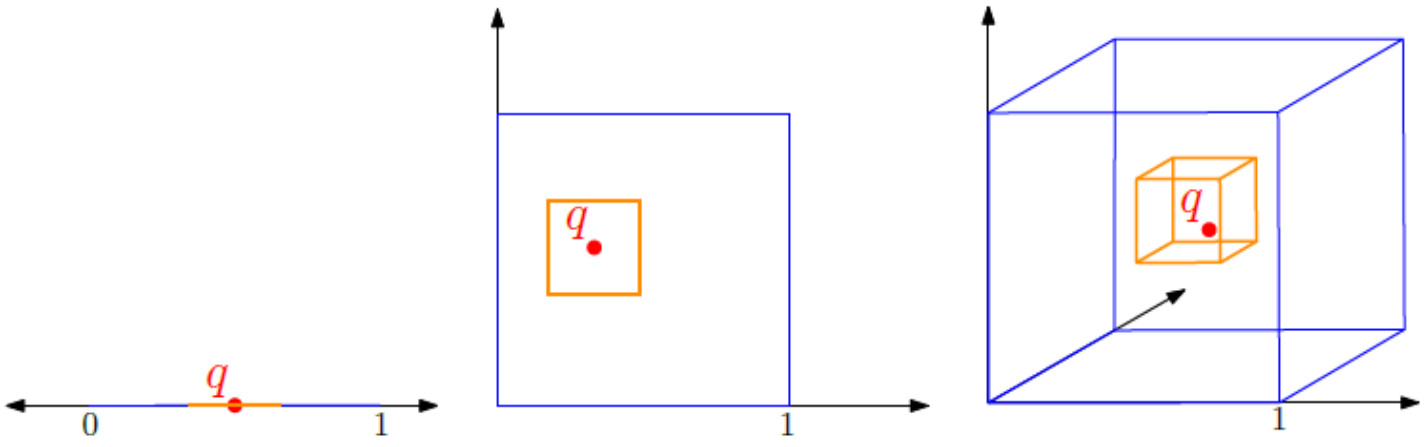
Lecture 12: Linear Dimensionality Reduction Methods

Instructor: Sergei V. Kalinin

Reminder: dimensionality is a problem

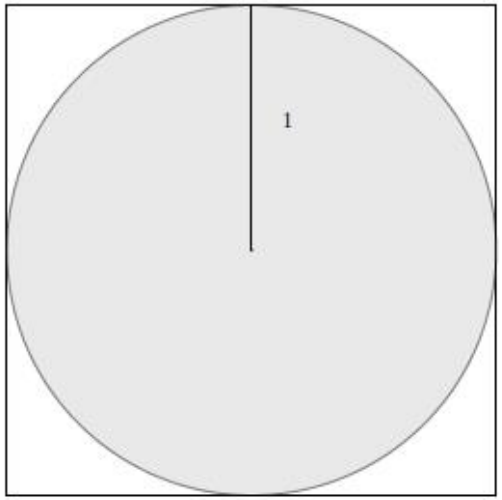


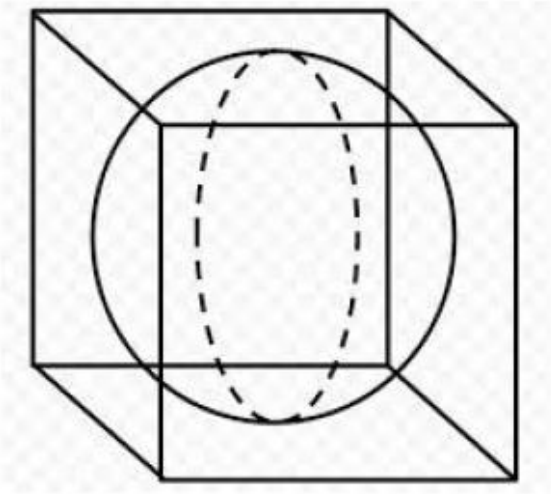
Suppose we have 5000 points:

- In 1d we have to explore 0.001 on average to capture 5 NN
- In 2d, on average we must explore 0:031 units along both dimensions to get 5 nearest neighbors points (about 3% of the whole cube).
- In 3d, on average we must go 10% of the total (unit) length in each of the 3 dimensions
- In 4d, we must explore 17:7% of unit length
- In 10d, we must go 50.1% of unit length along each dimension

From “Curse of Dimensionality”, Lecture Notes for Big Data Analytics, Faizad Ullah, February 2019

Reminder: dimensionality is a problem





dim m	volume of m-ball	volume of m-cube	ratio
2	π	2^2	~ 0.785
3	$4/3\pi$	2^3	~ 0.523
4	$\pi^2/2$	2^4	~ 0.308
6	$\pi^3/6$	2^6	~ 0.080
m	$\frac{\pi^{m/2}}{m/2!}$	2^m	$\to 0$

From “Curse of Dimensionality”, Lecture Notes for Big Data Analytics, Faizad Ullah, February 2019

Reminder: dimensionality is a problem

However if a dataset exhibit this phenomenon that the issue has be overcome by getting a larger training set (exponential in m). One way to look at this is as follows.

To cover $[-1,1]^m$ with $B_{m,1}$'s, the number of balls n must be

$$n \geq \frac{2^m}{V_m(1)} = \frac{2^m}{\pi^{m/2}/_{m/2!}} = \frac{{}^{m}/_{2}!\, 2^m}{\pi^{m/2}} \overset{m\mapsto\infty}{\sim} \sqrt{m\pi}\left(\frac{m2^{m/2}}{2\pi e}\right)^{m/2}$$

For $m = 16$ (a very small number) this n is substantially larger than 2^{58}

- In higher dimensions all the volume is in `corners'
- Points in high dimensional spaces are isolated (empty surrounding)
- The probability that a randomly generated point is within r radius of q approaches 0 as dimensionality increases
- The probability of a close nearest neighbor in a data set is very small

From “Curse of Dimensionality”, Lecture Notes for Big Data Analytics, Faizad Ullah, February 2019

High Dimensional Data – what should we do?

Examples of high D data:

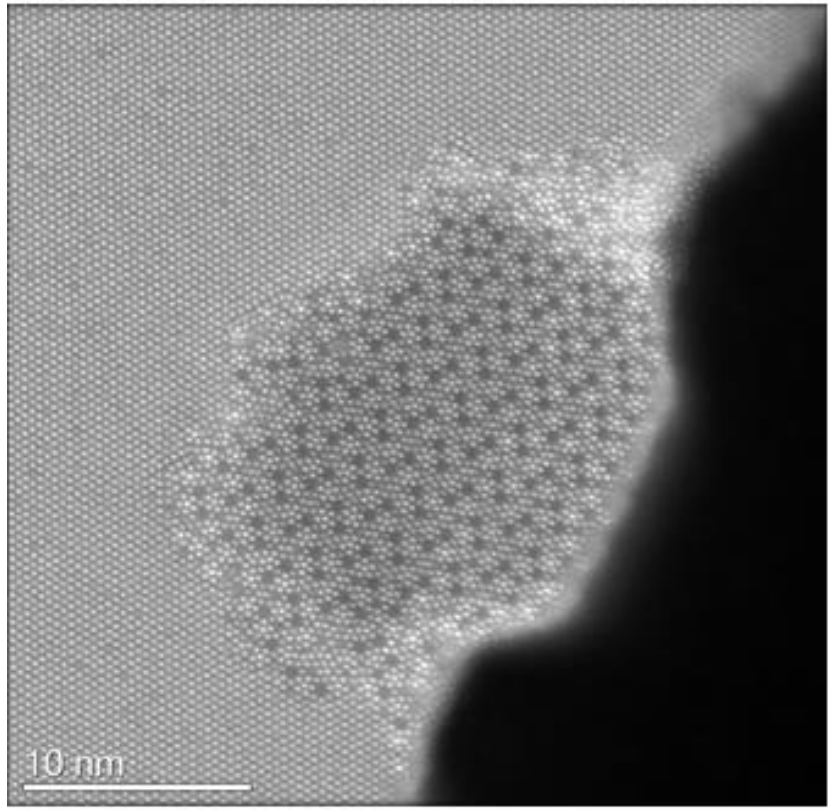
- Face recognition
- Image compression
- Gene expression analysis
- Spectroscopy
- 4D STEM
- X-Ray scattering

What do we want to accomplish?

- Reduce number of dimensions in data
- Find patterns in high-dimensional data
- Visualize data of high dimensionality

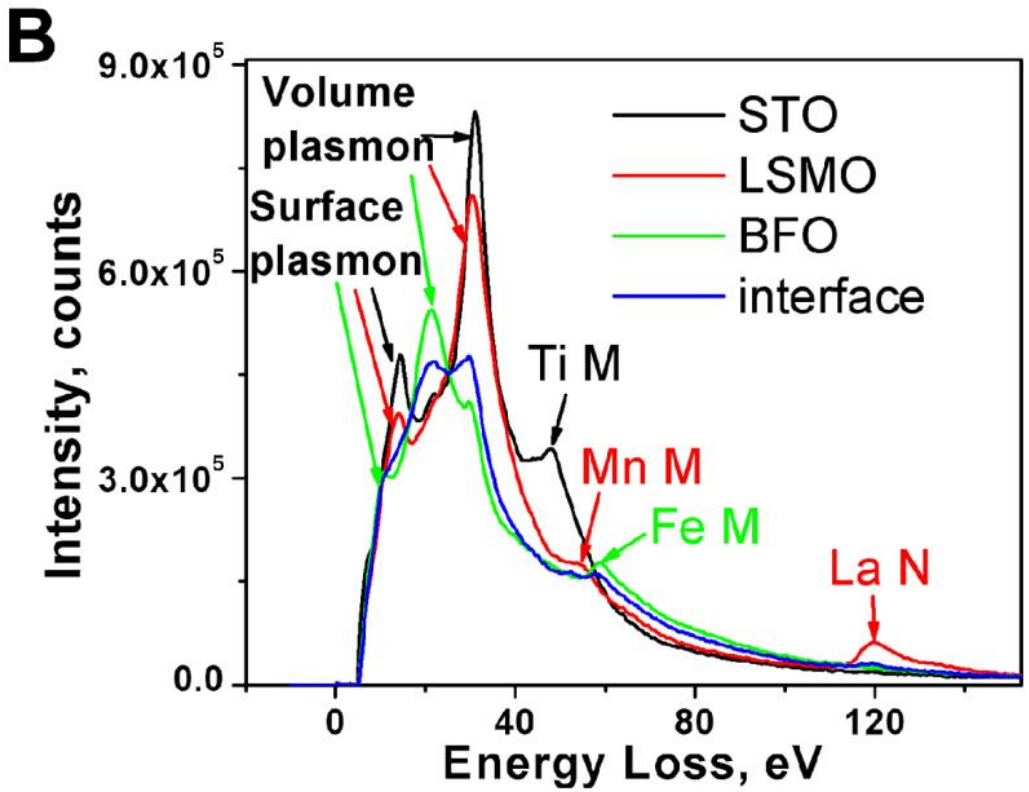
High D data in materials science?

Mo-V-Ta complex oxide



Q. He et al, ACS Nano 9, 3470-3478

Low-loss EELS spectra



A.Y. Borisevich et al., Phys. Rev. Lett. **105**, 087204 (2010).

- How many dimensions are in this data?
- Are all these dimensions necessary?
- For given acquisition time, how would the noise and signal balance?
- How do we extract “useful” information?

High Dimensional Data is often redundant

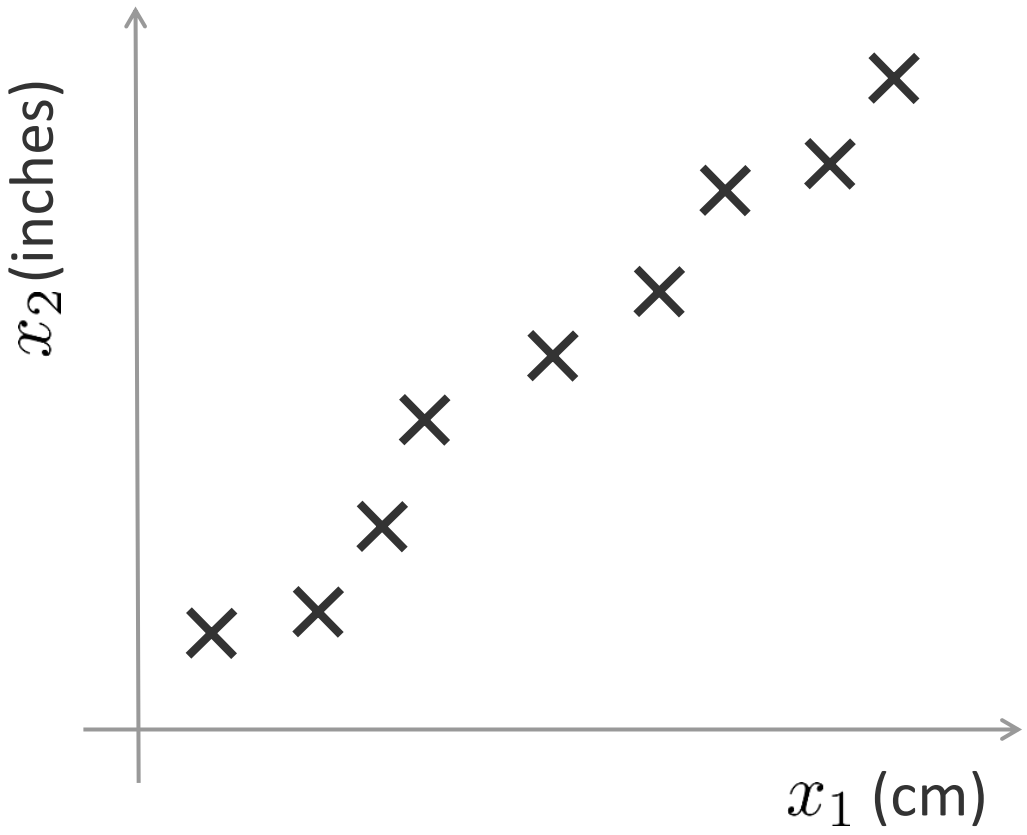
- We often need a method to simplify data on a large number of variables, and believe that there is some redundancy in those variables.
- Redundancy means that some of the variables are correlated with one another, possibly because they are measuring the same object or phenomenon.
- Because of redundancy, we believe that it should be possible to reduce the observed variables into a smaller number of artificial variables that will account for most of the variance in the observed variables.

Dimensionality Reduction Methods

- PCA (Principal Component Analysis):
  - Find projection that maximize the variance
- ICA (Independent Component Analysis):
  - Very similar to PCA except that it assumes non-Guassian features
- Multidimensional Scaling:
  - Find projection that best preserves inter-point distances
- LDA(Linear Discriminant Analysis):
  - Maximizing the component axes for class-separation
- Bayesian Linear Unmixing
  - Linear unmixing, non-negative, sum to one
- … constrained linear unmixing methods

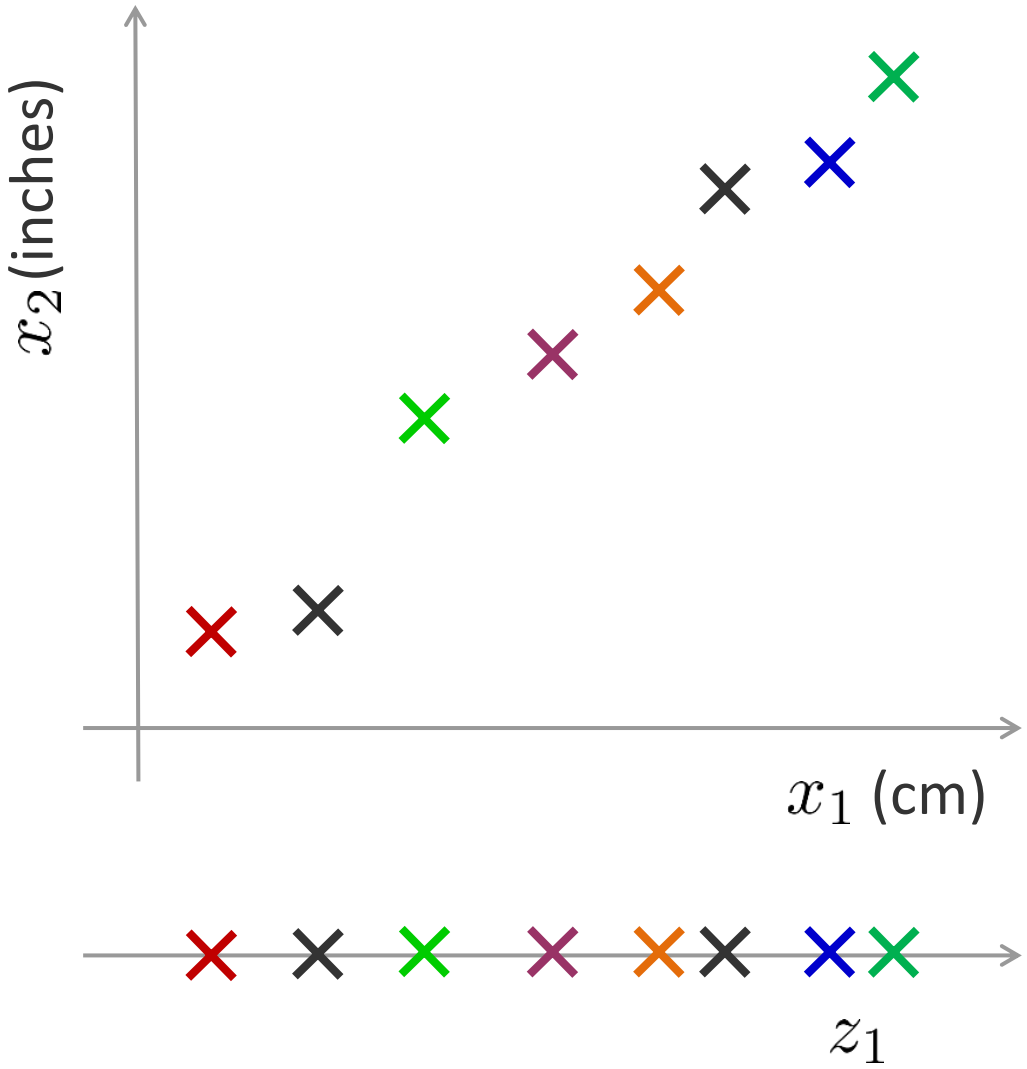
Manifold Hypothesis!

Simple Example



Reduce data from 2D to 1D

Simple Example



Reduce data from 2D to 1D

$$x^{(1)} \rightarrow z^{(1)}$$

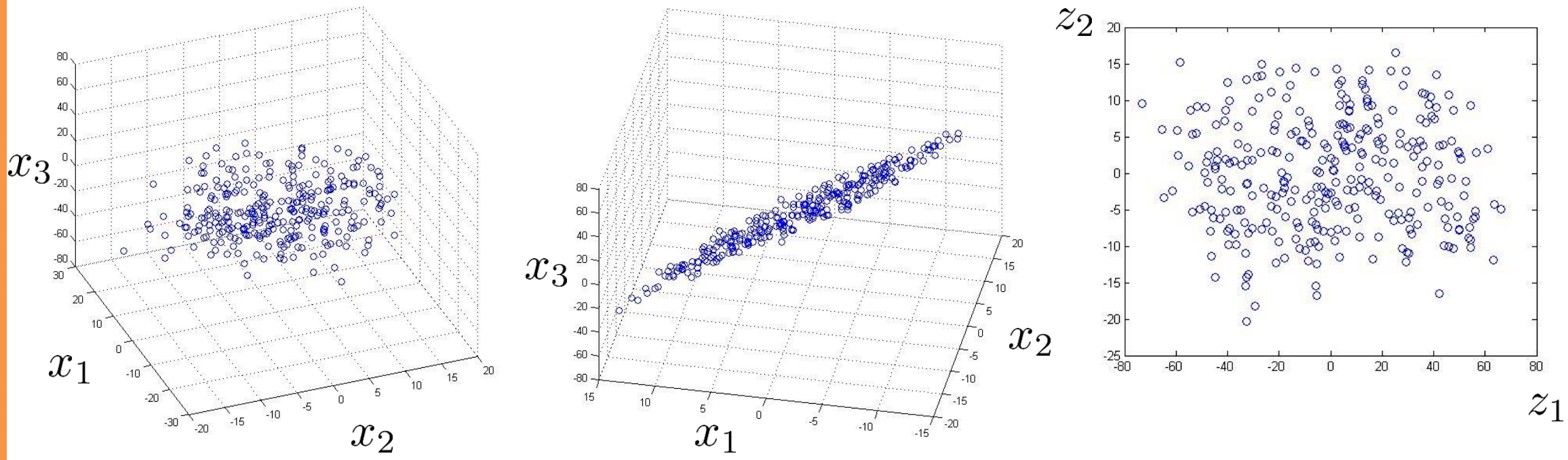
$$x^{(2)} \rightarrow z^{(2)}$$

$$\vdots$$

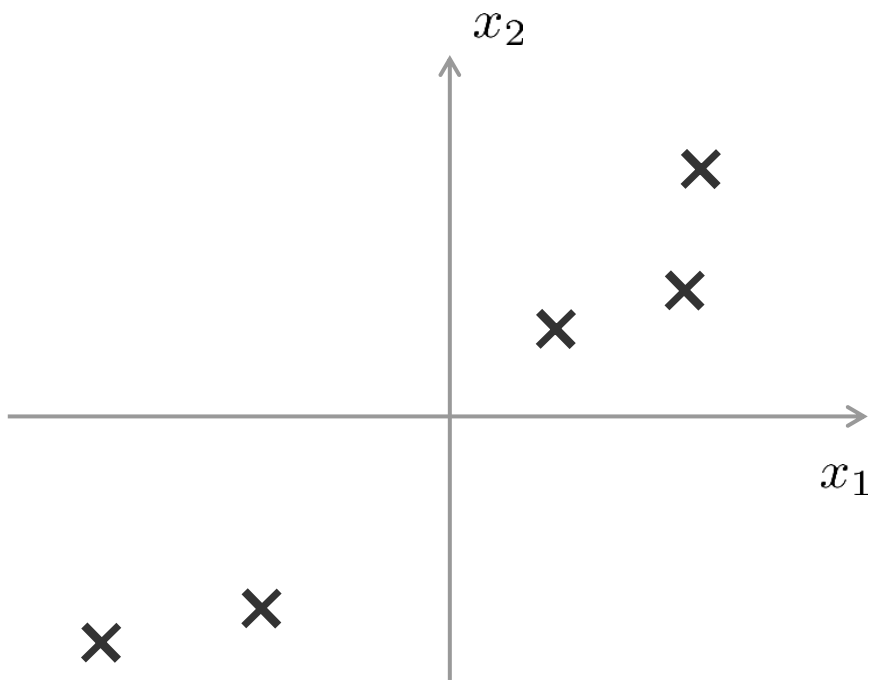
$$x^{(m)} \rightarrow z^{(m)}$$

Another Simple Example

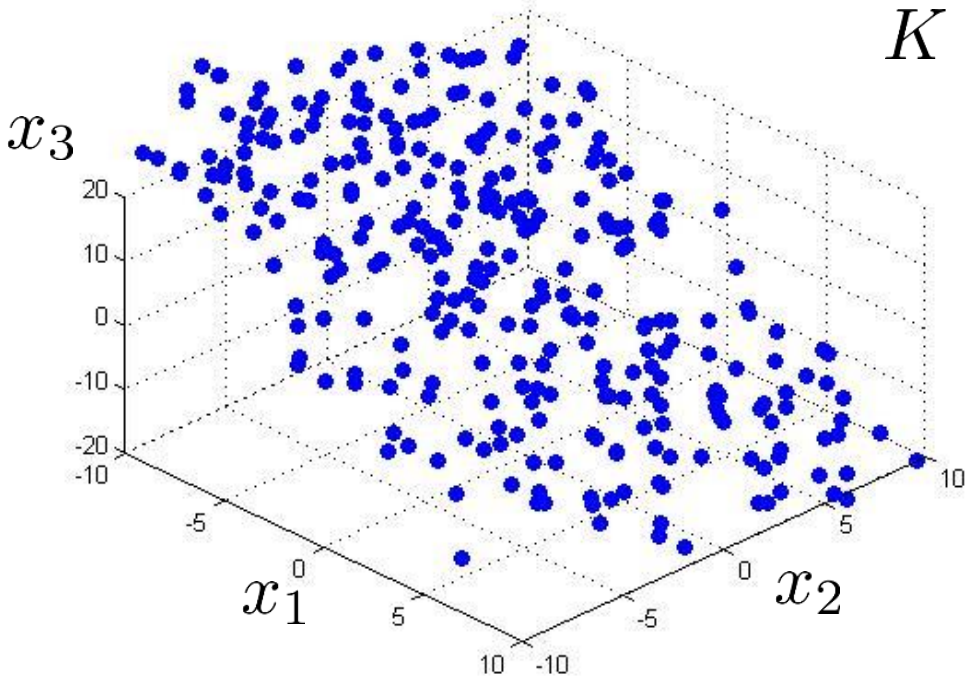
Reduce data from 3D to 2D



Generalize the problem



$3D \rightarrow 2D$
$K = 2$



Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

Andrew Ng

Variance and covariance

1D: Variance=(Standard deviation)²

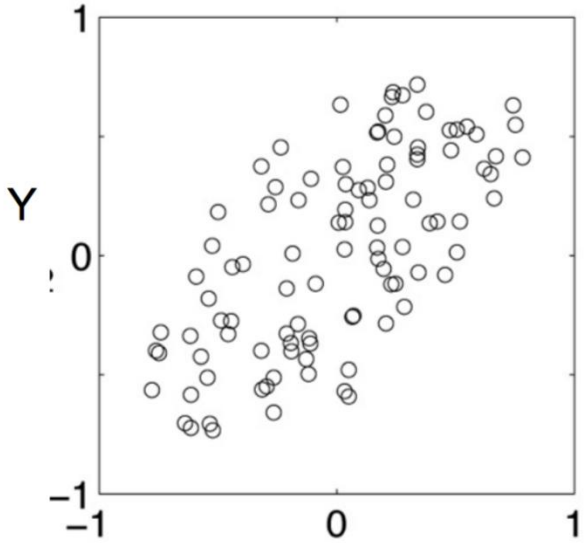
$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}$$

2D: Covariance: measures the correlation between X and Y

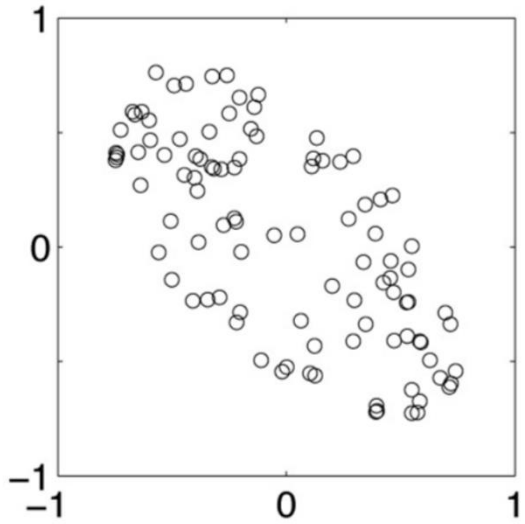
- Cov(X,Y)=0: independent
- Cov(X,Y)>0: move in the same direction
- Cov(X,Y)<0: move in opposite direction

$$\mathrm{cov}(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

positive covariance



negative covariance



Multidimensional data: covariance matrix

- Contains covariance values between all possible dimensions (=attributes):

$$C^{nxn} = (c_{ij} \mid c_{ij} = \mathrm{cov}(Dim_i, Dim_j))$$

- Example for three attributes (x,y,z):

$$C = \begin{pmatrix} \mathrm{cov}(x,x) & \mathrm{cov}(x,y) & \mathrm{cov}(x,z) \\ \mathrm{cov}(y,x) & \mathrm{cov}(y,y) & \mathrm{cov}(y,z) \\ \mathrm{cov}(z,x) & \mathrm{cov}(z,y) & \mathrm{cov}(z,z) \end{pmatrix}$$

- Eigenvalues of covariance matrix contain information on the independent factors of variability
- Eigenvectors of covariance matrix provide the information on direcitons

Principal Component Analysis

- Center the data (subtract the mean $\boldsymbol{\mu} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n$ from each data point)
- Compute the $D \times D$ covariance matrix $\mathbf{S}$ using the centered data matrix $\mathbf{X}$ as

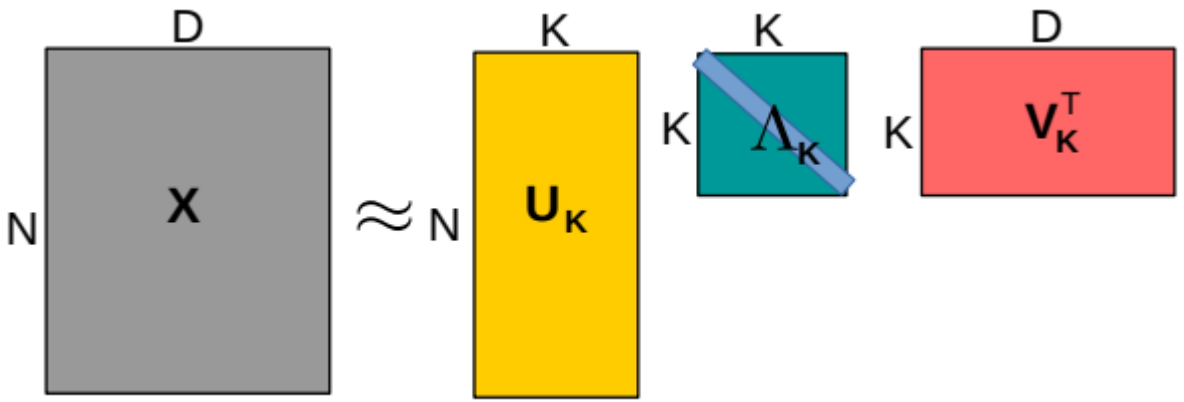
$$\mathbf{S} = \frac{1}{N}\mathbf{X}^\top\mathbf{X} \qquad \text{(Assuming } \mathbf{X} \text{ is arranged as } N \times D\text{)}$$

- Do an eigen decomposition of the covariance matrix $\mathbf{S}$ (many methods exist)
- Take top $K < D$ leading eigvectors $\{\boldsymbol{w}_1, \boldsymbol{w}_2, \dots, \boldsymbol{w}_K\}$ with eigen values $\{\lambda_1, \lambda_2, \dots, \lambda_K\}$
- The K-dimensional projection/embedding of each input is $\boldsymbol{z}_n \approx \mathbf{W}_K^\top \boldsymbol{x}_n$
- Where $\mathbf{W}_\mathrm{K} = [\boldsymbol{w}_1, \boldsymbol{w}_2, \dots, \boldsymbol{w}_K]$ is projection matrix of size $D \times K$

Adapted from Introduction to Machine Learning by Nisheeth

Singular Value Decomposition

- If we just use the top $K < \min\{N, D\}$ singular values, we get a rank-K SVD



$$\mathbf{X} \approx \hat{\mathbf{X}} = \sum_{k=1}^{K} \lambda_k \boldsymbol{u}_k \boldsymbol{v}_k^\top = \mathbf{U}_K \Lambda_K \mathbf{V}_K^\top$$

reconstruction error $\|\boldsymbol{X} - \hat{\boldsymbol{X}}\|$'

- Fact: SVD gives the best rank-K approximation of a matrix

- PCA is done by doing SVD on the covariance matrix **S** (left and right singular vectors are the sar and become eigenvectors, singular values become eigenvalues)

Adapted from Introduction to Machine Learning by Nisheeth

Principal Component Analysis

PCA: orthogonal transformation converting possibly correlated variables into linearly uncorrelated *principal components*

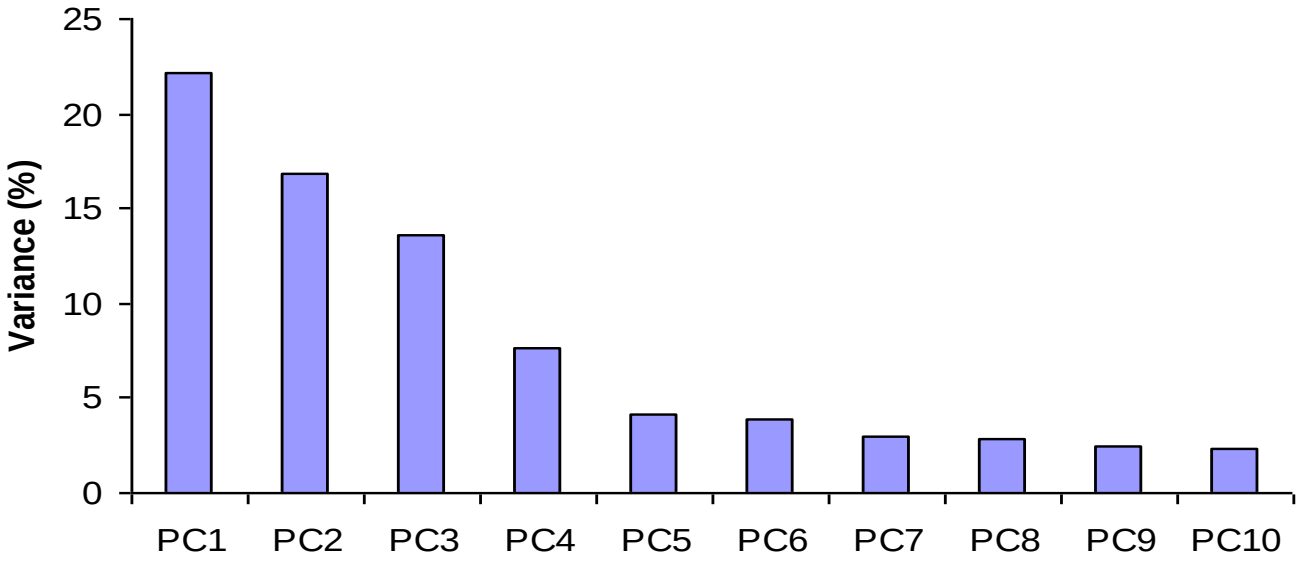
- PCA was invented by Karl Pearson in 1901, however the Singular Value Decomposition was independently derived some half a century earlier in Italy, Germany and France
- PCA transforms the data such that the greatest variance by any projection lies on the first coordinate
- Reveals internal structure of the data that best explains variance in the data set
- Since data often moves in clusters, PCA reveals those variables that drive the variance

Pearson, K. (1901). "On Lines and Planes of Closest Fit to Systems of Points is Space". *Philosophical Magazine Series 6* **2** (11): 559–572

PCA: Eigenvalues

Eigenvalues λ_j are used for calculation of [% of total variance] (V_j) for each component j:

$$V_j = 100 \cdot \frac{\lambda_j}{\sum_{x=1}^{n} \lambda_x} \qquad \sum_{x=1}^{n} \lambda_x = n$$



PCA: Components

- The first PC retains the greatest amount of variation in the sample
- The kth PC retains the kth greatest fraction of the variation in the sample
- The kth largest eigenvalue of the correlation matrix C is the variance in the sample along the kth PC
- The least-squares view: PCs are a series of linear least squares fits to a sample, each orthogonal to all previous ones

PCA Components and Loadings

- Technique useful for compression and classification of data
- Find new descriptors smaller than original variables
- Retain most of sample's information - correlation between original variables
- New descriptors are principal components (PCs)
- Loadings represent the “fraction” of PCs in initial data
- Uncorrelated, and ordered by fraction of total information retained in each PC

PCA in scikit-learn

sklearn.decomposition.PCA

class sklearn.decomposition.**PCA**(*n_components=None, *, copy=True, whiten=False, svd_solver='auto', tol=0.0, iterated_power='auto', n_oversamples=10, power_iteration_normalizer='auto', random_state=None*) [source]

Methods

fit(X[, y])	Fit the model with X.
fit_transform(X[, y])	Fit the model with X and apply the dimensionality reduction on X.
get_covariance()	Compute data covariance with the generative model.
get_feature_names_out([input_features])	Get output feature names for transformation.
get_metadata_routing()	Get metadata routing of this object.
get_params([deep])	Get parameters for this estimator.
get_precision()	Compute data precision matrix with the generative model.
inverse_transform(X)	Transform data back to its original space.
score(X[, y])	Return the average log-likelihood of all samples.
score_samples(X)	Return the log-likelihood of each sample.
set_output(*[, transform])	Set output container.
set_params(**params)	Set the parameters of this estimator.
transform(X)	Apply dimensionality reduction to X.

Examples: Eigenfaces

- When viewed as vectors of pixel values, face images are extremely high dimensional. Image of 100x100 pixels has 10,000 dimensions.
- However, very few of 100x100 vectors are valid face images
- We want to effectively represent the subspace of face images

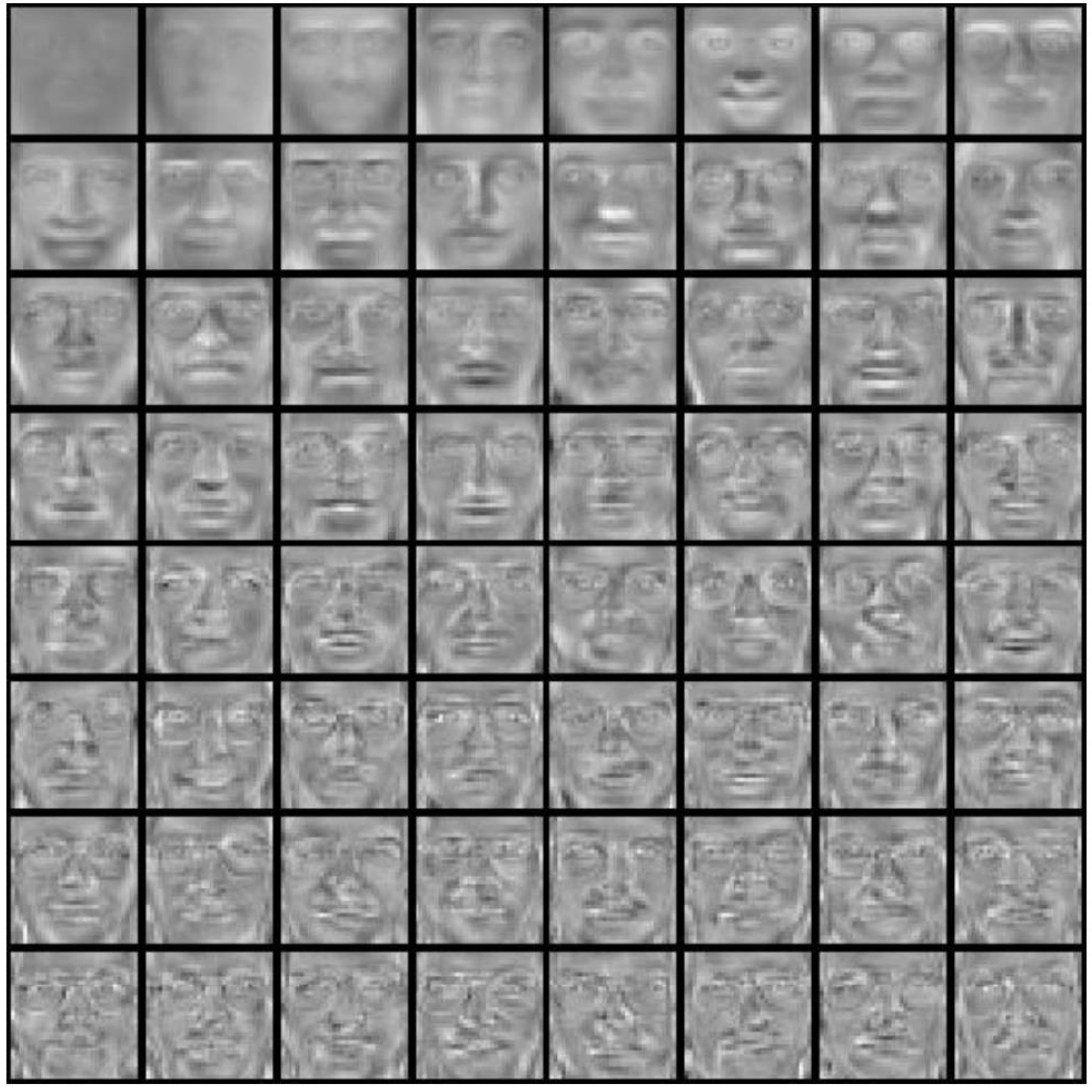
Adapted form Fereshteh Sadeghi

slide by Derek Hoiem

Examples: Eigenfaces

Mean: μ

Top eigenvectors: $u_1,\ldots u_k$



Adapted from Fereshteh Sadeghi slide by Derek Hoiem

Representation and reconstruction

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

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

- Reconstruction:

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

slide by Derek Hoiem

Adapted from Fereshteh Sadeghi

Reconstruction

P = 4

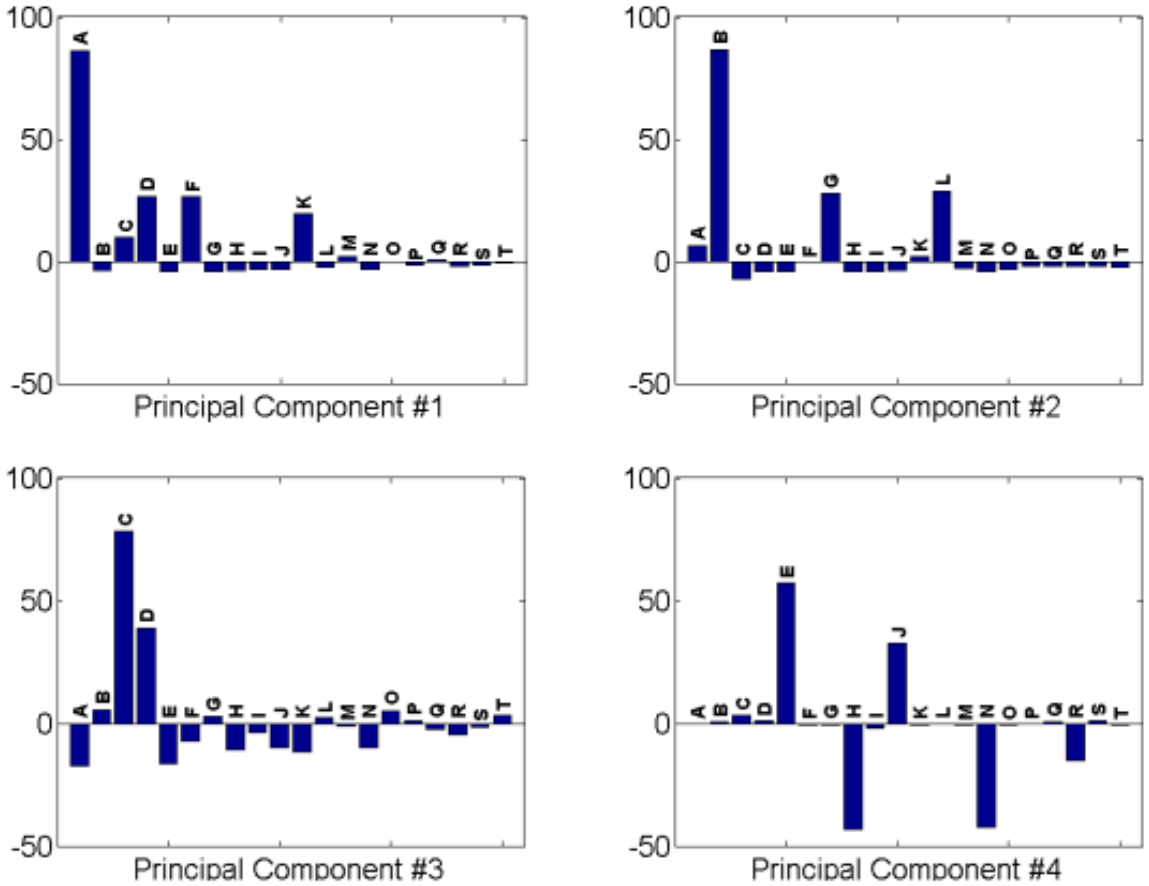
P = 200

P = 400

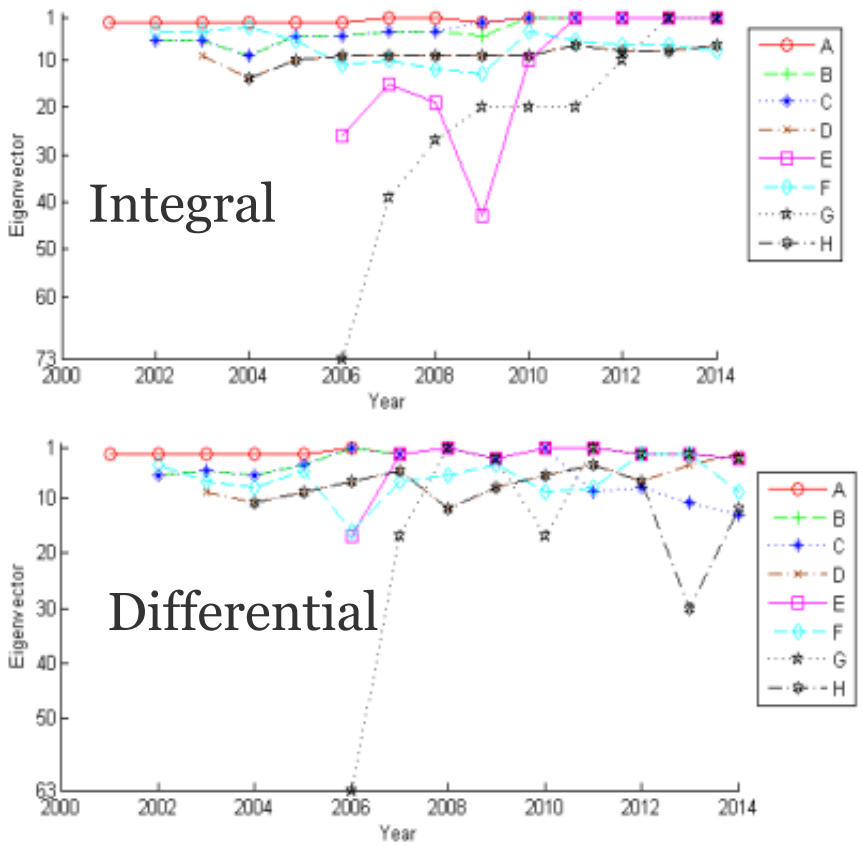
We can represent faces well by 400 components – rather then 10,000!

Adapted from Fereshteh Sadeghi

PCA can be applied to everything



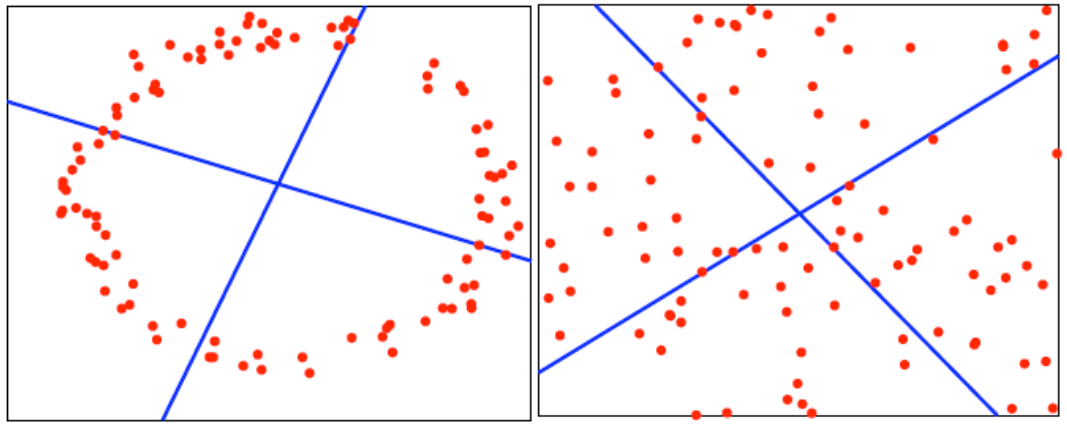
Publication activity



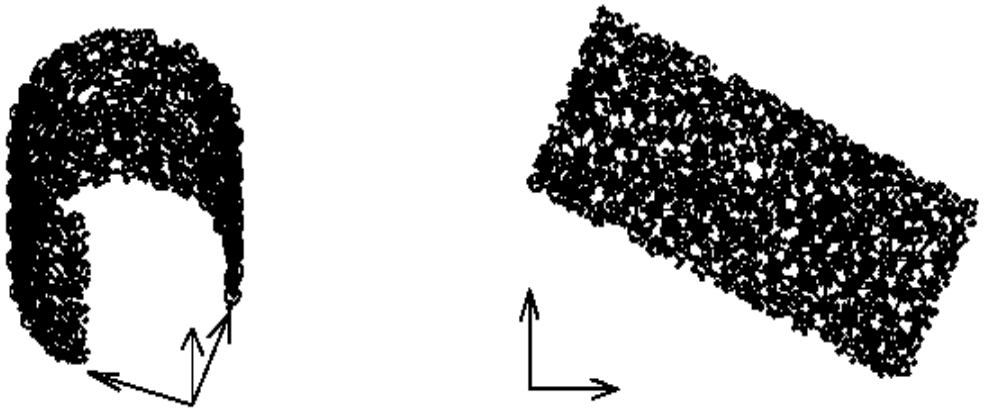
Publication analysis: The dimensionality of space, N, is defined by the total number of scientists. Each publication in this case then defines a single point in this space. For example, for the 28-dimensional space of authors of {A,B,C, … , Z} the publication authored by A and C will be represented as {1,0,1, …, 0}, and by A,B, and Z as {1,1,0, …, 0,1}, where all missing elements are zeroes.

https://arxiv.org/abs/1502.03439

Limitations of PCA



PCA will make no difference between these examples



Nonlinear projection of a horseshoe

Non-linear PCA

- Suppose that instead of using the points $\mathbf{x}_i$ as is, we wanted to go to some different *feature space* $\phi(\mathbf{x}_i) \in \Re^N$
- E.g. using polar coordinates instead of cartesian coordinates would help us deal with the circle
- In the higher dimensional space, we can then do PCA
- The result will be non-linear in the original data space!
- Similar idea to support vector machines

Kernel PCA

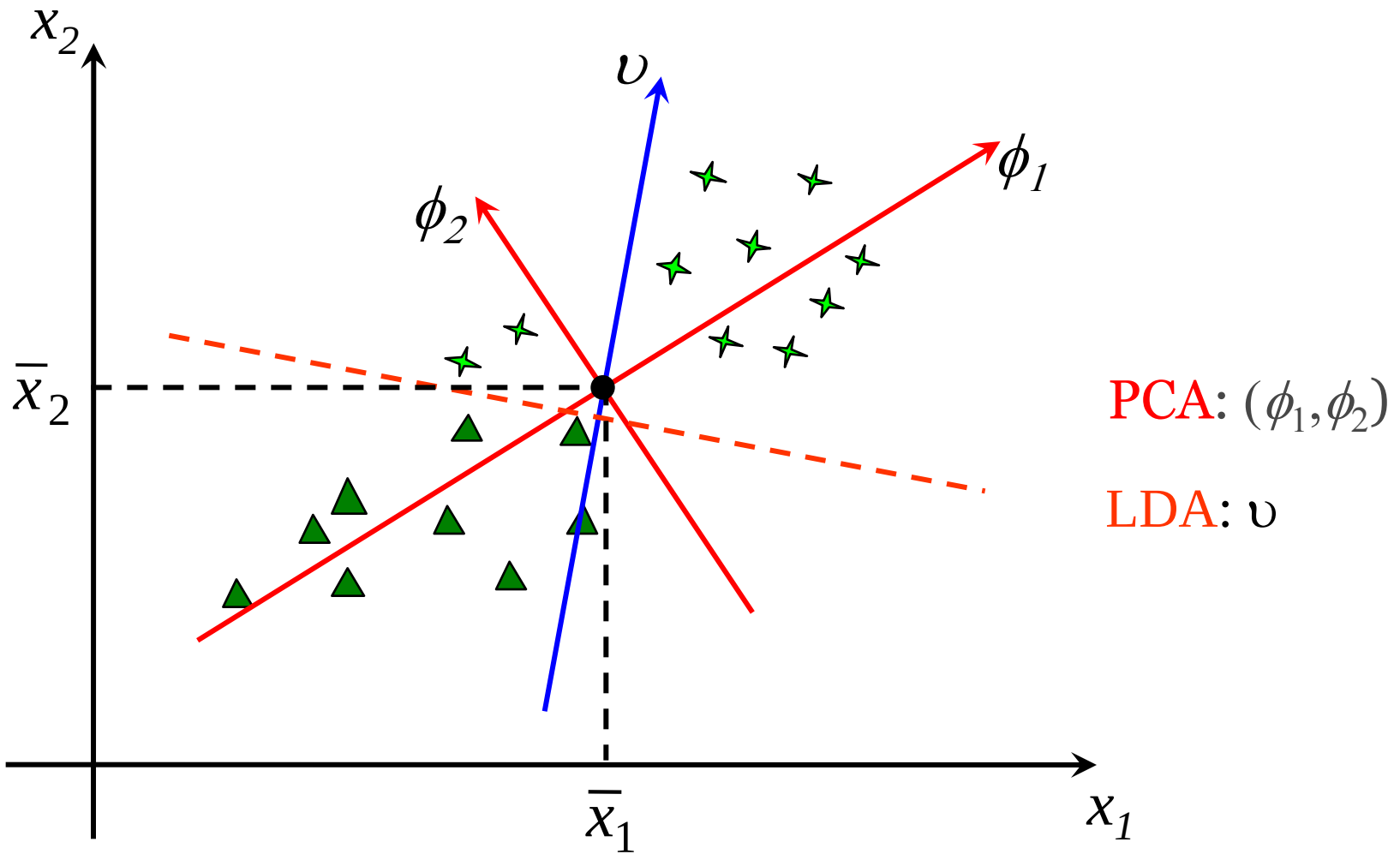
Kernel PCA is an unsupervised manifold learning technique that maps data points to a generally lower-dimensional space. It generalizes the Principal Components Analysis approach to non-linear transformations using the kernel trick (Schölkopf, Smola and Müller, 1996; Schölkopf, Smola and Müller, 1998; Schölkopf, Burges and Smola, 1999). The algorithm implicitly finds the leading eigenvectors and eigenvalues of the covariance of the projection $\phi(x)$ of the data in "feature space", where $\phi(x)$ is such that the kernel $K_n(x, y) = \phi(x) \cdot \phi(y)$ (i.e. K_n must not have negative eigenvalues). If the data is

(http://research.microsoft.com/users/Cambridge/nicolasl/papers/eigen_dimred.pdf)

Linear Discriminant Analysis

- Linear Discriminant Analysis, or simply LDA, is a feature extraction technique that has been used successfully in many statistical pattern recognition problems.
- LDA is often called Fisher Discriminant Analysis (FDA).
- The primary purpose of LDA is to separate samples of distinct groups by transforming then to a space which maximises their between-class separability while minimising their within-class variability.
- It assumes implicitly that the true covariance matrices of each class are equal because the same within-class scatter matrix is used for all the classes considered.
- If we remove this assumption, we get Quadratic Discriminant Analysis

Geometric Idea of LDA



From Intelligent Data Analysis and Probabilistic Inference by Longin Jan Latecki Temple University

LDA Steps

1. Compute the d-dimensional mean vectors.
2. Compute the scatter matrices
3. Compute the eigenvectors and corresponding eigenvalues for the scatter matrices.
4. Sort the eigenvalues and choose those with the largest eigenvalues to form a $d \times k$ dimensional matrix
5. Transform the samples onto the new subspace.