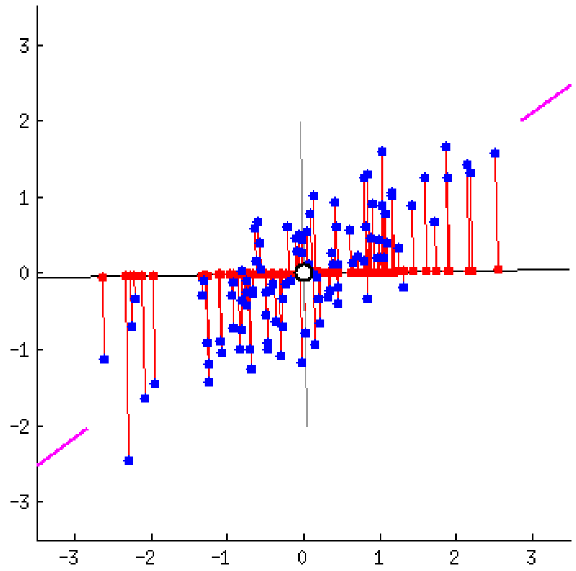
COMS20017 – Algorithms & Data



March 2025
Principal Component Analysis

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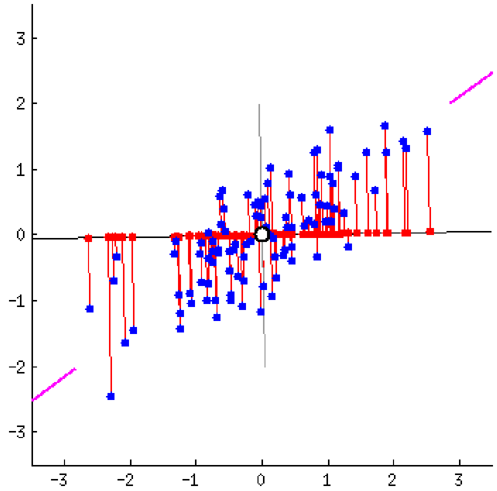
Lecture MM-07

Next in DATA



Feature Selection and Extraction

- Signal basics and Fourier Series
- 1D and 2D Fourier Transform
- Another look at features
- **PCA for dimensionality reduction**
- Convolutions

Dimensionality Reduction

- Benefit = reduce number of variables you have to worry about

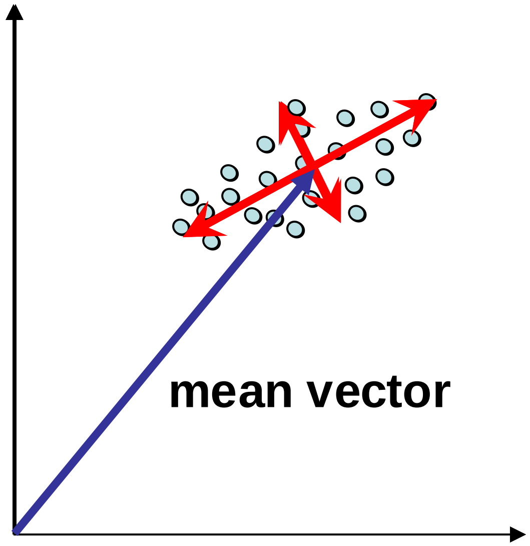
- Two typical approaches:
  - Selecting a subset of a given set of features → FS
  - Selecting a subset after transformation of a set of features → FE

An example of transformation for Feature Extraction:

- Principal Component Analysis - The goal of PCA is to reduce the dimensionality of the data while retaining as much of the variation present in the dataset as possible.

Principal Component Analysis

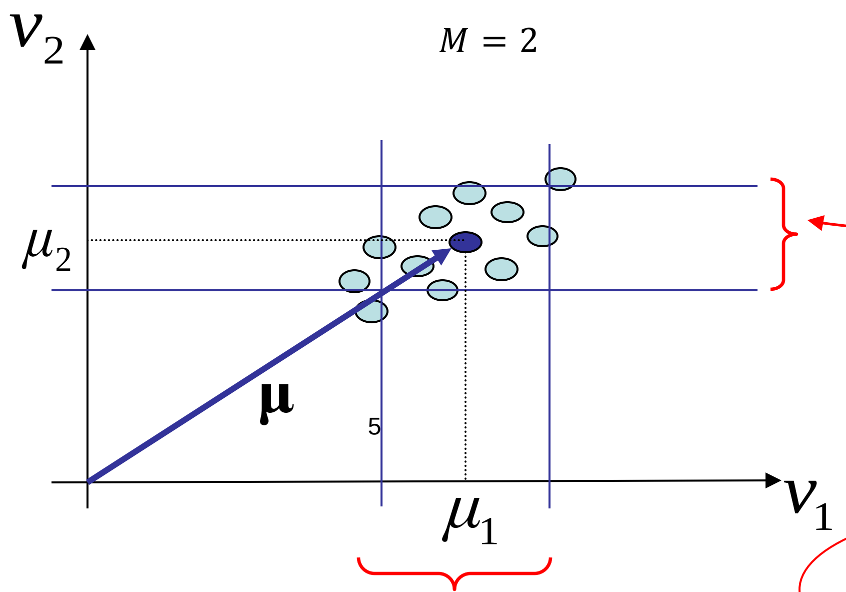
A geometrical view:



PCA decorrelates our data, i.e. it keeps the variance and removes the covariance.

REMINDER: Mean and Covariance

$$\boldsymbol{\mu} = \frac{1}{N}\sum_i \mathbf{v}_i$$



Covariance between components

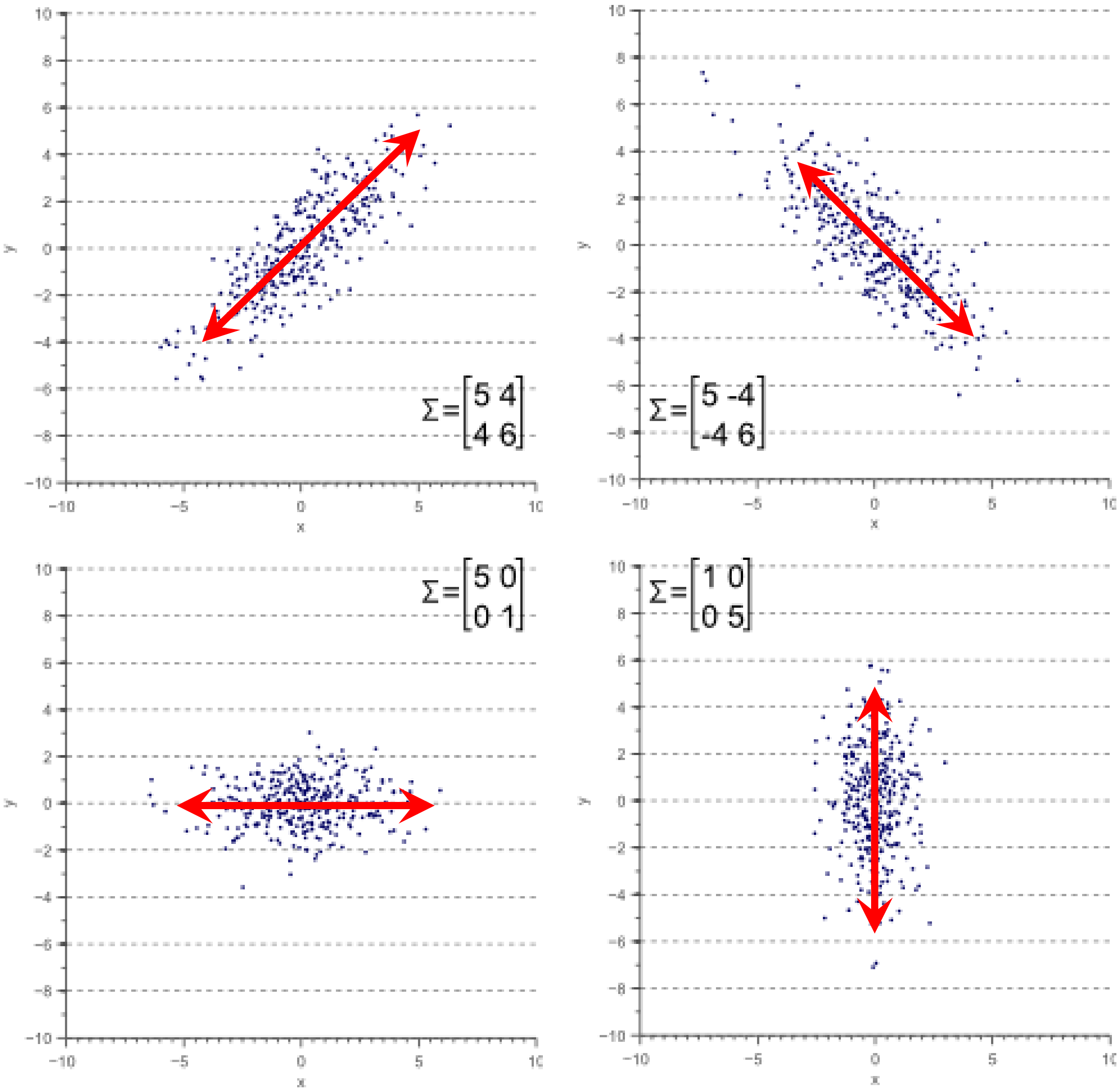
Variance along 1st dimension

Variance along 2nd dimension

$$\mathbf{C} = \frac{1}{N}\sum_i \begin{bmatrix} \boxed{(v_{i1} - \mu_1)^2} & (v_{i1} - \mu_1)(v_{i2} - \mu_2) \\ \boxed{(v_{i1} - \mu_1)(v_{i2} - \mu_2)} & \boxed{(v_{i2} - \mu_2)^2} \end{bmatrix}$$

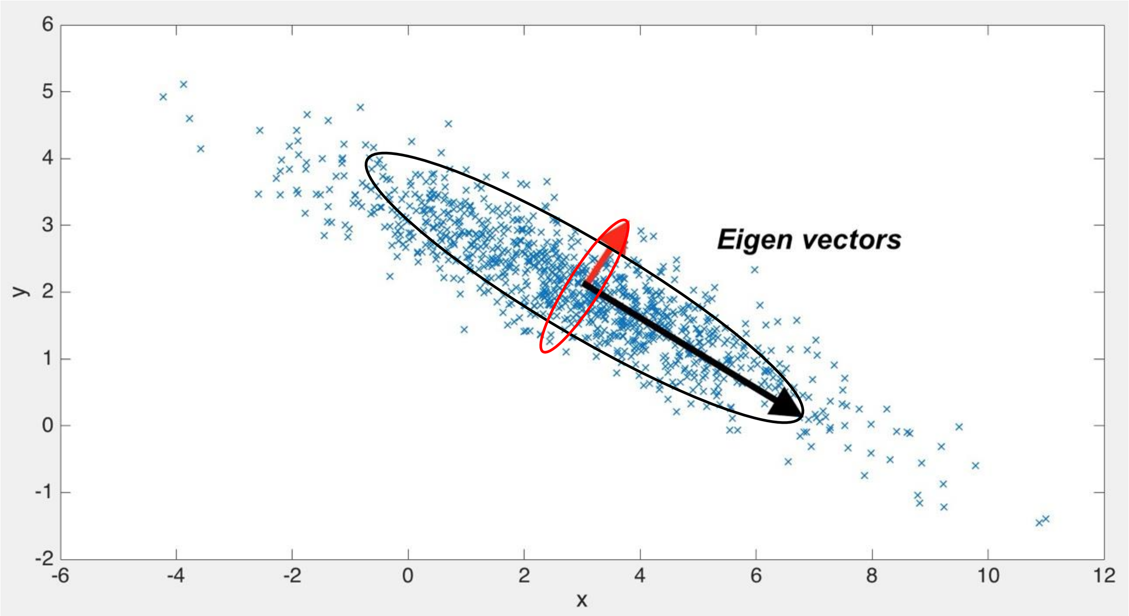
REMINDER: Spread and Covariance

- The shape of the data is defined by the covariance matrix.
- Diagonal spread is captured by the covariance, while axis-aligned spread is captured by the variance.



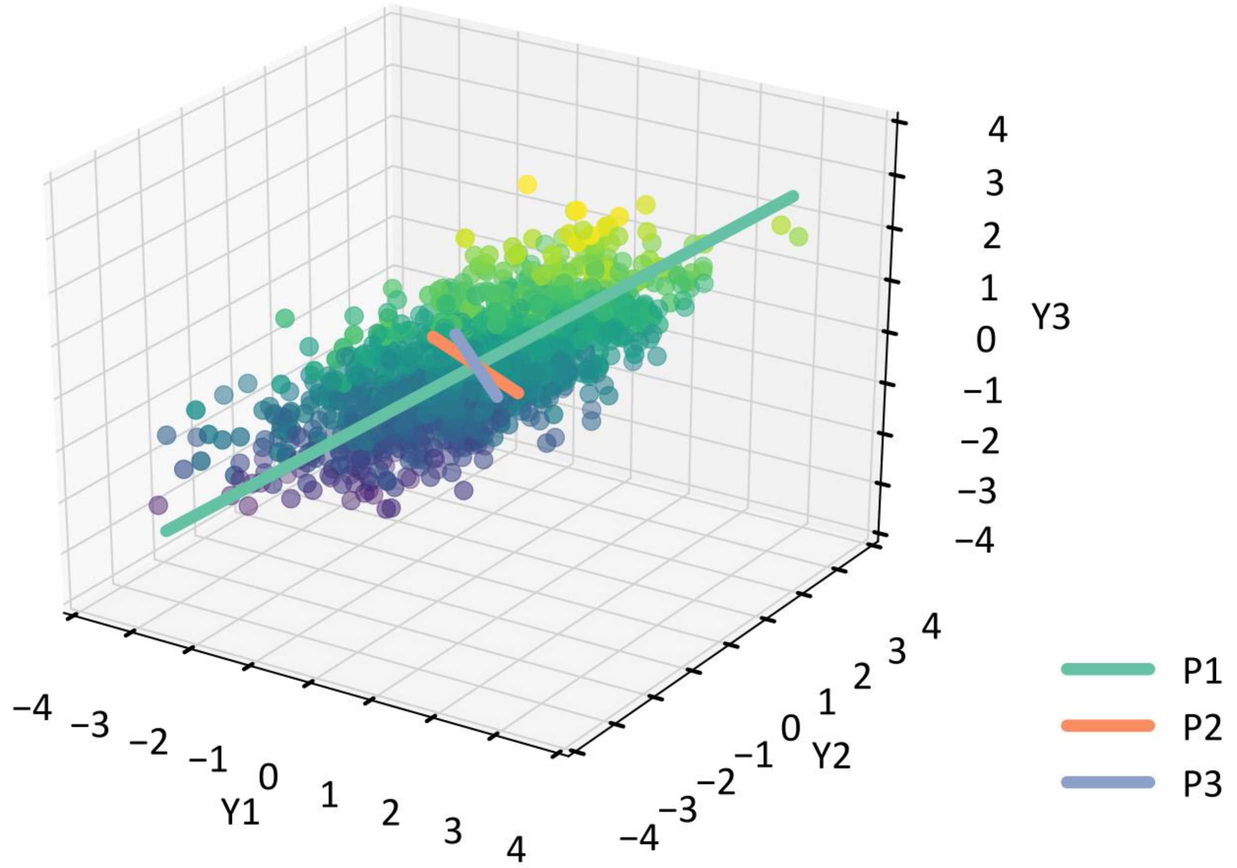
REMINDER – Covariance Matrix: Eigen analysis

- Eigenvectors and eigenvalues define **principal axes** and spread of points along directions, respectively.
- **Major axis** - eigenvector corresponding to larger eigenvalue (i.e. larger variance)
- **Minor axis** - eigenvector corresponding to smaller eigenvalue (i.e. smaller variance)
- These can be represented using major and minor axes of ellipses



Example in 3 Dimensions

- Eigenvectors and eigenvalues define **principal axes** and spread of points along directions



From: https://geostatisticslessons.com/lessons/sphereingmaf

Principal Component Analysis

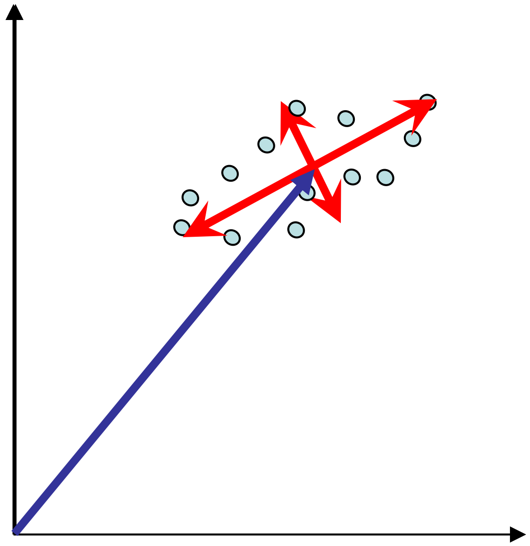
- PCA involves the transformation of a no. of correlated variables into a no. of new uncorrelated variables called → independent features.

- **Principal Axes**: the first direction that accounts for as much of the variance as possible (→ i.e. variance is maximum); then the direction orthogonal to the first for which the variance is maximum, and so on…

- Given N data vectors from p dimensions, find orthogonal vectors from d dimensions $(\text{where } d \leq p)$ that can be best used to represent the N data vectors.

Principal Component Analysis

A geometrical view:



PCA also allows us to represent our data using fewer dimensions by linearly projecting the data onto a lower-dimensional space, in a *least squares* sense.

Eigenvalues & Eigenvectors

If $\mathbf{C}$ is an nxn matrix, do there exist non-zero vectors $\mathbf{u}$ in R^n, such that $\mathbf{Cu}$ is a scalar multiple of $\mathbf{u}$?

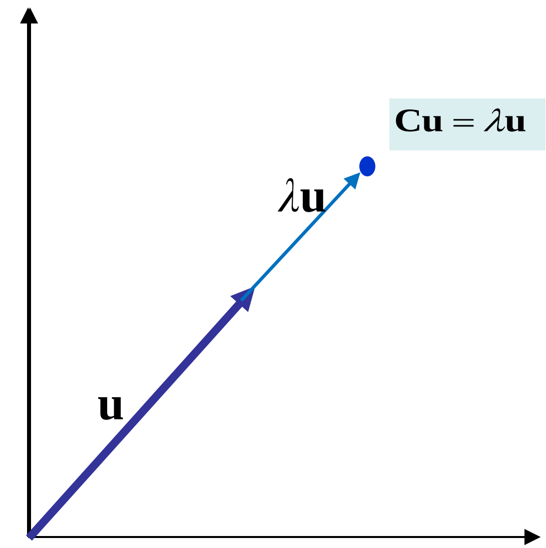
an nxn matrix

Eigenvalue – a scalar

$$\mathbf{Cu} = \lambda\mathbf{u}$$

Eigenvector – a non-zero vector in R^n

- A geometrical view:



Eigenvalue and Eigenvector Example

$$\mathbf{Cu} = \lambda\mathbf{u}$$

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \mathrm{x} \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \begin{pmatrix} 11 \\ 5 \end{pmatrix} \neq \lambda \mathrm{x} \begin{pmatrix} 1 \\ 3 \end{pmatrix}$$

Not an eigenvector

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \mathrm{x} \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4 \mathrm{x} \begin{pmatrix} 3 \\ 2 \end{pmatrix}$$

Eigenvalue and eigenvector

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \mathrm{x} \begin{pmatrix} 6 \\ 4 \end{pmatrix} = \begin{pmatrix} 24 \\ 16 \end{pmatrix} = 4 \mathrm{x} \begin{pmatrix} 6 \\ 4 \end{pmatrix}$$

Scaled eigenvector.
Still in the same direction.
Still the same eigenvalue.

Eigenvalue and Eigenvectors

Given the data covariance matrix $\mathbf{C}$, then :

$$\mathbf{C}\mathbf{u}_i = \lambda_i \mathbf{u}_i \longrightarrow \mathbf{C}\mathbf{u}_i - \lambda_i \mathbf{u}_i = 0 \longrightarrow \mathbf{u}_i(\mathbf{C} - \lambda_i \mathbf{I}) = 0$$

Solving this *characteristic equation* leads to the eigenvalues and eigenvectors:

$$\boxed{|\mathbf{C} - \lambda_i \mathbf{I}| = 0}$$

Quite easy in 2 dimensions, just bearable in 3, but not easy as we move into higher dimensions. Enter Matlab/Python…

⇨ Orientation given by eigenvector of covariance matrix

⇨ Spread given by eigenvalue of covariance matrix

Matlab: eigenvalues & eigenvectors

```
%% example to demonstrate the computation of eigenvalues and eigenvectors

disp('This is the example data set:')
V = [2.8 2.2 2.2 1.6 2.5 1.4 1.8 1.2 2.1 1.3;
     3.0 2.0 2.8 1.6 2.7 1.2 2.1 1.5 2.3 1.4
     7.0 7.4 6.2 6.4 6.6 7.0 6.9 7.1 6.5 7.1];
disp(V');
m1 = mean(V(1,:)); m2 = mean(V(2,:)); m3 = mean(V(3,:));
disp('The mean vector is:'); disp([m1 m2 m3]);

disp('Press a key to continue and see the covariance C:'); pause;
kov = cov(V')

disp('press a key to continue and show the eigenvectors and eigenvalues...'); pause;
[eigvec,eigval] = eig(kov)

disp('And finally, just to prove the equation: C u = lambda u')
disp('For example, take the 2nd eigenvalue and eigenvector'); pause;

disp('First C u');   kov*eigvec(:,2)
disp('then lambda u');   eigval(2,2)*eigvec(:,2)
```

See unit github page for Python code

Principal Component Analysis

Consider a data set of N 2-dimensional samples $\mathbf{v}_1, \mathbf{v}_2 \ldots, \mathbf{v}_N$.

Let the mean of the samples be at $\mathbf{m}$. Then we can get for example a 1D representation by projecting the data onto a line running through the sample mean:

$$\mathbf{v}_k = \mathbf{m} + a_k \mathbf{u}$$

where $\mathbf{u}$ is a unit vector in the direction of the line, and the scalar a_k is the distance of the point $\mathbf{v}_k$ from the mean $\mathbf{m}$.

- Thus, we find an optimal set of coefficients a_k, $k=1,\ldots,N$, such that:

$$a_k = \mathbf{u}^t(\mathbf{v}_k - \mathbf{m})$$

- The result is a least-squares solution which projects the vectors $\mathbf{v}_k$ onto the line in the direction $\mathbf{u}$ that passes through the sample mean.

Principal Component Analysis

- We can represent the data using a combination of other significant eigenvectors in higher dimensions.
- Thus, we can *approximate* any $\mathbf{v} \in \mathrm{R}^p$ as a linear combination of an orthonormal set of basis vectors $< u_1, u_2, \dots, u_d >$ where $d \leq p$.

$$\hat{\mathbf{v}} = \mathbf{m} + \sum_{i=1}^{d} \mathbf{a}_i \mathbf{u}_i$$

i.e. $\hat{\mathbf{v}} = \mathbf{m} + a_1 u_1 + a_2 u_2 + \dots + a_d u_d$

- The eigenvectors are a set of basis vectors for representing any feature vector $\mathbf{v}$ such that $\| \mathbf{v} - \hat{\mathbf{v}} \|$ is minimised → the principal components
- d characterises a lossy or lossless representation of the data $(d \leq p)$

Recipe for PCA

1 - Adjust the data to zero-mean

2.8	3.0
2.2	2.0
2.2	2.8
1.6	1.6
2.5	2.7
1.4	1.2
1.8	2.1
1.2	1.5
2.1	2.3
1.3	1.4

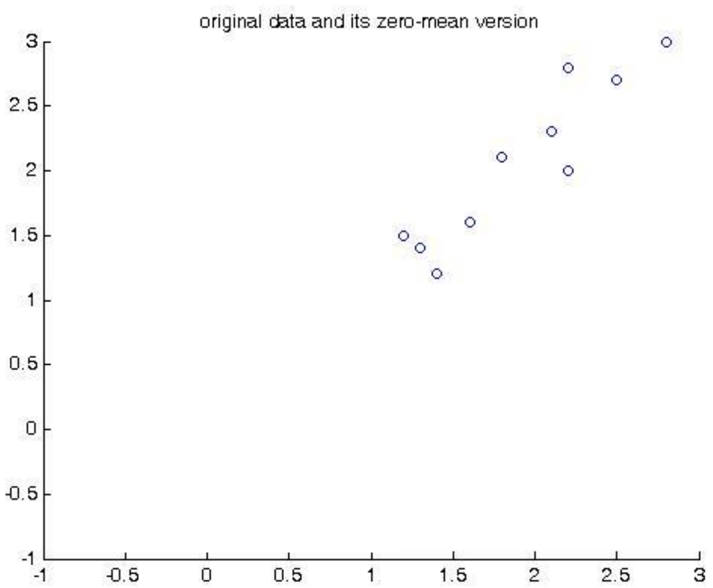
$\mathbf{v}$

mean:

1.91 2.06

0.89	0.94
0.29	-0.06
0.29	0.74
-0.31	-0.46
0.59	0.64
-0.51	-0.86
-0.11	0.04
-0.71	-0.56
0.19	0.24
-0.61	-0.66

$(\mathbf{v}-\mathbf{m})$



Recipe for PCA

2 - Find the Covariance Matrix

$$\mathbf{C} = \begin{pmatrix} 0.2887 & 0.3149 \\ 0.3149 & 0.4004 \end{pmatrix}$$

3 – Compute the eigenvalues and eigenvectors of $\mathbf{C}$

$$\boldsymbol{\lambda} = \begin{pmatrix} 0.0242 \\ 0.6640 \end{pmatrix} \qquad \mathbf{u} = \begin{pmatrix} -0.7669 & 0.6418 \\ 0.6418 & 0.7669 \end{pmatrix}$$

Note $\mathbf{u}^t\mathbf{u} = \| \mathbf{u} \| = 1$.

Recipe for PCA

4 – Order eigenvalues from highest to lowest value

- Eigenvector with the *highest* eigenvalue → 1st principal axis
- Eigenvector with the next *highest* eigenvalue → 2nd principal axis
- and so on (if there were more dimensions!)

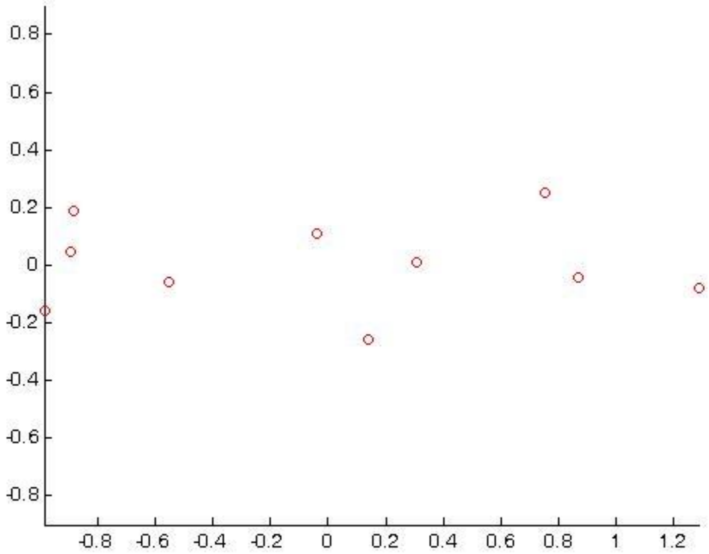
$$\text{Reordered} \quad \boldsymbol{\lambda} = \begin{pmatrix} 0.6640 \\ 0.0242 \end{pmatrix}$$

$$\mathbf{u} = \begin{pmatrix} 0.6418 & -0.7669 \\ 0.7669 & 0.6418 \end{pmatrix}$$

Recipe for PCA

5 – Generate the new representation of the data

1.2921	-0.0793
0.1401	-0.2609
0.7536	0.2525
-0.5517	-0.0575
0.8695	-0.0417
-0.9868	-0.1608
-0.0399	0.1100
-0.8851	0.1851
0.3060	0.0083
-0.8976	0.0442



Note also our data is now totally uncorrelated, i.e. its covariance matrix is diagonal

$$\mathbf{C}_{new} = \begin{pmatrix} 0.6640 & 0 \\ 0 & 0.0242 \end{pmatrix}$$

This step relates to $\mathbf{a} = \mathbf{u}^t(\mathbf{v} - \mathbf{m})$

Recipe for PCA

$$\mathbf{V} = \begin{pmatrix} 2.8 & 3.0 \\ 2.2 & 2.0 \\ 2.2 & 2.8 \\ 1.6 & 1.6 \\ 2.5 & 2.7 \\ 1.4 & 1.2 \\ 1.8 & 2.1 \\ 1.2 & 1.5 \\ 2.1 & 2.3 \\ 1.3 & 1.4 \end{pmatrix}$$

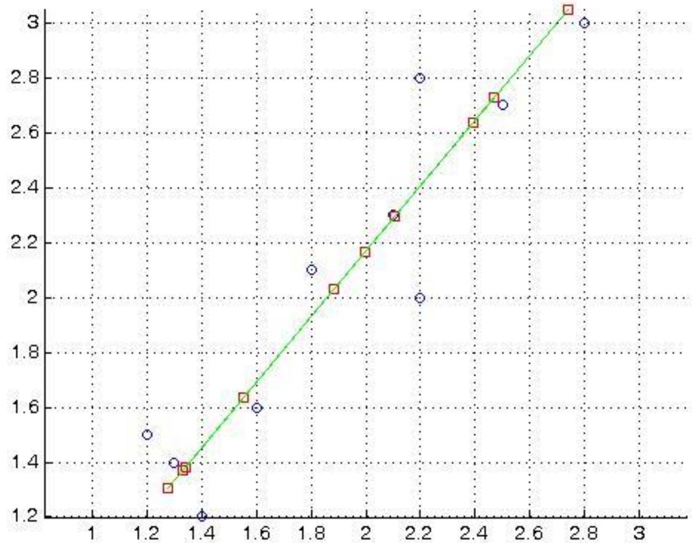
6 – Get the old data back (lossless or lossy):

Both principal components to get lossless data back.

One principal component to get approximate data back (as shown here).

$$\begin{pmatrix} 1.2921 \\ 0.1401 \\ 0.7536 \\ -0.5517 \\ 0.8695 \\ -0.9868 \\ -0.0399 \\ -0.8851 \\ 0.3060 \\ -0.8976 \end{pmatrix} * \begin{pmatrix} 0.6418 & 0.7669 \end{pmatrix} + \underbrace{\begin{pmatrix} 1.91 & 2.06 \end{pmatrix}}_{\text{Add mean}} = \begin{pmatrix} 2.73 & 3.05 \\ 1.99 & 2.16 \\ 2.39 & 2.63 \\ 1.55 & 1.63 \\ 2.46 & 2.72 \\ 1.27 & 1.30 \\ 1.88 & 2.02 \\ 1.34 & 1.38 \\ 2.10 & 2.29 \\ 1.33 & 1.37 \end{pmatrix} = \hat{\mathbf{V}}$$

The new reduced dimensionality representation of our original data →our feature vector



This step relates to $$\mathbf{v} = \mathbf{m} + \sum_{i=1}^{d} \mathbf{a}_i \mathbf{u}_i$$

Dimensionality Reduction

- Importance of PCA lies in dimensionality reduction while maintaining as much of the variance as possible!

➢ Sum of the variances = sum of all eigenvalues = 100% of variance in original data

$$\sum_{i=1}^{p} \lambda_i$$

➢ The proportion of the variance that each eigenvector represents can be calculated by dividing the eigenvalue corresponding to that eigenvector by the sum of all eigenvalues.

Hence, the first d eigenvalues can be said to account for some fraction of the total variance in the data:

$$\frac{\sum_{i=1}^{d} \lambda_i}{\sum_{i=1}^{p} \lambda_i}$$

Example: how to account for a % of variance

- Around 2000 people were asked a set of questions about their *Internet use*. Let's say they asked each person 50 questions.

- There are therefore $p = 50$ **variables, making it a** $\mathbf{50}$**-dimensional dataset**. There will then be 50 eigenvectors and eigenvalues out of that dataset.

- Let's say the eigenvalues of the dataset were (in descending order):
  $39.8, 19.2, 17.0, 10.0, 3.2, 1.0, 0.4, 0.21, 0.0979, \ldots\ldots$ with a total sum of $\sum_{i=1}^{50} \lambda_i = 98.5$

- **The first five have comparatively large values – indicating there is a lot of info (variance) along their corresponding eigenvectors (directions)!**

- The dataset can thus be reduced from 50 dimensions to only 5 by ignoring all the eigenvectors that have insignificant eigenvalues. Nice way of simplifying the data!

- **Percentage of variance captured by the first 5 components:**

$$\frac{\sum_{i=1}^{5} \lambda_i}{\sum_{i=1}^{50} \lambda_i} \Rightarrow \frac{89.2}{98.5} \Rightarrow \sim 91\%$$

Adapted from: http://jurnal-singkat.blogspot.co.uk/2013/10/principal-component-analysis-4-dummies.html

Example Application: Face Recognition using PCA

Set of normalized
face images

Eigenfaces

Training:

1. Acquire initial set of N face images (training set) → $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N$
2. The image pixels are then the feature vectors ($S\ x\ 1$)
3. Compute the average image $\bar{\mathbf{x}} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}_i$
4. Adjust the data set → $\boldsymbol{\phi}_i = \mathbf{x}_i - \bar{\mathbf{x}}$
5. Compute the covariance of the image set

$$\mathbf{C} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})\,(\mathbf{x}_i - \bar{\mathbf{x}})^T$$

$$\mathbf{C} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{\phi}_i\, \boldsymbol{\phi}_i^T = \frac{1}{N}\ \mathbf{A}\mathbf{A}^T$$

where $\mathbf{A} = [\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_N]$, i.e the columns of $\mathbf{A}$ are the $\boldsymbol{\phi}_i$, a $S\ x\ N$ matrix.

Mean face $\bar{\mathbf{x}}$

Eigenfaces

Training:

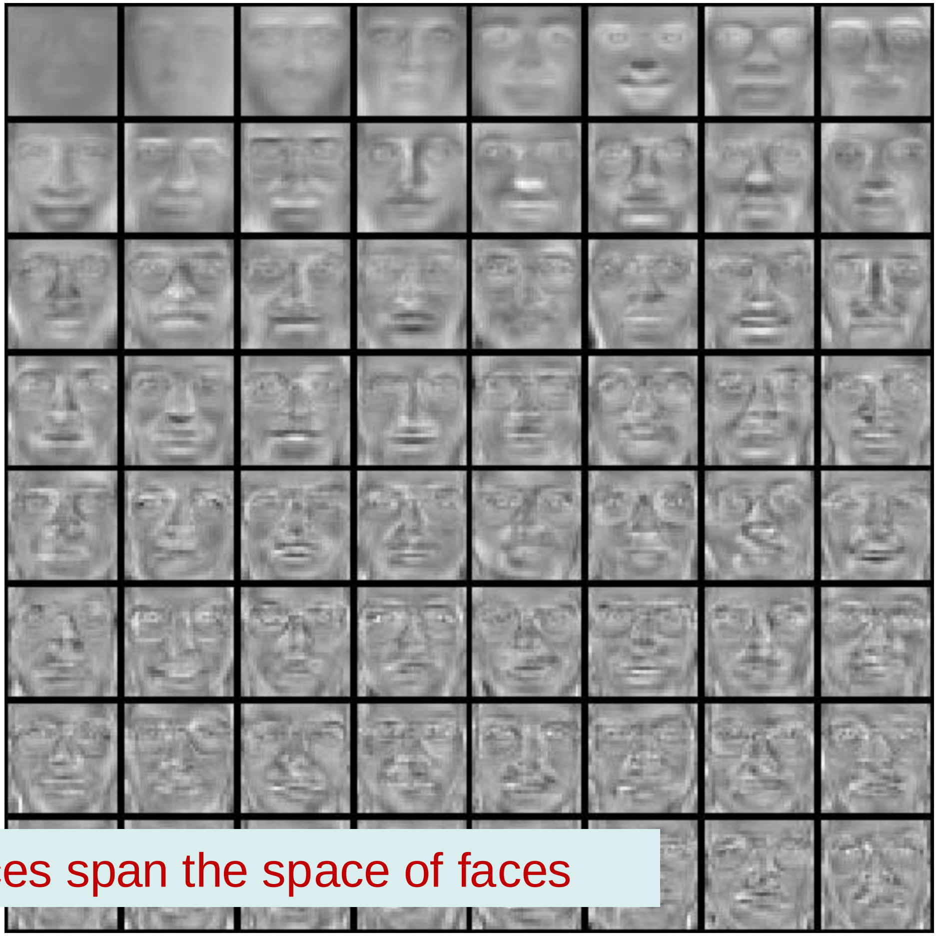
- Compute the eigenvalues and eigenvectors of this covariance matrix → *eigenfaces*

$$(\frac{1}{N}\mathbf{A}\mathbf{A}^T)\mathbf{u} = \boldsymbol{\lambda}\mathbf{u}$$

- Then compute the coefficients, as in

$$\mathbf{a}_i = \mathbf{u}^{\mathrm{T}}(\mathbf{x}_i - \bar{\mathbf{x}})$$

K largest eigenvectors: $\mathbf{u_1}, \mathbf{u_2}, \ldots \mathbf{u_k}$ (or basis vectors visualized as images)



The eigenfaces span the space of faces

Eigenfaces

We can reconstruct a representation of each known individual in face space using a weighted linear combination of the eigenfaces.

 =  +  …

$$\hat{\mathbf{x}} \quad = \quad \bar{\mathbf{x}} \quad + \quad a_1\mathbf{u}_1 + a_2\mathbf{u}_2 + a_3\mathbf{u}_3 + \cdots$$

Eigenfaces

Testing (for example, find a matching face)

Given a novel image $\mathbf{y}$,

- Project $\mathbf{y}$ into face space to obtain the eigen coefficients

$$\mathbf{b} = \mathbf{u}^{\mathrm{T}}(\mathbf{y} - \bar{\mathbf{x}})$$

- Find most likely candidate by distance computation between the feature vectors (distance in face space)

$$\operatorname{argmin} \parallel \mathbf{b} - \boldsymbol{a}_{\boldsymbol{i}} \parallel \qquad i = 1,2, \dots, N$$

Use Euclidean or Mahalanobis distance

PCA characteristics: a summary

PCA is a projection of data that best represents it in a least squares sense:

★ Reveals the structure in data.

★ Provides independent, uncorrelated features.

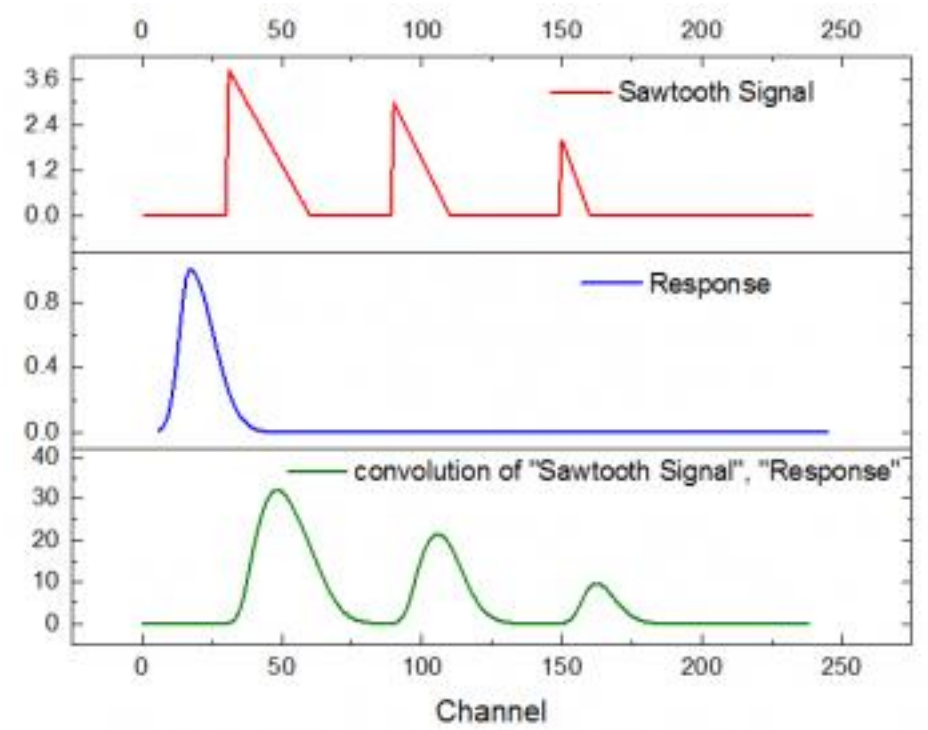
★ Provides reduced dimensionality and speeds up machine learning methods.

★ Reduced and uncorrelated feature set makes the process of clustering and classification *much easier.*

Need to reduce outliers to ensure better modelling of data

The technique is linear, therefore any non-linear correlation between variables will not be captured.

Next…



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