Dimentionality Reduction

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

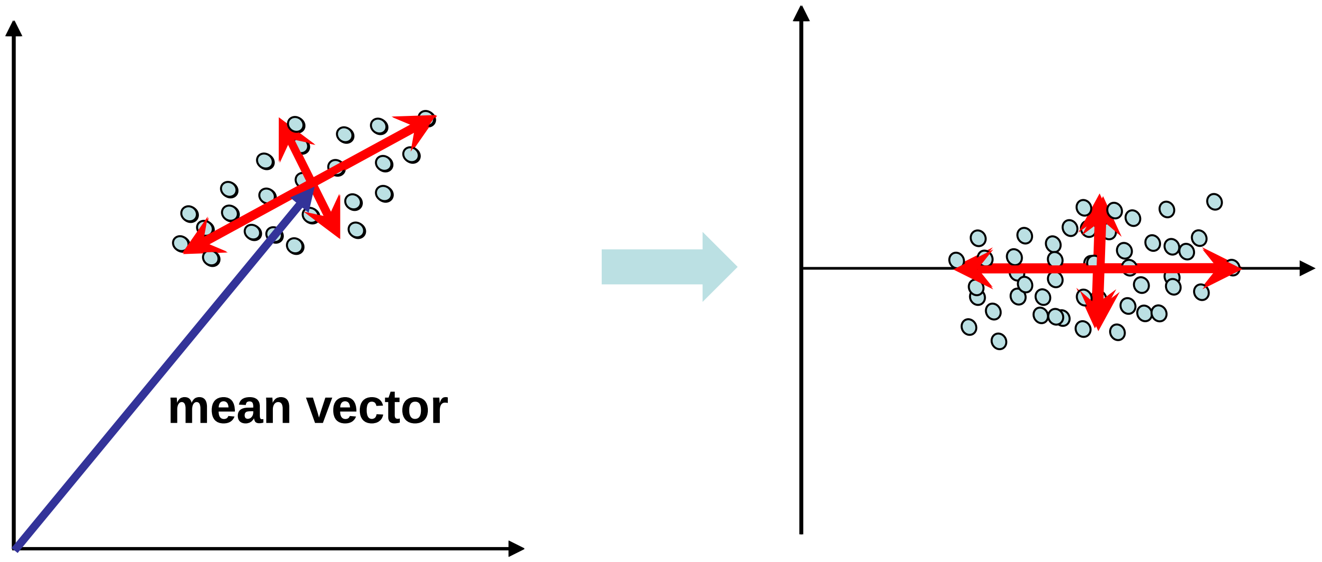
- Two typical approaches:
  - Selecting a subset of a given set of features → FS
  - Selecting a subset after transformation of a set of features → FE

An example of transformation for Feature Extration:

- 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

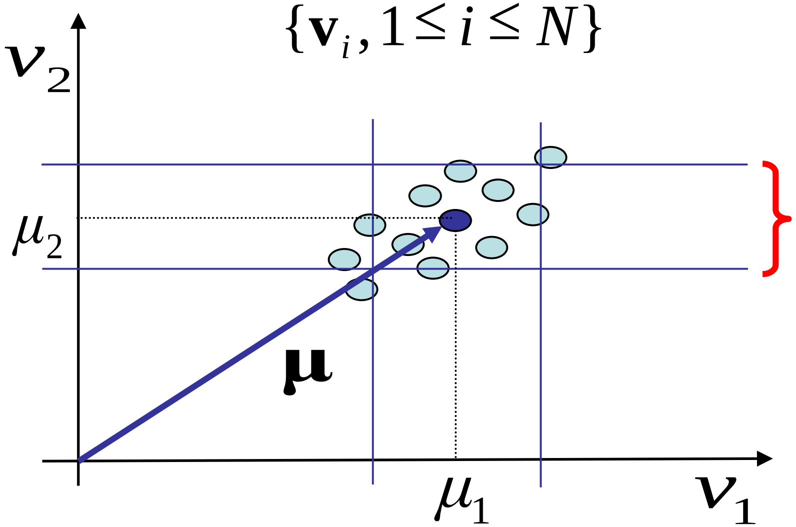
- A geometrical view:



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

Reminder: Covariance Matrix

$$\{\mathbf{v}_i, 1 \le i \le N\}$$



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

Covariance between components

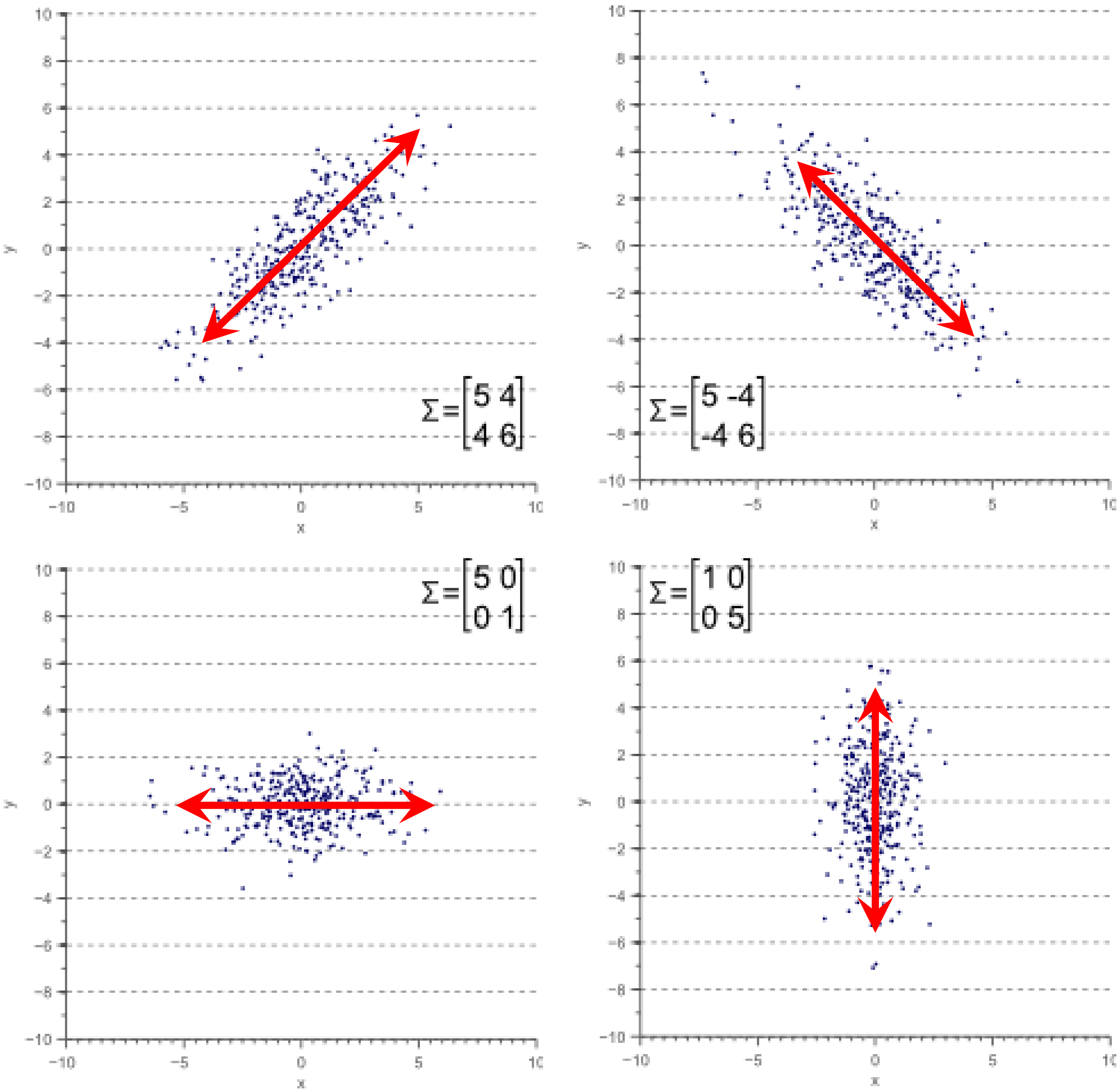
Variance along 1st dimension

Variance along 2nd dimension

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

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.



Principal Component Analysis

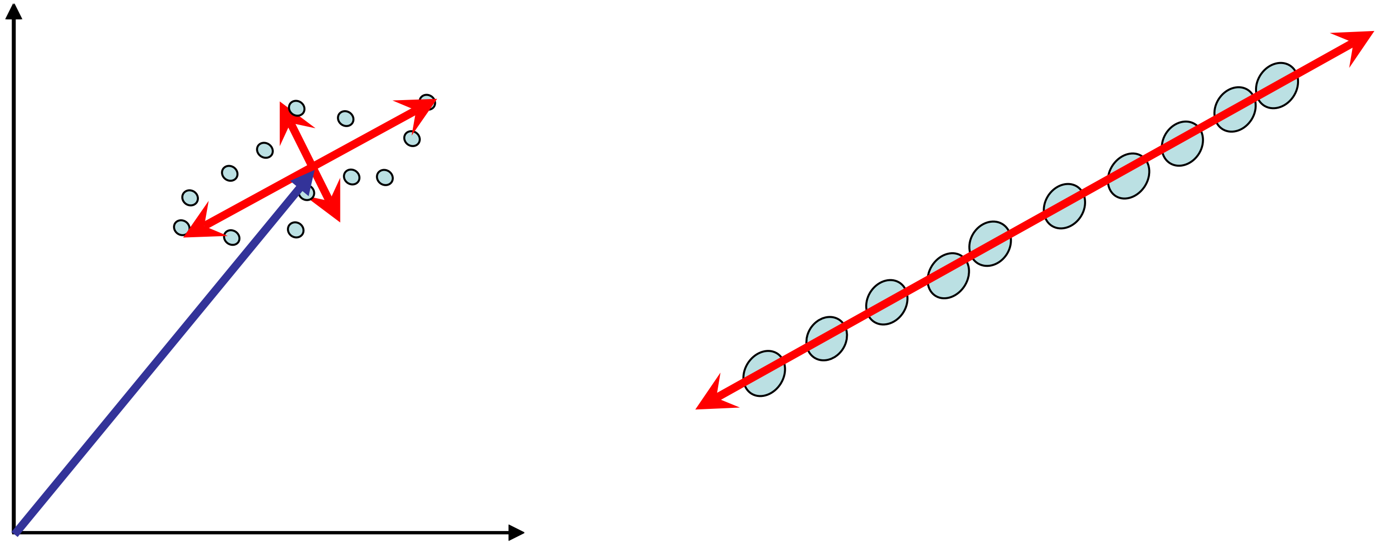
- PCA involves the transformation of a no. of correlated variables into a no. of new uncorrelated variables called → independent features

- **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 (where $d < p$) 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 $\mathbf{u}$?

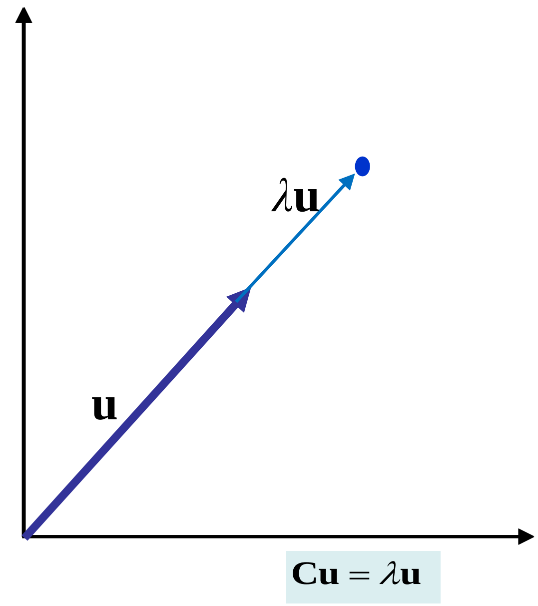
an nxn matrix

Eigenvalue – a scalar

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

Eigenvector – a non-zero vector in R^n

- A geometrical view:



Reminder: Eigenvalue and Eigenvectors

see Dima's Lecture 2 slides

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

Eigenvalue and Eigenvector Example

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

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

Not an eigenvector

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

Eigenvalue and eigenvector

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

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

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 web page for Python code

Principal Component Analysis

Consider a data set of N p-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 any 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

- $\mathbf{u}$ is the eigenvector of the data corresponding to the (largest) eigenvalue λ.
- We can represent the data using a combination of other significant eigenvectors in higher dimensions, i.e. from a 1D projection to a d-dimensional projection:

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

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

Recipe for PCA

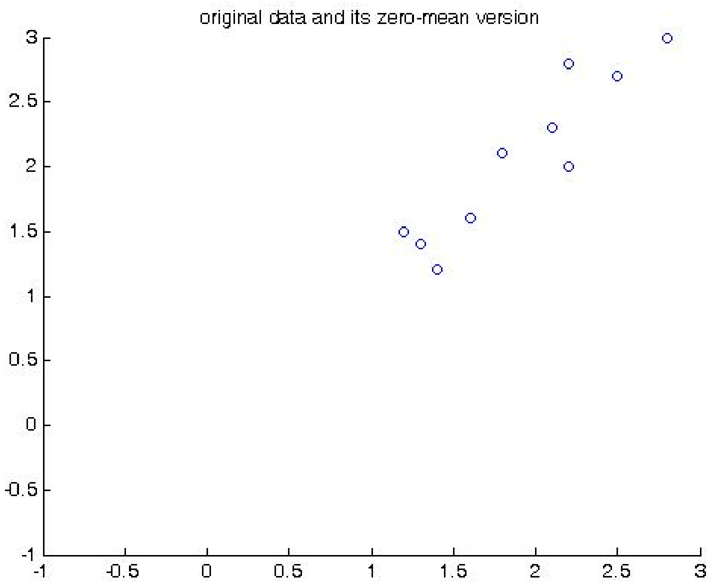
1 - Adjust the data to zero-mean

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

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!)

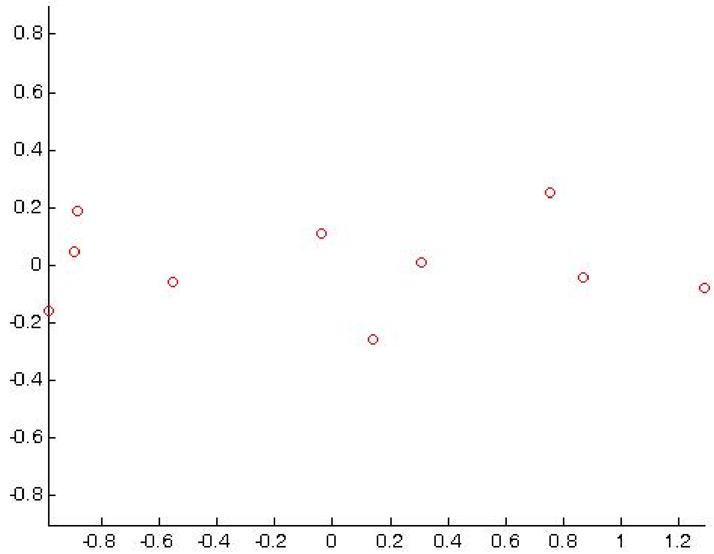
$$\text{Reordered} \quad \boldsymbol{\lambda} = \begin{pmatrix} 0.6640 \\ 0.0242 \end{pmatrix}$$

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

Recipe for PCA

5 – Generate the new representation of the data

$$\begin{array}{rr} 1.2921 & -0.0793 \\ 0.1401 & -0.2609 \\ 0.7536 & 0.2525 \\ -0.5517 & -0.0575 \\ 0.8695 & -0.0417 \\ -0.9868 & -0.1608 \\ -0.0399 & 0.1100 \\ -0.8851 & 0.1851 \\ 0.3060 & 0.0083 \\ -0.8976 & 0.0442 \end{array}$$



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

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

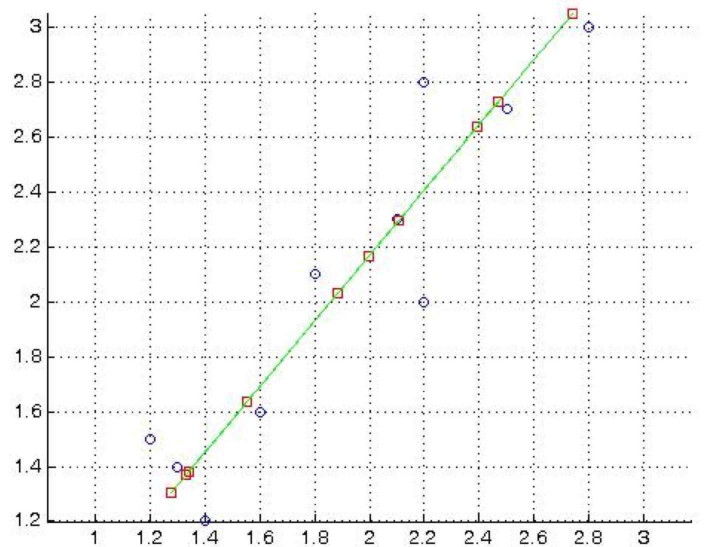
Both principal components to get lossless data back.

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

Add mean

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

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



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

Principal Component Analysis

- 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.

- Then the first d eigenvalues can be said to account for this fraction of the total variance in data:

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

Example: the OxIS Report

- The OxIS 2013 report asked around 2000 people a set of questions about their *Internet use*. Let's say they asked each person 50 questions.
- There are therefore **50 variables, making it a 50-dimensional data set**. There will then be 50 eigenvectors and eigenvalues that will come out of that data set.
- Let's say the eigenvalues of that data set were (in descending order): 40, 19, 17, 10, 3.2, 1, 0.4, 0.2,0.098,….. With a total sum of

$$\sum_{i=1}^{50} \lambda_i = 98.5$$

- There are lots of eigenvalues, but **there are only 5 which have big enough values – indicating there is a lot of info (variance) along those five directions!**
- These are then identified as the five principal components of the data set (which in the report were labelled as enjoyable escape, instrumental efficiency, social facilitator etc)
- The data set 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.

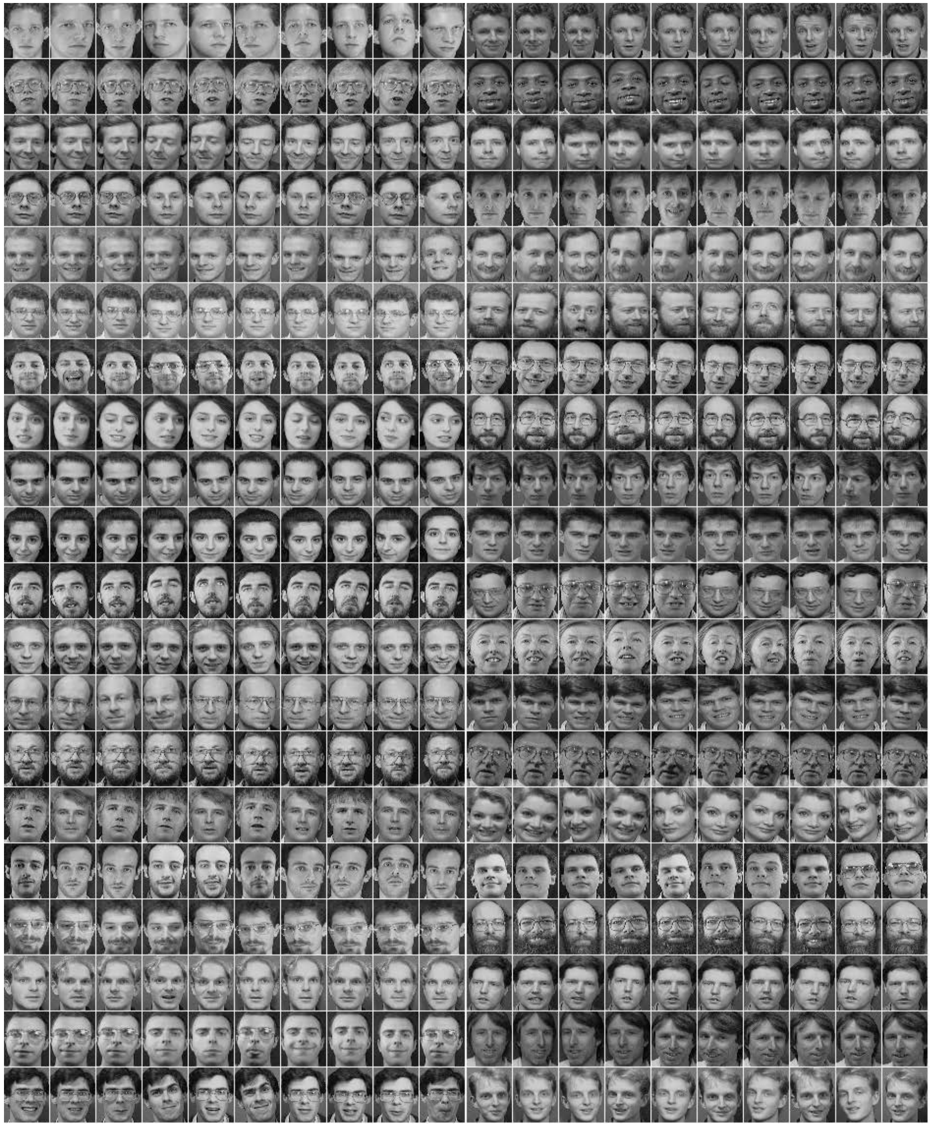
- Percentage of variance captured by the first 5 components:

$$\frac{89.2}{98.5} \Rightarrow \sim 91\%$$

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

Example Application: Face Recognition using PCA

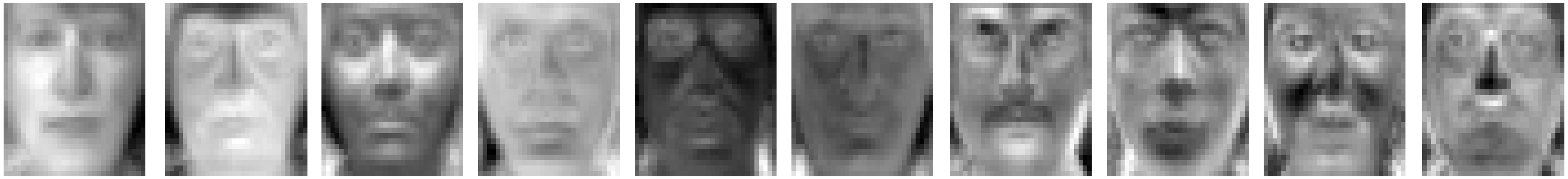
Set of normalized face images



Eigenfaces

Training:

- Acquire initial set of face images (training set) → **S**
- Compute the average image (**m**) and adjust data set → **S – m**
- The image pixels are the feature vectors.
- Compute the covariance of the image set → **C**
- Compute the eigenvectors and eigenvalues of this covariance matrix → *eigenfaces*



Eigenfaces

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

Testing:

- Project new input image into face space
- Find most likely candidate by distance computation between the feature vectors

PCA characteristics: a summary

PCA: 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.
- Reduced and uncorrelated feature set makes the process of clustering and classification *much easier.*

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

A little exercise…

- Matrix K is a covariance matrix of some 3D data:

$$K = \begin{pmatrix} 5 & 2 & 4 \\ -3 & 6 & 2 \\ 3 & -3 & 1 \end{pmatrix}$$

Prove the following is an eigenvalue and eigenvector set for K:

$$\lambda = 3 \qquad e = \begin{pmatrix} 0.37 \\ 0.74 \\ -0.56 \end{pmatrix}$$

A little exercise…

- Matrix K is a covariance matrix of some 3D data:

$$K = \begin{pmatrix} 5 & 2 & 4 \\ -3 & 6 & 2 \\ 3 & -3 & 1 \end{pmatrix}$$

Prove the following is an eigenvalue and eigenvector set for K:

$$\lambda = 3 \qquad e = \begin{pmatrix} 0.37 \\ 0.74 \\ -0.56 \end{pmatrix}$$

Answer: **show that** $Ke = \lambda e$