

## **Q5**, **Quiz 1**

- The last option is also correct
- Everyone get 1 free mark capped to 6/6

```
ID INT PRIMARY KEY,
FIRST_NAME CHAR(100),
LAST_NAME CHAR(100),
PHONE_NUMBER CHAR(32),
ADRESS CHAR(100),
POST_CODE INT,
);
```

• **nullable**¶ – When set to False, will cause the "NOT NULL" phrase to be added when generating DDL for the column. When True, will normally generate nothing (in SQL this defaults to "NULL"), except in some very specific backend-specific edge cases where "NULL" may render explicitly. Defaults to True unless primary\_key is also True, in which case it defaults to False. This parameter is only used when issuing CREATE TABLE statements.



# Data Visualization(2)

COMP9321 2019T1

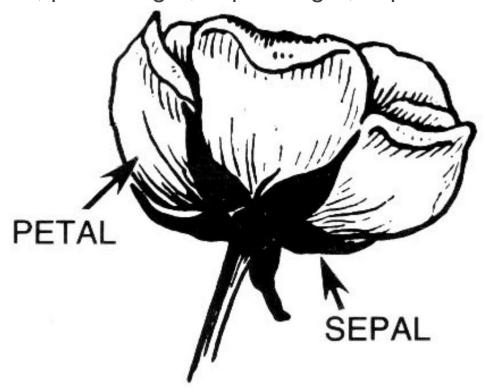


### **Iris Dataset**

The measurements in centimeters of the variables sepal length and width and petal length and width, respectively, for 50 flowers from each

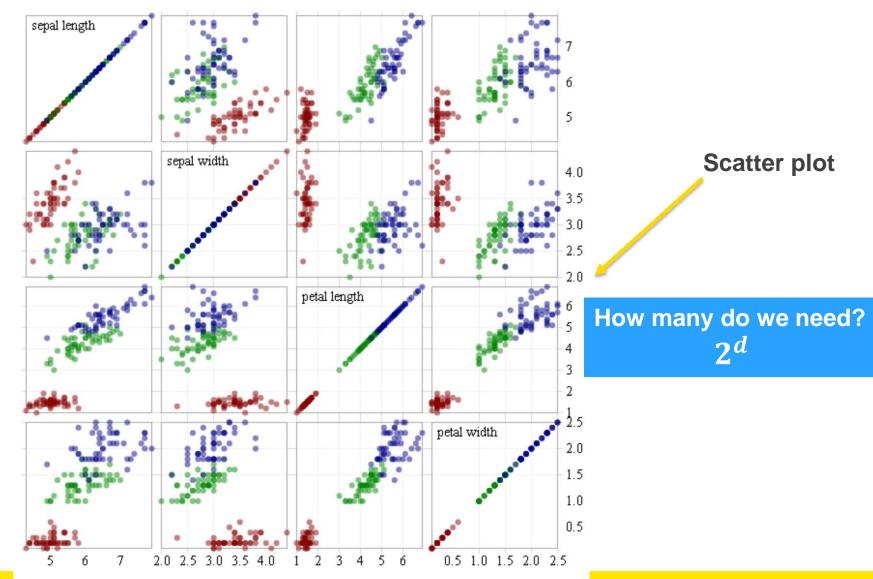
of 3 species of iris  $\rightarrow n = 150$ 

**d** = 4 (petal width, petal length, sepal length, sepal width)



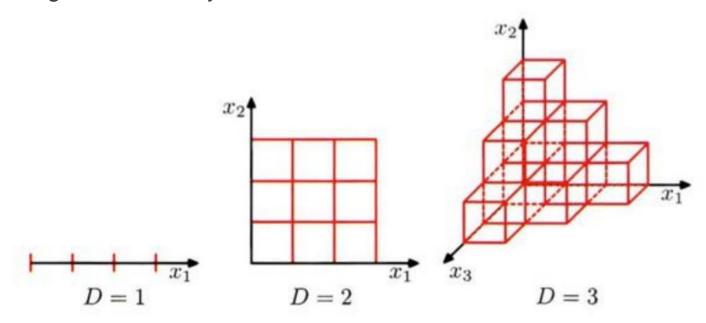


### **How to Visualization?**



## **High Dimensional Data**

- What if the dimensionality increases to hundreds or thousands?
- Curse of dimensionality:
- When dimensionality increases, the volume of the space increases so fast that the available data become sparse.
- Statistically sound results requires the sample size to grow exponentially with increasing dimensionality.



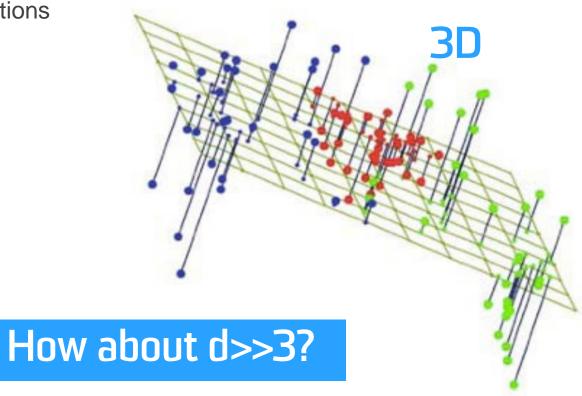


## **Dimensionality Reduction**

Project high-dimensional data to lower-dimensional subspace

Linear projections

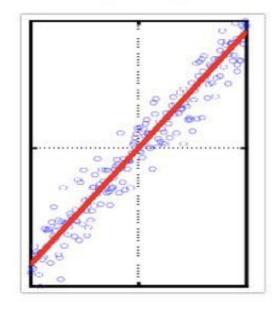
Non-linear projections





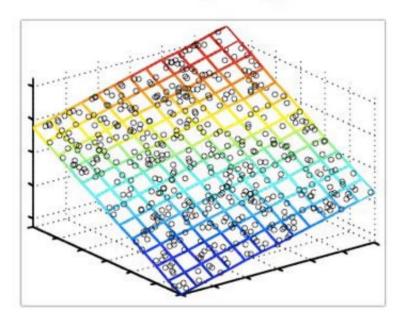
## **Dimensionality Reduction**

- Does the data lie in / close to a hyperplane?
- What is the dimensionality of the hyperplane?



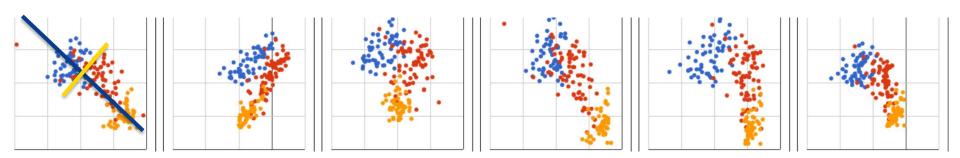
$$D=3$$

$$d=2$$



## Visualization using linear projections

- Consider a linear projection from a high-dimensional attribute space into a 2D (or 3D) visual space.
- Try to find an optimal projection with respect to some metric.
- They give the best 2D (or 3D) view on the data.
- It is a slice through the high-dimensional space. The visual encoding is that of a scatterplot.





### **PCA**

- Machine learning
- Dimension reduction pre-step
- Visualization
- Objects represented by many descriptors
- PCA helps to find structure among objects which could not be visualized otherwise (e.g., patients or car accidents)
- Compression
- Representation of object only by their coordinates in the respective subspace
   E.g. in the eigenfaces (see later), each faces can be reasonable approximated by 10 coordinates



#### **Dimensionality Reduction**

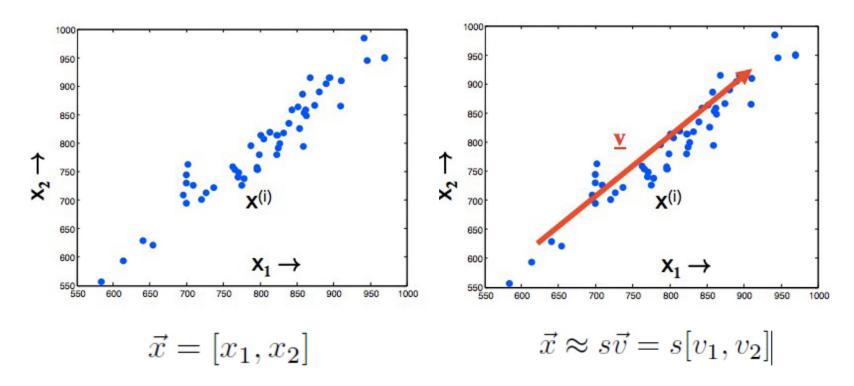
#### Idea:

- Given data points in d-dimensional space,
- Project into lower dimensional space while preserving as much information as possible
  - -E.g., find best planar approximation to 3D data
  - -E.g., find best planar approximation to 104D data
- In particular, choose projection that minimizes the squared error in reconstructing original data



### **Principal Component Analysis**

- PCA tries to find the most relevant directions (principal components) in the data.
- For projection to 2D, the first two principal components span the projection space



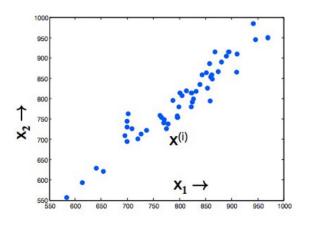


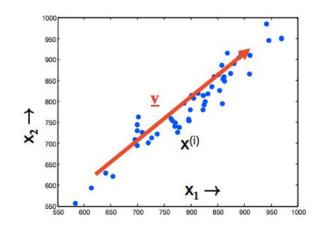
### **PCA**

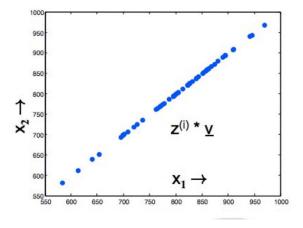
1. V is chosen to minimize residual variance

$$\min_{a,v} \sum_{i} (x^{(i)} - a^{(i)}v)^2$$

- 2. Find v that most closely reconstructs x.
- 3. Equivalent to v being the direction of maximum variance

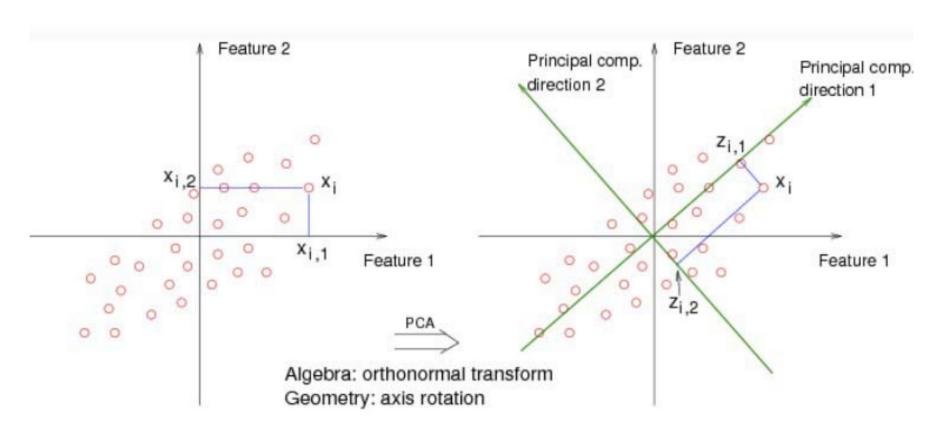






#### **PCA**

Project data to subspace such as to maximize the variance of projected data





### **PCA Process**

Input: Data X of sample size N.

Output: k principal components

Centering: Subtract mean from data

Scaling: Scale each dimension by its variance

Compute covariance matrix by

$$S = \frac{1}{N} X^{\mathrm{T}} X$$

Compute *k* largest eigenvectors of *S* 



#### **Basics of Linear Algerbra**

Variance measures the spread of data in a dataset from the mean

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

 Covariance measures how each of the dimensions varies from the mean with respect to each other

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



#### **Basics of Linear Algerbra**

- Positive covariance of two dimensions indicates that they change together (number of hours spent studying – grade)
- Negative covariance indicates that change in one dimension causes inverse change in the other (number of hours spent in a pub – balance of your bank account)
- Covariance matrix is a matrix of all pairwise covariences, e.g. for 3 dimensions X, Y, Z:

$$\begin{pmatrix}
cov(X,X) & cov(X,Y) & cov(X,Z) \\
cov(Y,X) & cov(Y,Y) & cov(Y,Z) \\
cov(Z,X) & cov(Z,Y) & cov(Z,Z)
\end{pmatrix}$$

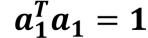


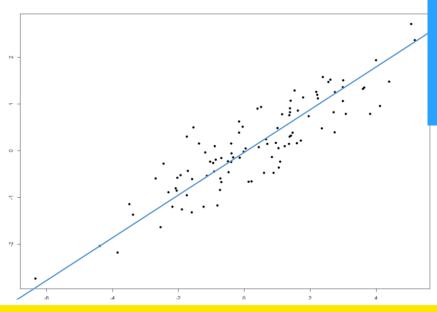
Let us have a random variable (observations)  $x^T = (x_1, ..., x_p)$  with mean  $\mu$  and covariance matrix  $\Sigma$ 

First PC is the linear combination

$$y_1 = a_1^T x = \sum_{i=1}^r a_{1i} x_i$$

where a1 is chosen such that var(y1) is maximum subject to



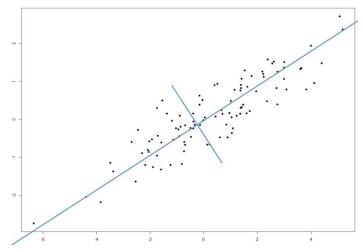


If we project the data onto this line, we lose as little information as possible = we keep as much variance as possible.



Second PC is the linear combination

$$y_2 = a_2^T x = \sum_{i=1}^p a_{2i} x_i$$



where a2 is chosen such that var(y2) is maximum subject to

$$a_2^T a_2 = \mathbf{1}$$
 and  $a_2^T a_1 = \mathbf{0} = cov(a_k, a_l)$ 



Searching for the first PC

Assumption that the data are normalized, i.e., the mean is subtracted

Find 1D subspace so that the observations have maximum spread in it

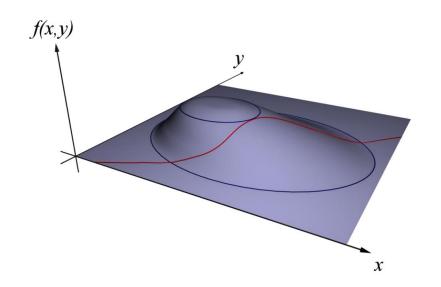
→ maximizing variance

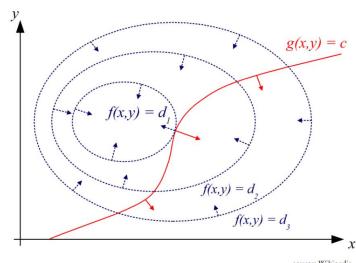
$$var(y_1) = var(a_1^T X) = E[(a_1^T X - E[a_1^T X])(a_1^T X - E[a_1^T X])^T]$$
  
=  $E[(a_1^T X)(a_1^T X)^T] = E[a_1^T X X^T a_1] = E[a_1^T \Sigma a_1] = a_1^T \Sigma a_1$ 

The goal is to maximize variance given  $a_1^T a_1 = 1$  Lagrange multipliers



### Lagrange multipliers





source: Wikipedia

13

Maximize f(x, y) subject to  $g(x, y) = c \rightarrow \text{introduction of a new variable}$ 

Lagrange multiplier 
$$\lambda$$
 ( $\nabla f = \lambda \nabla g \rightarrow \nabla f - \lambda \nabla g = 0$ )
$$\Lambda(x, y, \lambda) = f(x, y) + \lambda(g(x, y) - c) \rightarrow \frac{\Delta \Lambda(x, y, \lambda)}{\Delta x, y, \lambda} = 0$$



Transcription into the Lagrangian form

$$\Lambda(a_1,\lambda) = a_1^T \Sigma a_1 - \lambda(a_1^T a_1 - 1)$$

Now we need to differentiate the Lagrangian

$$\frac{\partial \Lambda(a_1, \lambda)}{\partial a_1} = \frac{\partial \Lambda(a_1)}{\partial \begin{bmatrix} a_{11} \\ \dots \\ a_{1k} \end{bmatrix}} = 2\Sigma a_1 - 2\lambda a_1 = 0$$

• This leads to the eigenproblem  $\Sigma a_1 = \lambda a_1 o a_1$  is an eigenvector of  $\lambda$ 

$$var(y_1) = var(a_1^T X) = a_1^T \Sigma a_1 = \lambda a_1^T a_1 = \lambda$$

$$\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_p \rightarrow \text{to maximize } var(y_1)$$

$$\lambda = \lambda_1$$



Searching for the next PCs

$$\Lambda(a_{2}) = a_{2}^{T} \Sigma a_{2} - \lambda(a_{2}^{T} a_{2} - 1) - \kappa(a_{2}^{T} a_{1})$$

$$\Sigma a_{2} - \lambda a_{2} - \kappa a_{1} = 0$$

$$a_{1}^{T} \Sigma a_{2} - \lambda a_{1}^{T} a_{2} - \kappa a_{1}^{T} a_{1} = 0$$

$$0 - 0 - \kappa = 0$$

$$a_{1}^{T} \Sigma a_{2} = a_{2}^{T} (\Sigma a_{1}) = \lambda_{1} a_{2}^{T} a_{1}$$

$$\Sigma a_{2} - \lambda a_{2} = 0$$

$$\Sigma a_{2} = \lambda a_{2} \Rightarrow \lambda = \lambda_{2}$$

Thus the coefficients of the linear combination which transform the observations onto the PCs are formed by eigenvalues of the covariance matrix

Let A contain the eigenvalues ai as its columns and let x be a p- dimensional vector, then

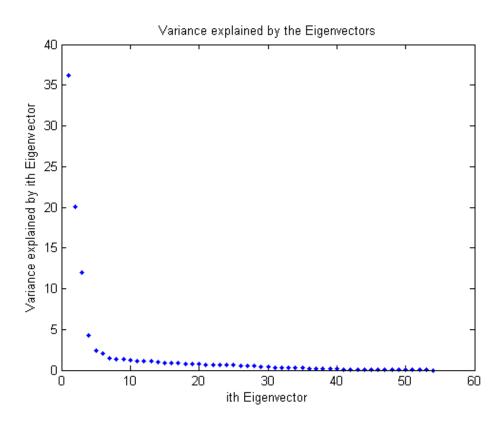
$$y = A^T(x - \mu)$$



### How many components do I need?

Check the distribution of eigen-values

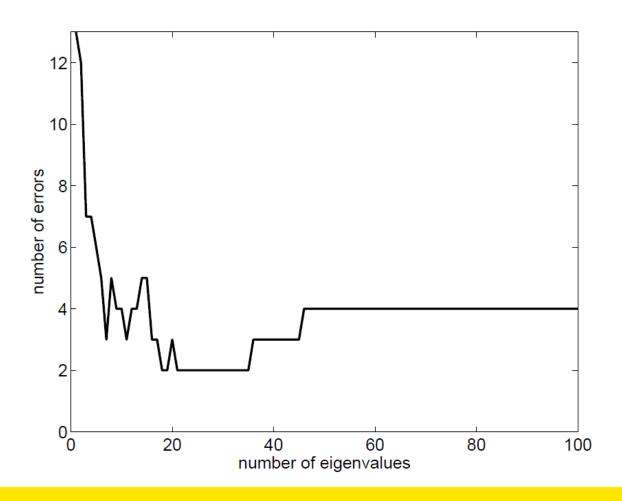
Take enough many eigen-vectors to cover 80-90% of the variance





### How many components do I need?

Check the validation errors





# **A 2D Numerical Example**



### Subtract the mean

from each of the data dimensions. All the x values have x subtracted and y values have y subtracted from them. This produces a data set whose mean is zero.

Subtracting the mean makes variance and covariance calculation easier by simplifying their equations. The variance and co-variance values are not affected by the mean value.



http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

	Λ	Т	Δ.		
$\boldsymbol{\mathcal{L}}$	$\Box$	\ I	$\overline{}$	l.	=

<b>—</b> , , , , , ,			
X	У		
2.5	2.4		
0.5	0.7		
2.2	2.9		
1.9	2.2		
3.1	3.0		
2.3	2.7		
2	1.6		
1	1.1		
1.5	1.6		
1.1	0.9		

#### **ZERO MEAN DATA:**

Χ	У
.69	.49
-1.31	-1.21
.39	.99
.09	.29
1.29	1.09
.49	.79
.19	31
81	81
31	31
71	-1.01



http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

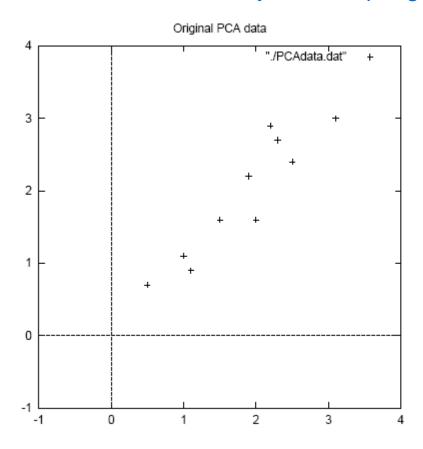


Figure 3.1: PCA example data, original data on the left, data with the means subtracted on the right, and a plot of the data



### Calculate the covariance matrix

```
cov = (.616555556 .61544444
.615444444 .716555556
```

since the non-diagonal elements in this covariance matrix are positive, we should expect that both the x and y variable increase together.



Calculate the eigenvectors and eigenvalues of the covariance matrix



http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

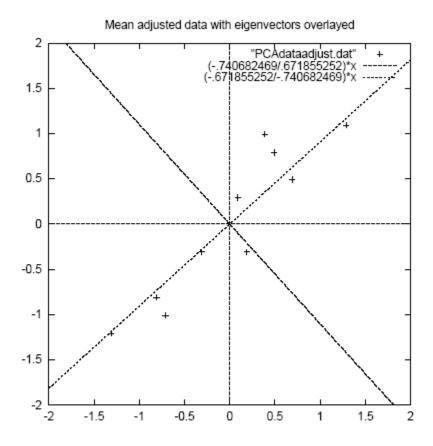


Figure 3.2: A plot of the normalised data (mean subtracted) with the eigenvectors of Side of the main line by some the covariance matrix overlayed on top.

- •eigenvectors are plotted as diagonal dotted lines on the plot.
- •Note they are perpendicular to each other.
- •Note one of the eigenvectors goes through the middle of the points, like drawing a line of best fit.
- •The second eigenvector gives us the other, less important, pattern in the data, that all the points follow the main line, but are off to the side of the main line by some amount.



Now, if you like, you can decide to *ignore* the components of lesser significance.

You do lose some information, but if the eigenvalues are small, you don't lose much

n dimensions in your data calculate n eigenvectors and eigenvalues choose only the first p eigenvectors final data set has only p dimensions.



### Feature Vector

FeatureVector =  $(eig_1 eig_2 eig_3 ... eig_n)$ 

We can either form a feature vector with both of the eigenvectors:

- -.677873399
   -.735178656

   -.735178656
   .677873399

or, we can choose to leave out the smaller, less significant component and only have a single column:

- .677873399 .735178656



# PCA Example –STEP 5

### Deriving the new data

FinalData = RowFeatureVector x RowZeroMeanData

RowFeatureVector is the matrix with the eigenvectors in the columns *transposed* so that the eigenvectors are now in the rows, with the most significant eigenvector at the top

RowZeroMeanData is the mean-adjusted data *transposed*, ie. the data items are in each column, with each row holding a separate dimension.



# PCA Example –STEP 5

FinalData transpose: dimensions along columns

X	У
827970186	175115307



# PCA Example –STEP 5

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

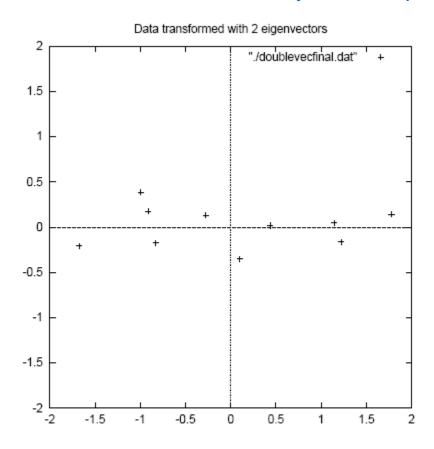


Figure 3.3: The table of data by applying the PCA analysis using both eigenvectors, and a plot of the new data points.



# Reconstruction of original Data

If we reduced the dimensionality, obviously, when reconstructing the data we would lose those dimensions we chose to discard. In our example let us assume that we considered only the x dimension...



# Reconstruction of original Data

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

X



1.77758033

-.992197494

-.274210416

-1.67580142

-.912949103

.0991094375

1.14457216

.438046137

1.22382056

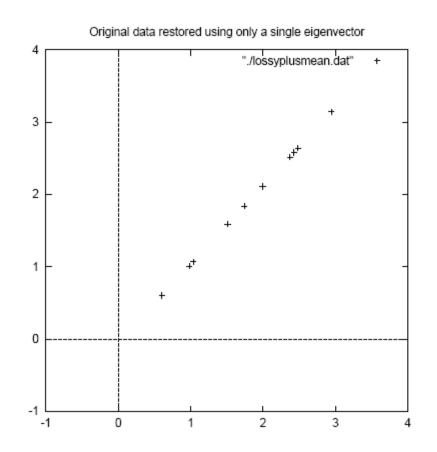


Figure 3.5: The reconstruction from the data that was derived using only a single eigenvector



#### What Can PCA Do?

#### Visualization

- Objects represented by many descriptors
- PCA helps to find structure among objects which could not be visualized otherwise (e.g., patients or car accidents)

### Compression

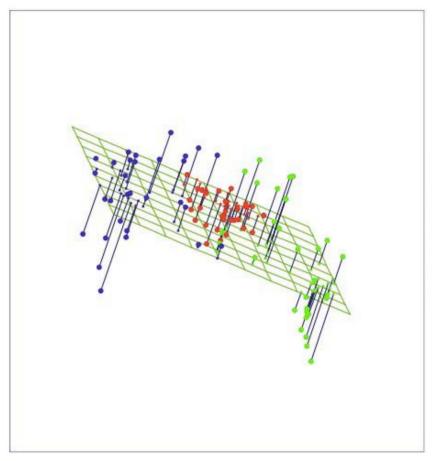
- Representation of object only by their coordinates in the respective subspace
- E.g. in the eigenfaces (see later), each faces can be reasonable approximated by 10 coordinates

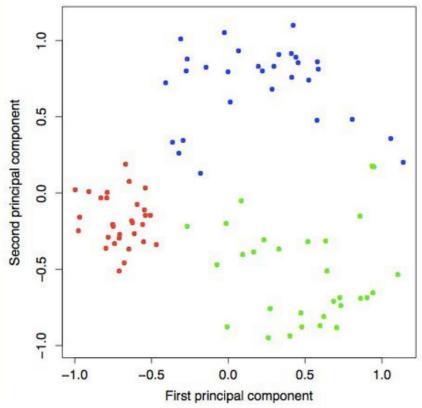
### Machine learning

Dimension reduction pre-step

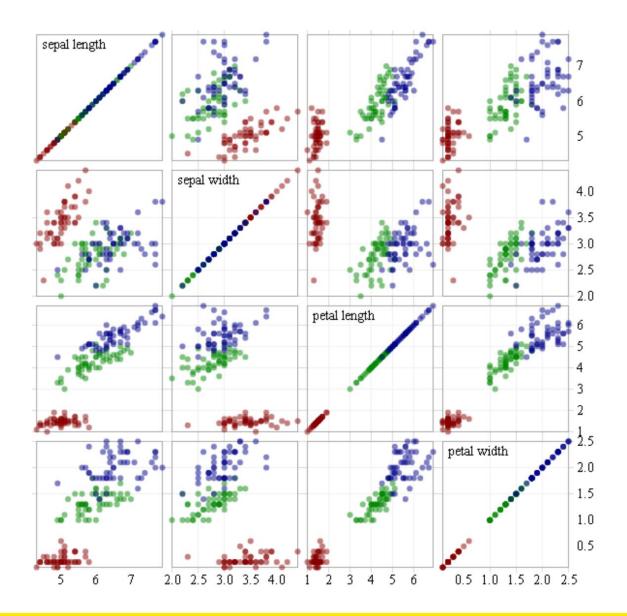


#### What Can PCA Do?



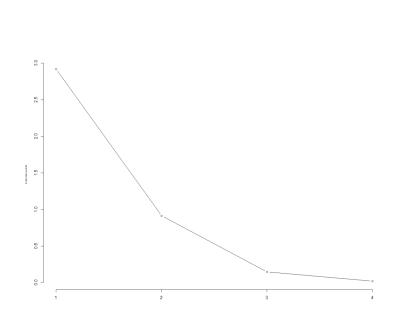


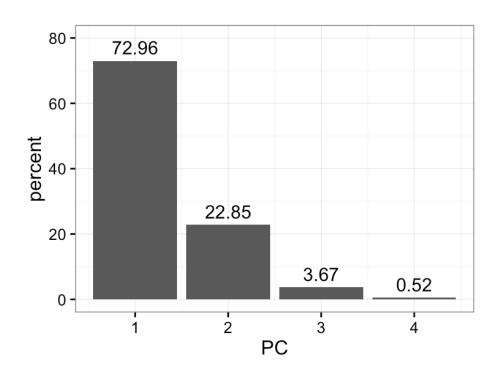




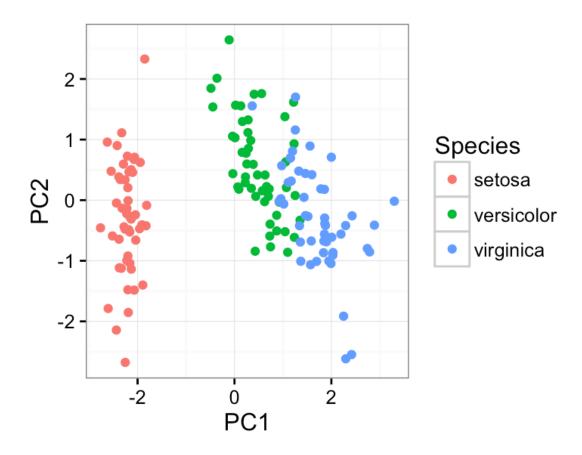


- Display of variance of each of the component
- Plot of magnitudes of eigenvalues
- Gives impression of the intrinsic dimensionality



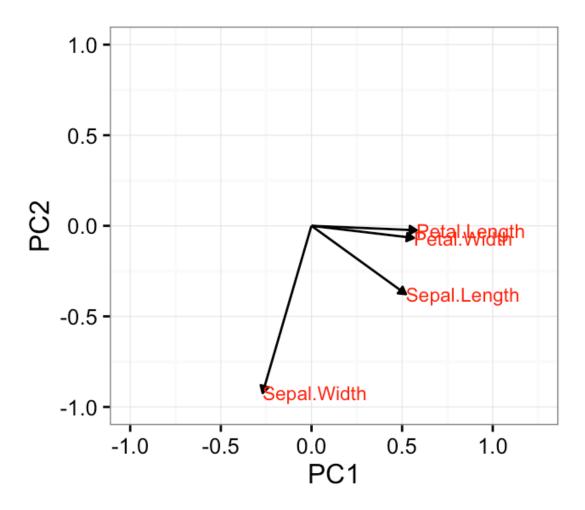






In the PC2 vs PC1 plot, versicolor and virginica are much better separated.

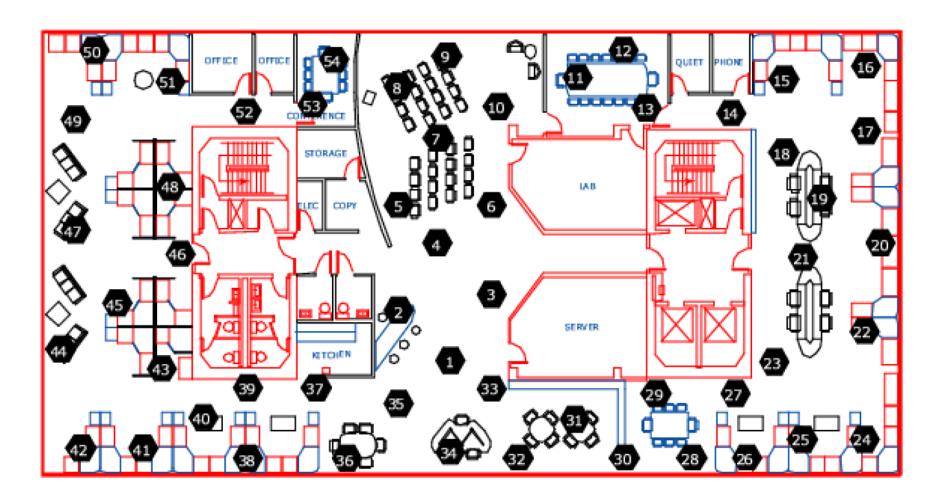




Rotation matrix

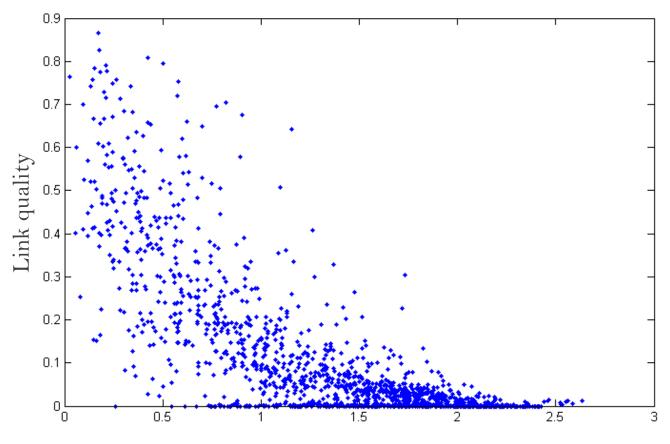


### What Does PCA Do? - Magic Time





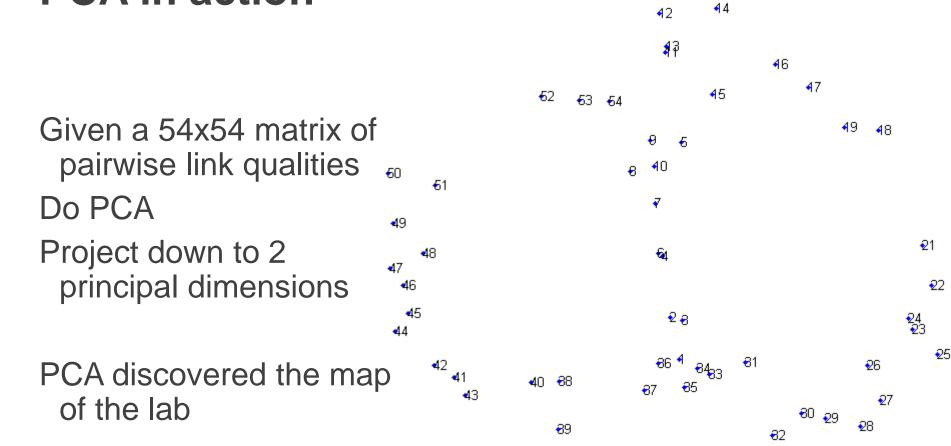
#### Pairwise link quality vs. distance



Distance between a pair of sensors



### **PCA** in action





#### **Problems and limitations**

What if very large dimensional data?

• e.g., Images (d ≥ 10<sup>4</sup>)

#### Problem:

- Covariance matrix  $\Sigma$  is size (d<sup>2</sup>). The computational complexity is O(d<sup>3</sup>)!
- $d=10^4 \rightarrow |\Sigma| = 10^4 \times 10^4 = 10^8$  !!!

May bound to Min O(D, N)<sup>3</sup>

### Singular Value Decomposition (SVD)!

- efficient algorithms available (Matlab)
- some implementations find just top N eigenvectors



# **SVD**

Singular Value Decomposition



## Singular Value Decomposition

#### Problem:

• #1: Find concepts in text

• #2: Reduce dimensionality

term	data	information	retrieval	brain	lung
document					
CS-TR1	1	1	1	0	0
CS-TR2	2	2	2	0	0
CS-TR3	1	1	1	0	0
CS-TR4	5	5	5	0	0
MED-TR1	0	0	0	2	2
${f MED-TR2}$	0	0	0	3	3
MED-TR3	0	0	0	1	1



### **SVD** - Definition

$$\mathbf{A}_{[n \times m]} = \mathbf{U}_{[n \times r]} \Lambda_{[r \times r]} (\mathbf{V}_{[m \times r]})^{\mathsf{T}}$$

**A**: *n* x *m* matrix (e.g., n documents, m terms)

**U**: *n x r* matrix (n documents, r concepts)

Λ: *r* x *r* diagonal matrix (strength of each 'concept') (r: rank of the matrix)

V: m x r matrix (m terms, r concepts)



### **SVD - Properties**

**THEOREM** [Press+92]: always possible to decompose matrix **A** into  $\mathbf{A} = \mathbf{U} \Lambda \mathbf{V}^{\mathsf{T}}$ , where

**U**, Λ, **V**: unique (\*)

**U**, **V**: column orthonormal (ie., columns are unit vectors, orthogonal to each other)

•  $U^TU = I$ ;  $V^TV = I$  (I: identity matrix)

**Λ:** singular value are positive, and sorted in decreasing order



## **SVD - Properties**

'spectral decomposition' of the matrix:



## **SVD** - Interpretation

'documents', 'terms' and 'concepts':

U: document-to-concept similarity matrix

V: term-to-concept similarity matrix

Λ: its diagonal elements: 'strength' of each concept

### Projection:

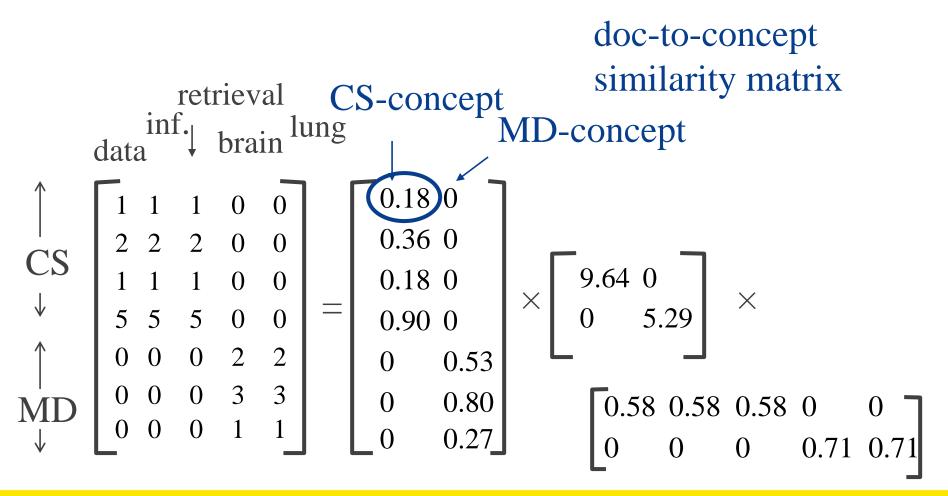
best axis to project on: ('best' = min sum of squares of projection errors)



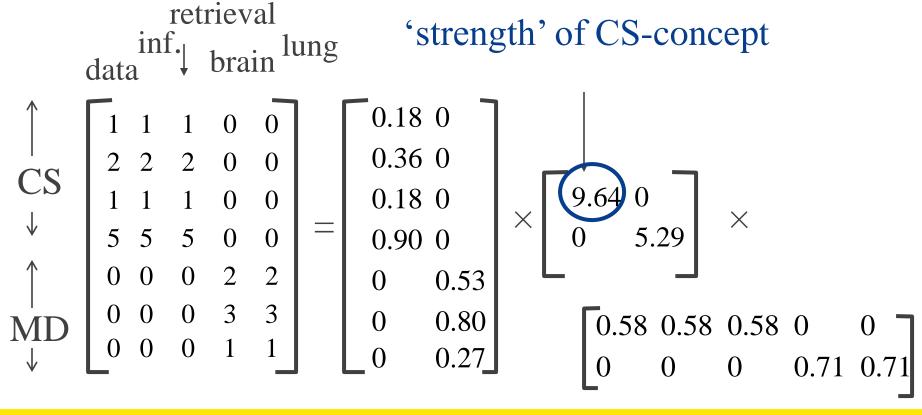
retrieval 
$$\inf$$
.  $\downarrow$  brain lung

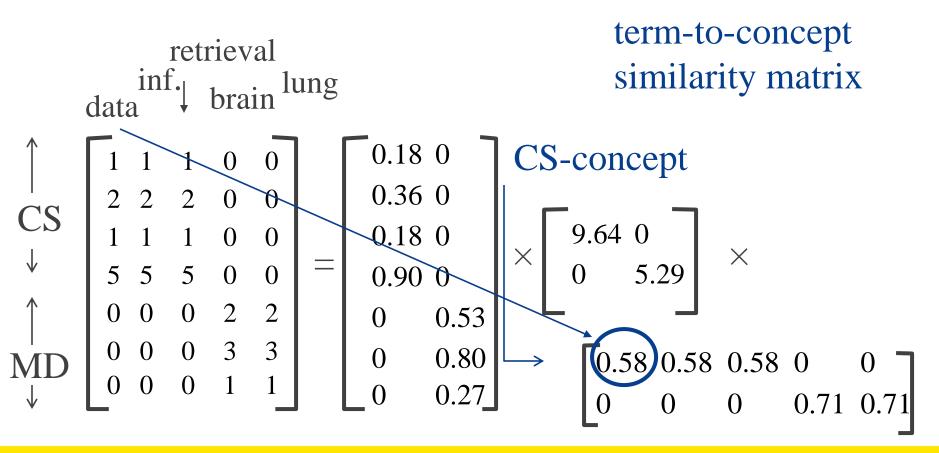
$$\uparrow \quad \begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
2 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 0 & 0 & 2 & 2 \\
0 & 0 & 0 & 3 & 3 \\
0 & 0 & 0 & 1 & 1
\end{bmatrix} = \begin{bmatrix}
0.18 & 0 \\
0.36 & 0 \\
0.18 & 0 \\
0.90 & 0 \\
0 & 0.53 \\
0 & 0.80 \\
0 & 0.27
\end{bmatrix} \times \begin{bmatrix}
9.64 & 0 \\
0 & 5.29
\end{bmatrix} \times \begin{bmatrix}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0.71 & 0.71
\end{bmatrix}$$











## **SVD** – Dimensionality reduction

Q: how exactly is dim. reduction done?

A: set the smallest singular values to zero:

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.21 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \\ 0 & 5.29 \\ \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \\ \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

### **SVD - Dimensionality reduction**

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} 0.18 \\ 0.36 \\ 0.18 \\ 0.90 \\ 0 \\ 0 \end{bmatrix} \times \begin{bmatrix} 9.64 \\ \end{bmatrix} \times \begin{bmatrix} 9.64 \\ \end{bmatrix}$$



### **SVD - Dimensionality reduction**

 $\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \sim$ 

