into the objective function

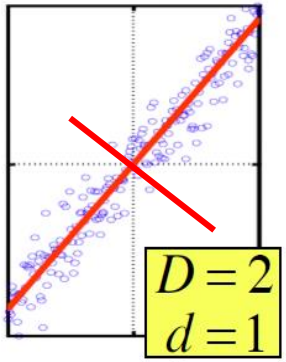
$$\partial/\partial\mathbf{v} = 0 \qquad (\mathbf{X}\mathbf{X}^T - \lambda\mathbf{I})\mathbf{v} = 0 \qquad \Rightarrow \boxed{(\mathbf{X}\mathbf{X}^T)\mathbf{v} = \lambda\mathbf{v}}$$

# Principal Component Analysis (PCA)

$(X X^T)v = \lambda v$ , so v (the first PC) is the eigenvector of sample correlation/covariance matrix $X X^T$

Sample variance of projection $v^T X X^T v = \lambda v^T v = \lambda$

Thus, the eigenvalue $\lambda$ denotes the amount of variability captured along that dimension (aka amount of energy along that dimension).

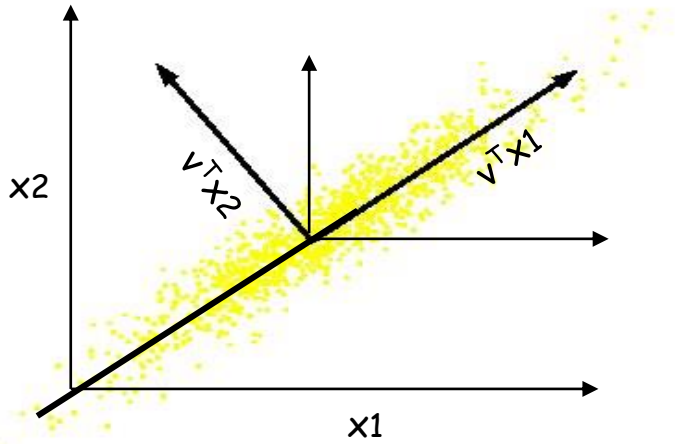



Eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots$

- The 1st PC $v_1$ is the the eigenvector of the sample covariance matrix $X X^T$ associated with the largest eigenvalue
- The 2nd PC $v_2$ is the the eigenvector of the sample covariance matrix $X X^T$ associated with the second largest eigenvalue
- And so on …

# Principal Component Analysis (PCA)

- So, the new axes are the eigenvectors of the matrix of sample correlations $X\,X^T$ of the data.
- Transformed features are uncorrelated.




- Geometrically: centering followed by rotation.
  - Linear transformation

**Key computation**: eigendecomposition of $XX^T$ (closely related to SVD of $X$).

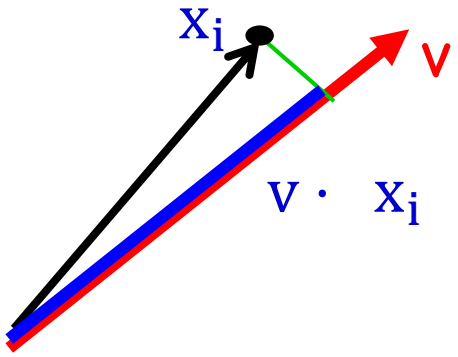
# Two Interpretations

So far: Maximum Variance Subspace. PCA finds vectors v such that projections on to the vectors capture maximum variance in the data

$$\frac{1}{n}\sum_{i=1}^{n}(\mathbf{v}^T\mathbf{x}_i)^2 = \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v}$$

Alternative viewpoint: Minimum Reconstruction Error. PCA finds vectors v such that projection on to the vectors yields minimum MSE reconstruction

$$\frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_i - (\mathbf{v}^T\mathbf{x}_i)\mathbf{v}\|^2$$



# Two Interpretations

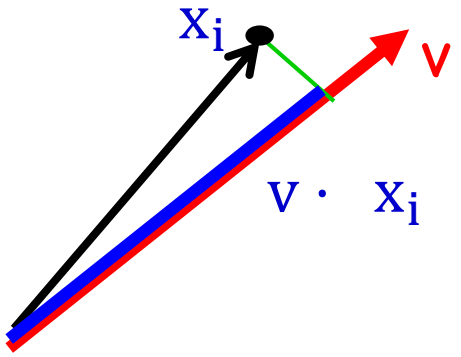
E.g., for the first component.

Maximum Variance Direction: 1st PC a vector v such that projection on to this vector capture maximum variance in the data (out of all possible one dimensional projections)

$$\frac{1}{n}\sum_{i=1}^{n}(\mathbf{v}^T\mathbf{x}_i)^2 = \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v}$$

Minimum Reconstruction Error: 1st PC a vector v such that projection on to this vector yields minimum MSE reconstruction

$$\frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_i - (\mathbf{v}^T\mathbf{x}_i)\mathbf{v}\|^2$$



# Why? Pythagorean Theorem

E.g., for the first component.

Maximum Variance Direction: 1st PC a vector v such that projection on to this vector capture maximum variance in the data (out of all possible one dimensional projections)

$$\frac{1}{n}\sum_{i=1}^{n}(\mathbf{v}^T\mathbf{x}_i)^2 = \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v}$$

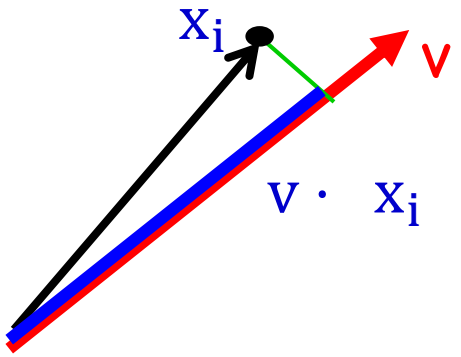
$$\frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_i - (\mathbf{v}^T\mathbf{x}_i)\mathbf{v}\|^2$$

Minimum Reconstruction Error: 1st PC a vector v such that projection on to this vector yields minimum MSE reconstruction

blue$^2$ + green$^2$ = black$^2$

black$^2$ is fixed (it's just the data)

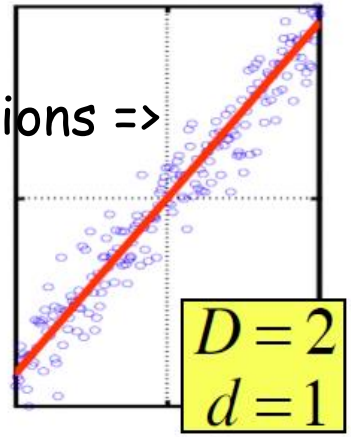
So, maximizing blue$^2$ is equivalent to minimizing green$^2$



# Dimensionality Reduction using PCA

The eigenvalue $\lambda$ denotes the amount of variability captured along that dimension (aka amount of energy along that dimension).

Zero eigenvalues indicate no variability along those directions => data lies exactly on a linear subspace




Only keep data projections onto principal components with non-zero eigenvalues, say $v_1, \ldots, v_k$, where k=rank($X\ X^T$)

Original representation

Data point

$$x_i = (x_i^1, \ldots, x_i^D)$$

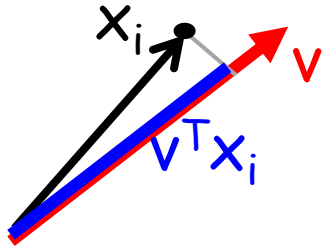
D-dimensional vector

Transformed representation

projection

$$(v_1 \cdot x^i, \ldots, v_d \cdot x^i)$$

d-dimensional vector

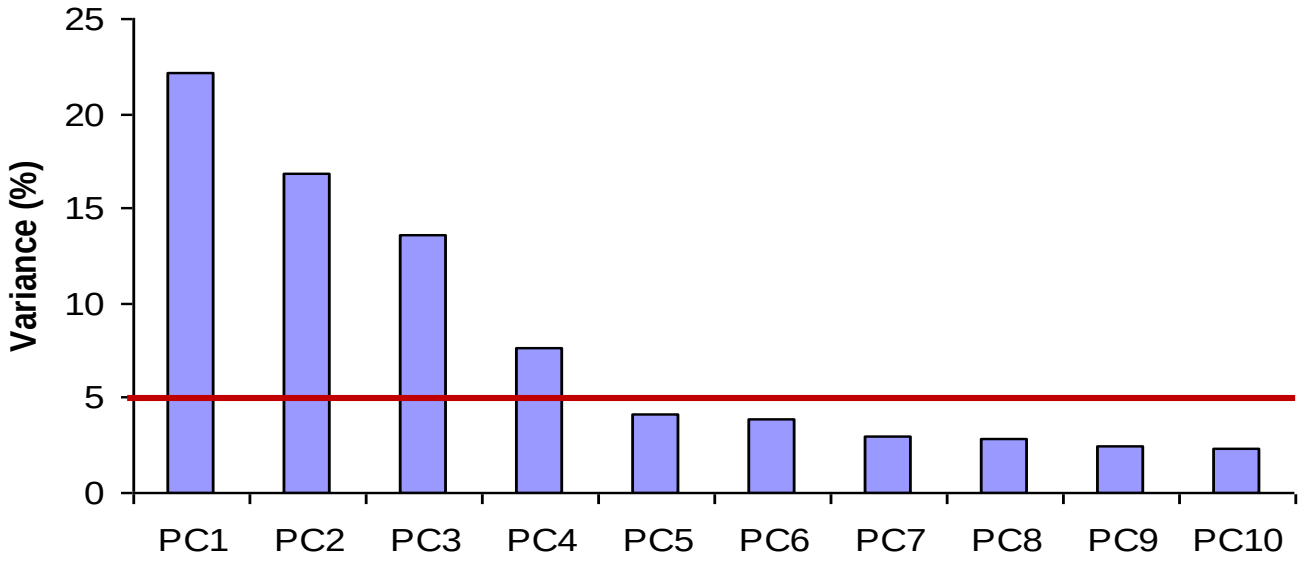


# Dimensionality Reduction using PCA

In high-dimensional problems, data sometimes lies near a linear subspace, as noise introduces small variability

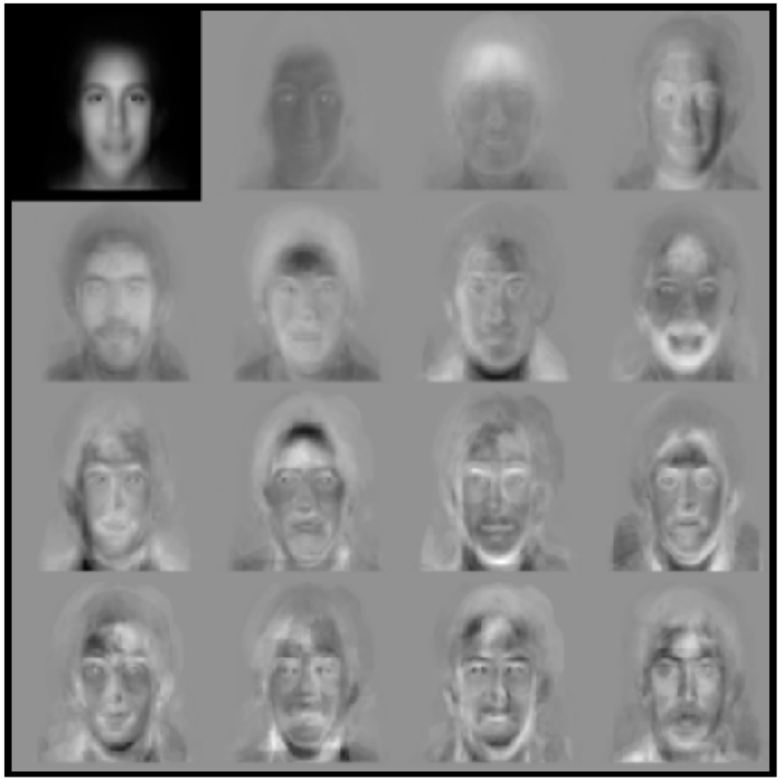
Only keep data projections onto principal components with **large** eigenvalues

Can *ignore* the components of smaller significance.




Might lose some info, but if eigenvalues are small, do not lose much

# Example: faces



**Eigenfaces from 7562 images:**

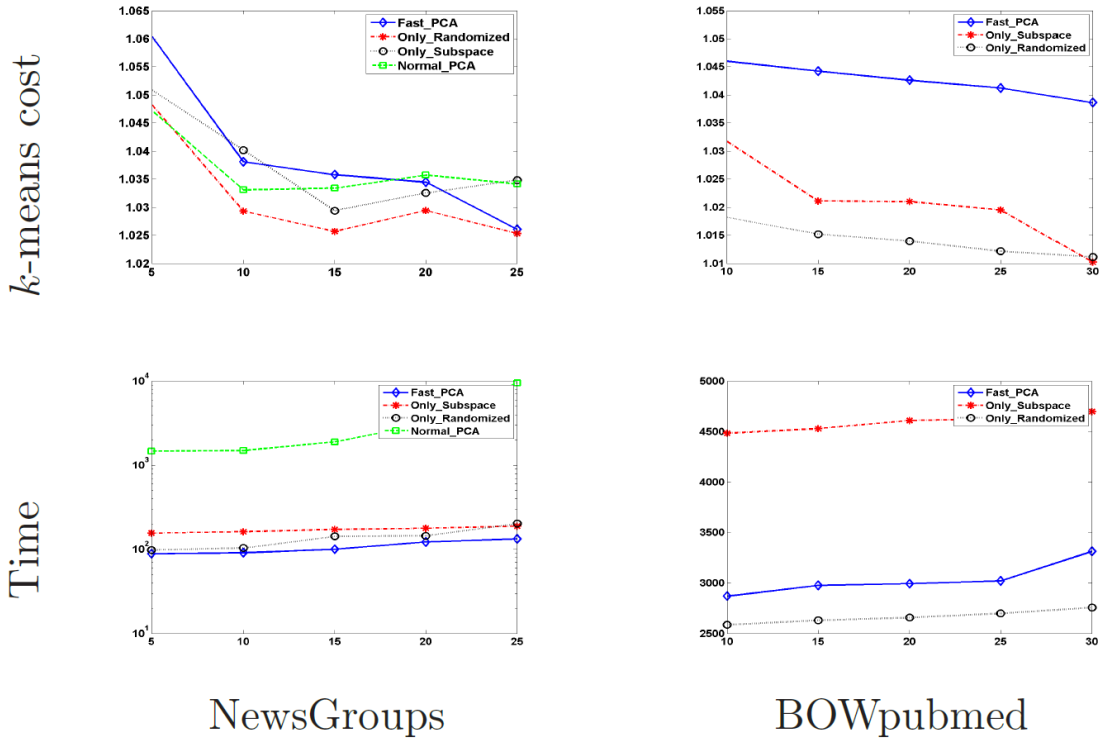
**top left image is linear combination of rest.**

Sirovich & Kirby (1987)
Turk & Pentland (1991)

Can represent a face image using just 15 numbers!

- PCA provably useful before doing k-means clustering and also empirically useful. E.g.,

  - ▷ **Performance:** cost increase $< 5\%$; $\times 10$ to $\times 100$ speedup
  - ▷ **$k$-Means Clustering**: $k$-means cost/time vs dimension



# PCA Discussion

**Strengths**

Eigenvector method

No tuning of the parameters

No local optima

**Weaknesses**

Limited to second order statistics

Limited to linear projections

# What You Should Know

- Principal Component Analysis (PCA)
  - What PCA is, what is useful for.
  - Both the maximum variance subspace and the minimum reconstruction error viewpoint.