GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 16: DIMENSION REDUCTION

DATA EXPLORATION

SUPERVISED LEARNING: REGRESSION

SUPERVISED LEARNING: CLASSIFICATION

UNSUPERVISED LEARNING

- CLUSTERING
- DIMENSION REDUCTION (TODAY)

VARIOUS TOPICS

0. PRESENTATIONS DATA EXPLORATION FOR FINAL PROJECT

I. DIMENSIONALITY REDUCTION

II. SINGULAR VALUE DECOMPOSITION (SVD)

III. PRINCIPAL COMPONENT ANALYSIS (PCA)

IV. NOTEBOOK EXAMPLES & EXERCISES

- EXPLAIN PITFALLS OF WORKING IN HIGH DIMENSIONS
- DESCRIBE EXAMPLES OF USEFUL APPLICATIONS OF DIM. RED.
- BE ABLE TO APPLY SVD AND PCA IN PYTHON, AND TO DRAW INFERENCES OF LOWER-DIMENSIONAL STRUCTURES

I. DIMENSIONALITY REDUCTION

Q: What is dimensionality reduction?

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Dimensionality reduction is frequently performed as a pre-processing step before another learning algorithm is applied.

Q: What are the motivations for dimensionality reduction?

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The number of features in our dataset can be difficult to manage, or even misleading (eg, if the relationships are actually simpler than they appear).

We'd like to represent a user's taste profile by a select number of dimensions, rather than their rating of each and every movie

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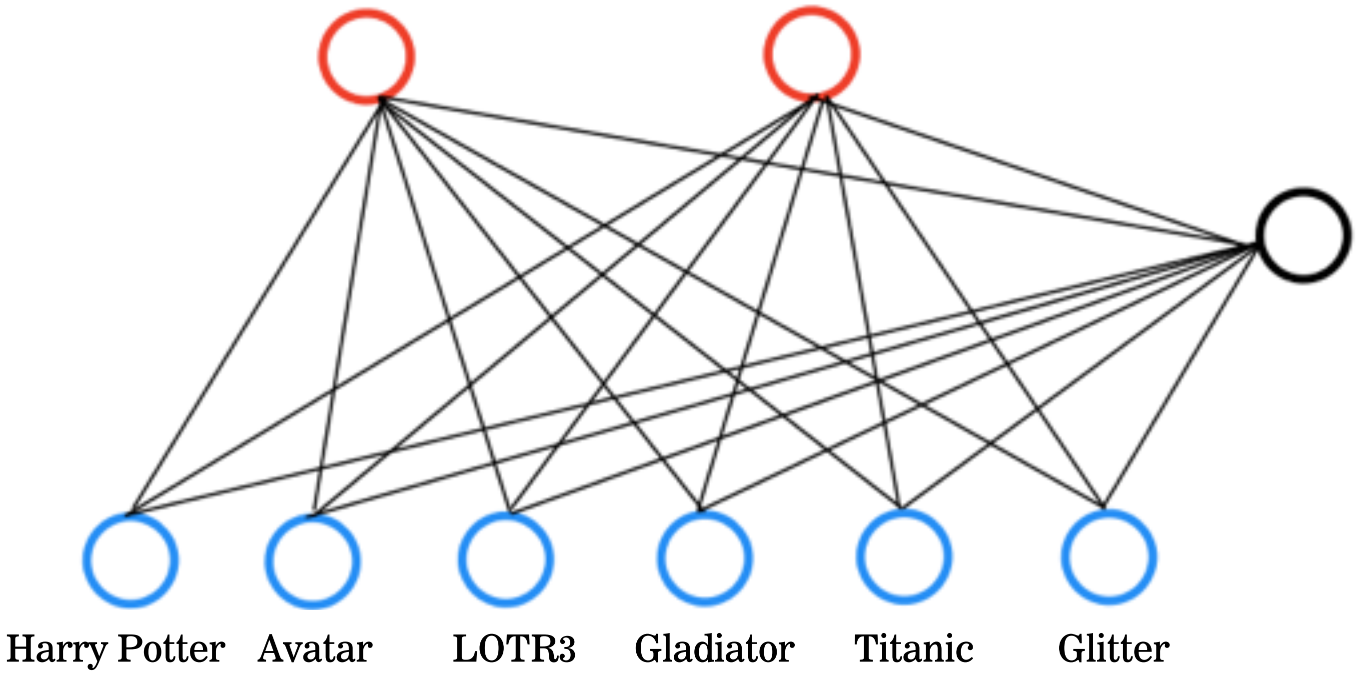
Harry Potter Avatar LOTR3 Gladiator Titanic Glitter


Harry Potter
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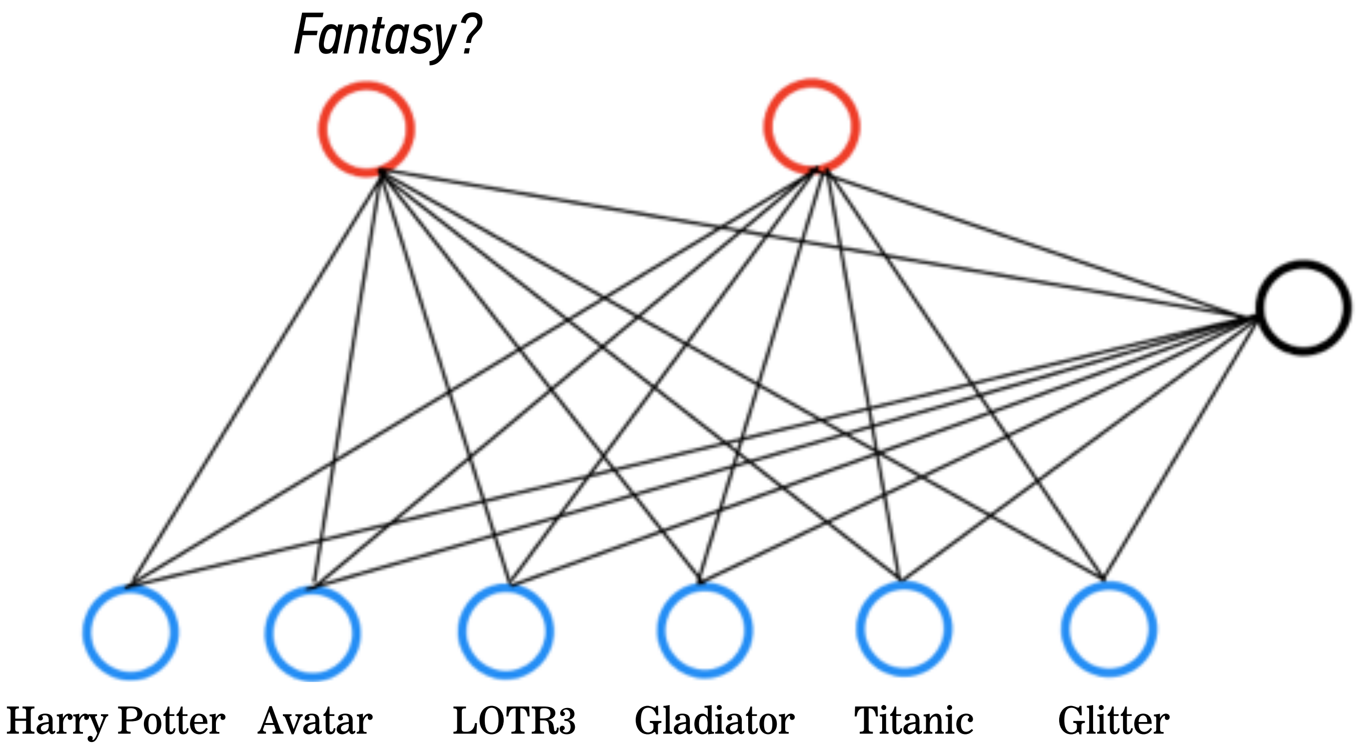
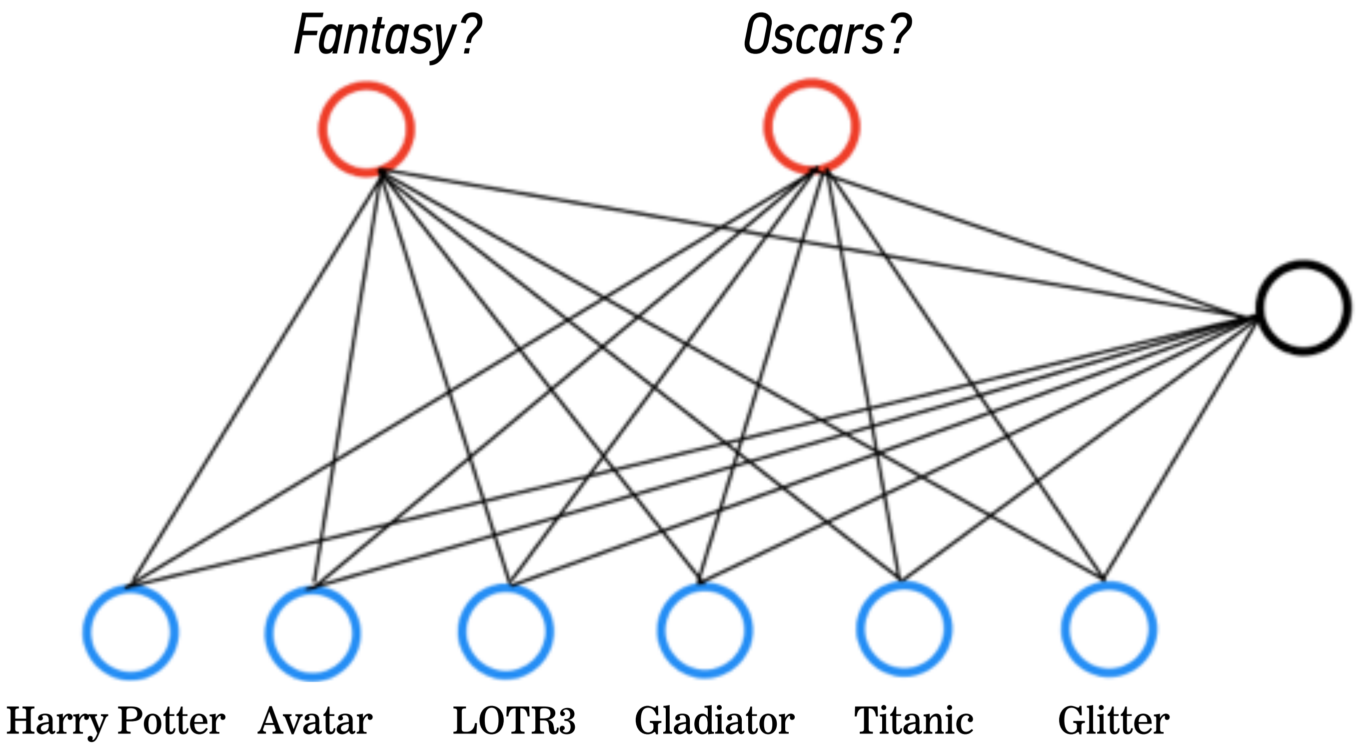
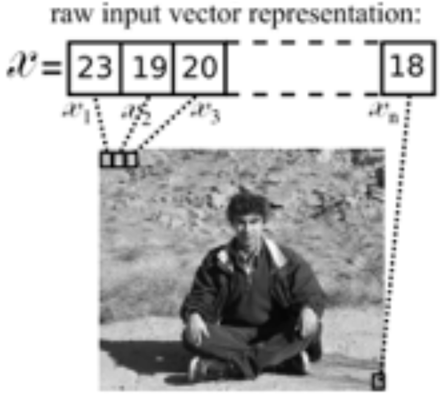

Fantasy?
Harry Potter
Avatar
LOTR3
Gladiator
Titanic
Glitter

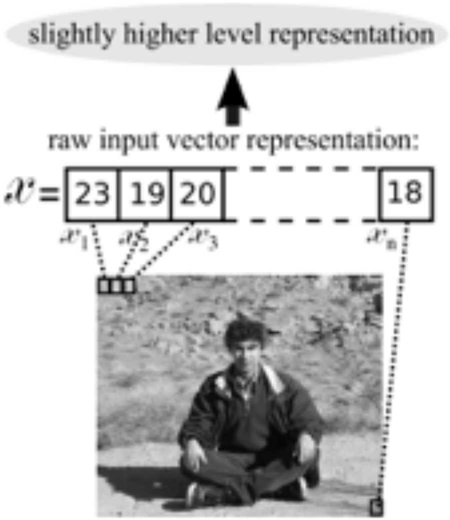
DIMENSIONALITY REDUCTION – EXAMPLE

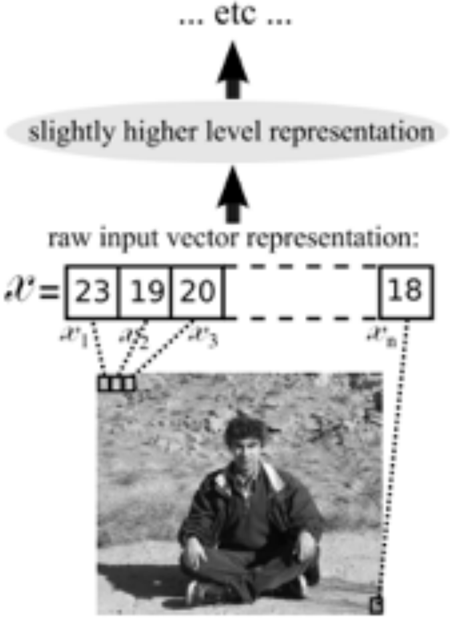




raw input vector representation:
x =
23
19
20
18
x1
x2
x3
xn

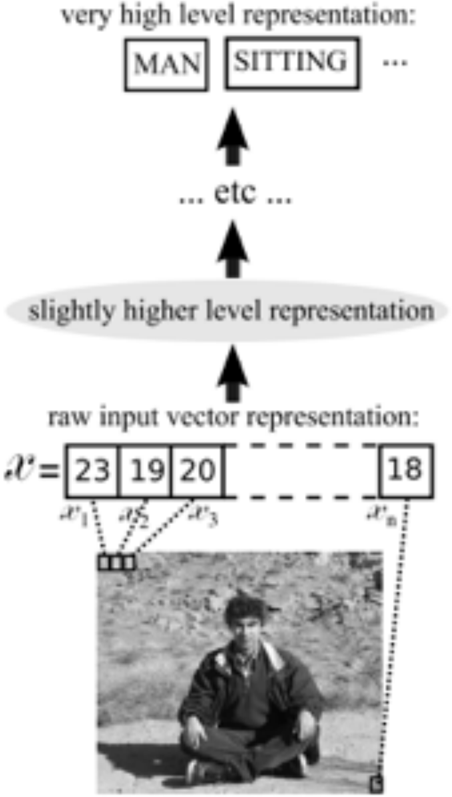
DIMENSIONALITY REDUCTION – EXAMPLE





... etc ...
slightly higher level representation
raw input vector representation:
x = 23 19 20 18
x1 x2 x3 xn

DIMENSIONALITY REDUCTION – EXAMPLE



Q: What is the goal of dimensionality reduction?

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- *reduce computational expense*
- *reduce susceptibility to overfitting*
- *reduce noise in the dataset*
- *enhance our intuition*

The goal of feature extraction is to create a new set of coordinates that simplify the representation of the data.

Q: What are some applications of dimensionality reduction?

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- *document clustering*
- *image recognition/computer vision*
- *recommender systems*

II. SINGULAR VALUE DECOMPOSITION (SVD)

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st. U, V are **orthogonal** *matrices and Σ is a* **diagonal** *matrix.*

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NOTE

Look in the notebook about SVD to dive into the mathematics behind this

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Because the singular values are ranked-ordered,
we could **truncate** *the diagonal matrix* Σ *to some dimension k,*
preserving most of the information in A.

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(N x n) ~~(N x N) (N x n) (n x n)~~

(N x d) (d x d) (d x n)

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$$\underset{(N \times n)}{A} \approx \underset{\substack{\cancel{(N \times N)} \\ (N \times d)}}{U} \; \underset{\substack{\cancel{(N \times n)} \\ (d \times d)}}{\Sigma} \; \underset{\substack{\cancel{(n \times n)} \\ (d \times n)}}{V^T}$$

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With this step, we **reduce the dimensionality** *from n to d.*

SINGULAR VALUE DECOMPOSITION

$$
\begin{array}{c}
\\
\text{CS} \\
\\
\\
\\
\text{MD} \\
\\
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{array} \\
\left[\begin{array}{ccccc}
1 & 1 & 1 & 0 & 0 \\
2 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 0 & 0 & 2 & 2 \\
0 & 0 & 0 & 3 & 3 \\
0 & 0 & 0 & 1 & 1
\end{array}\right]
\end{array}
$$

$$
\begin{array}{cc}
 & \begin{array}{ccccc} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{array} \\
\begin{array}{c} \\ \text{CS} \\ \\ \\ \\ \text{MD} \\ \\ \end{array} &
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
2 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 0 & 0 & 2 & 2 \\
0 & 0 & 0 & 3 & 3 \\
0 & 0 & 0 & 1 & 1
\end{bmatrix}
\end{array}
=
\begin{bmatrix}
0.18 & 0 \\
0.36 & 0 \\
0.18 & 0 \\
0.90 & 0 \\
0 & 0.53 \\
0 & 0.80 \\
0 & 0.27
\end{bmatrix}
\text{x}
\begin{bmatrix}
9.64 & 0 \\
0 & 5.29
\end{bmatrix}
\text{x}
\begin{bmatrix}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.71 & 0.71
\end{bmatrix}
$$

SINGULAR VALUE DECOMPOSITION

$$
\begin{array}{cc}
 & \begin{array}{ccccc} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{array} \\
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\begin{bmatrix}
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0.18 & 0 \\
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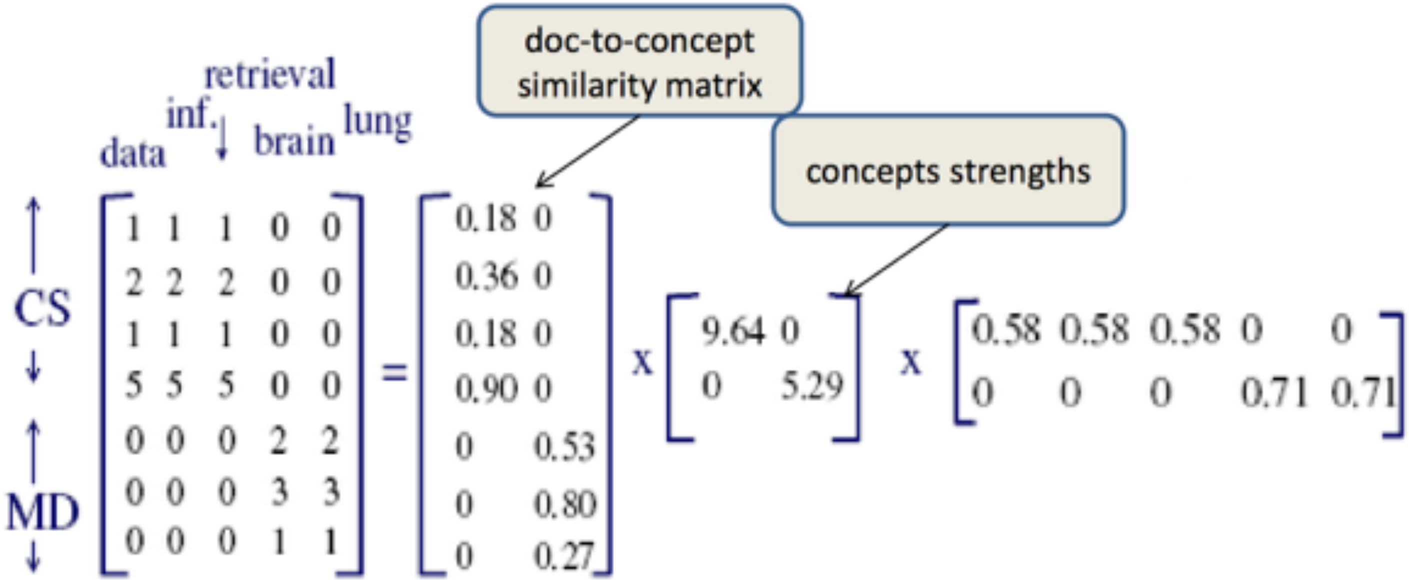
\end{bmatrix}}_{\text{doc-to-concept similarity matrix}}
\times
\begin{bmatrix}
9.64 & 0 \\
0 & 5.29
\end{bmatrix}
\times
\begin{bmatrix}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.71 & 0.71
\end{bmatrix}
$$


doc-to-concept similarity matrix
concepts strengths
data
inf.
retrieval
brain
lung
CS
MD
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
=
0.18 0
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x
9.64 0
0 5.29
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0.58 0.58 0.58 0 0
0 0 0 0.71 0.71

$$
\begin{array}{cc}
 & \begin{matrix} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{matrix} \\
\begin{matrix} \\ \text{CS} \\ \\ \\ \\ \text{MD} \\ \\ \end{matrix} &
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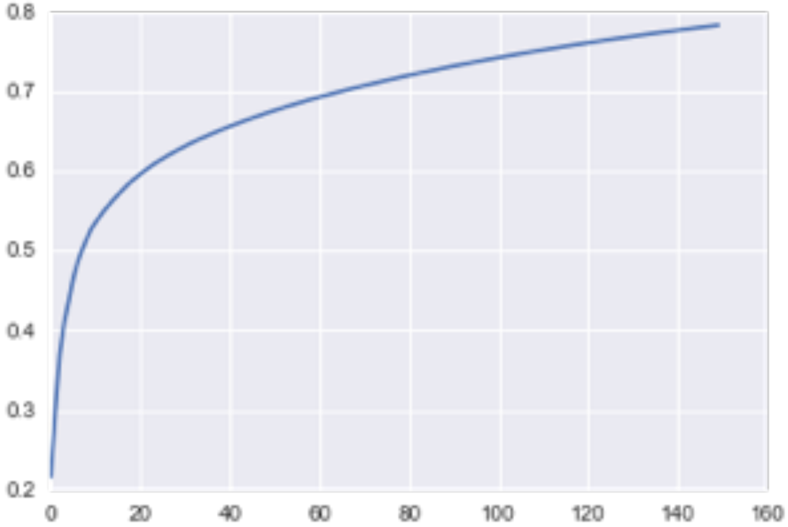
\end{bmatrix}}_{\text{term-to-concept similarity matrix}}
$$

Singular Values by # of components

(cumulative as % of total)



source: 20-newsgroups dataset, analysis in ipython notebook

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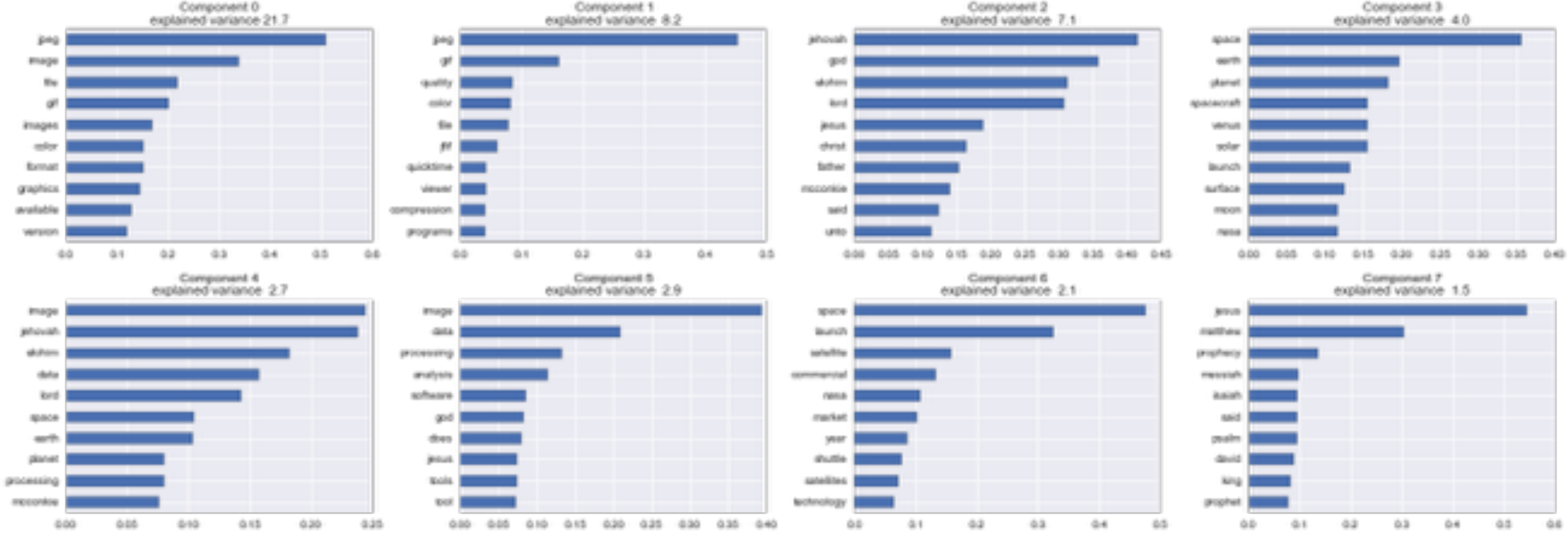

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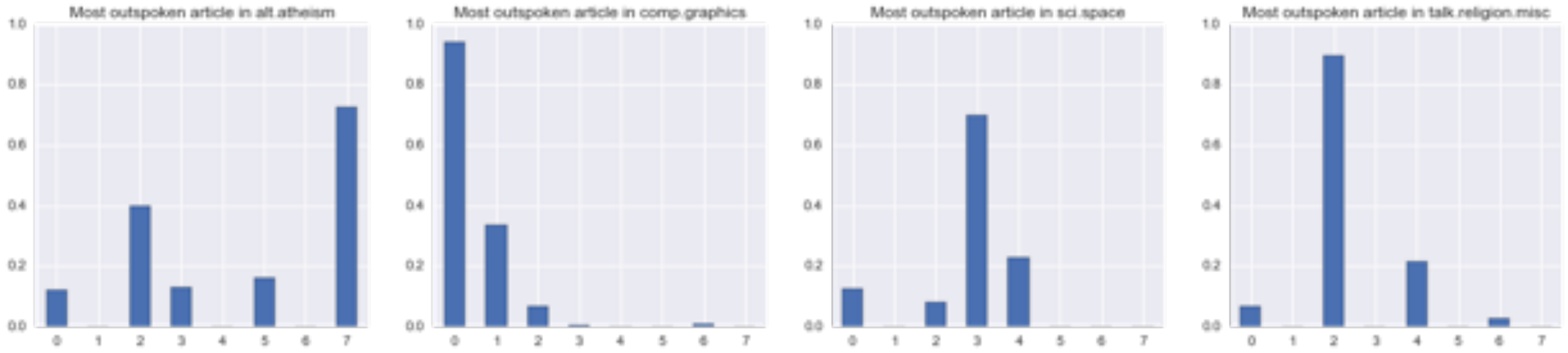

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III. PRINCIPAL COMPONENT ANALYSIS (PCA)

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The PCA of a matrix A boils down to the **eigenvalue decomposition** *of the* **covariance matrix** *of A.*

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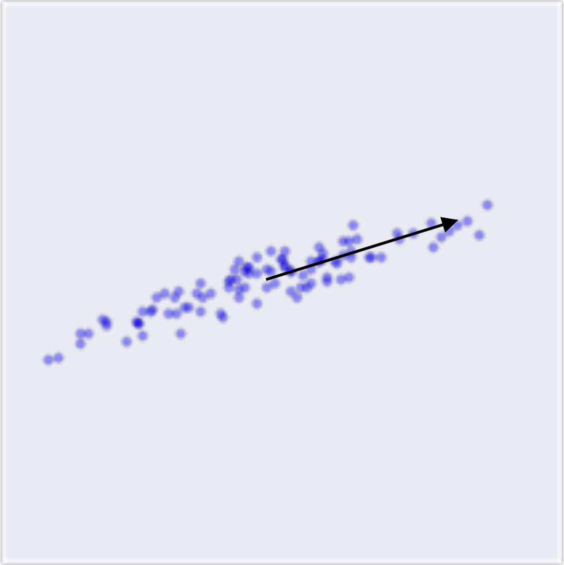
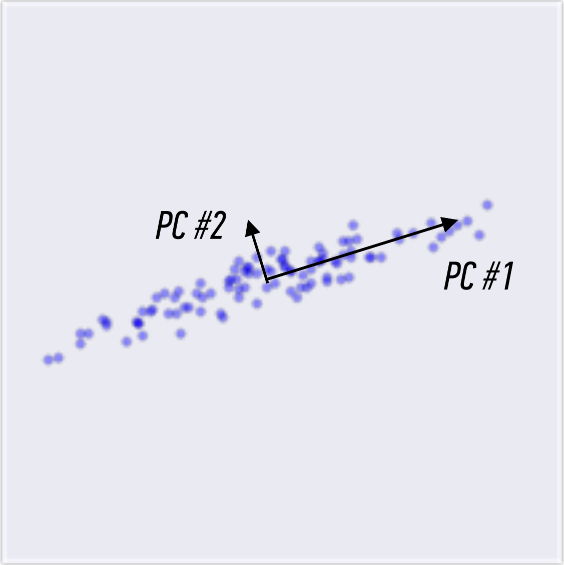
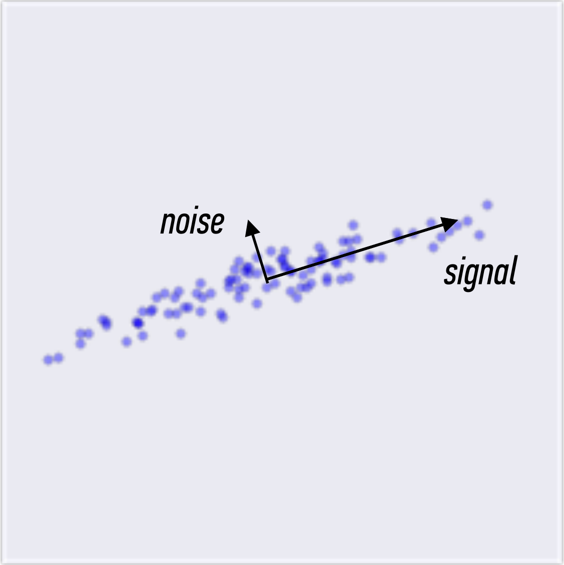




Principal Component Analysis (PCA) seeks the dimensions in which the most variance occurs

It can be seen as a transformation to a new orthogonal basis, ordered by variance



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The idea is that the first principal components contain the most information, while the latter ones contain noise

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COVARIANCE MATRICES

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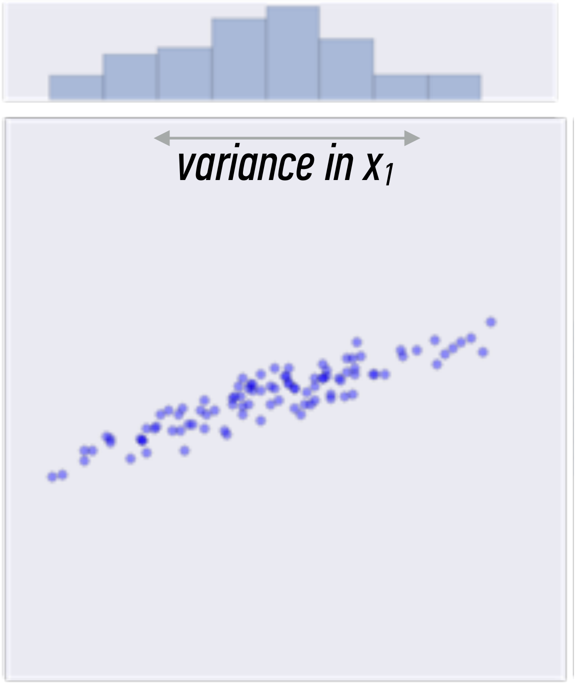
The covariance of ***X*** *and* ***Y*** *is given by* $\mathrm{Cov}(X, Y) = E\,[\,(X - \mu_X)(Y - \mu_Y)\,]$

Let’s show that in an example



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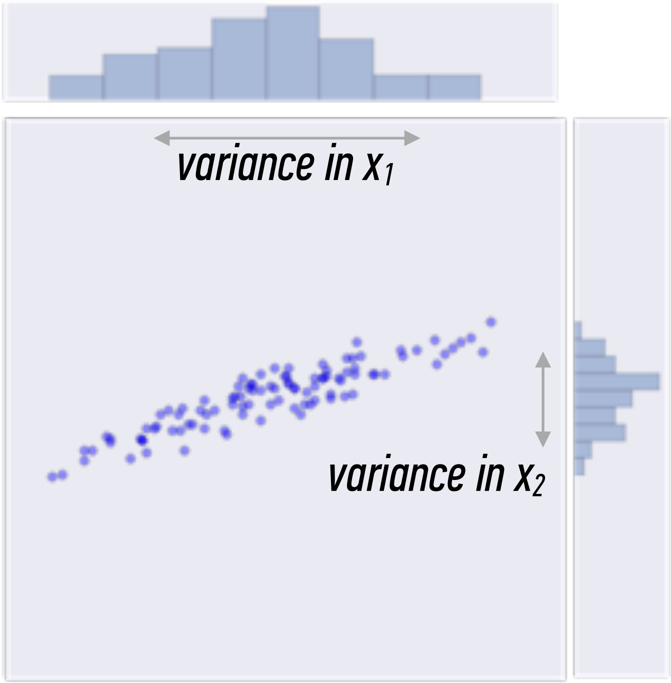

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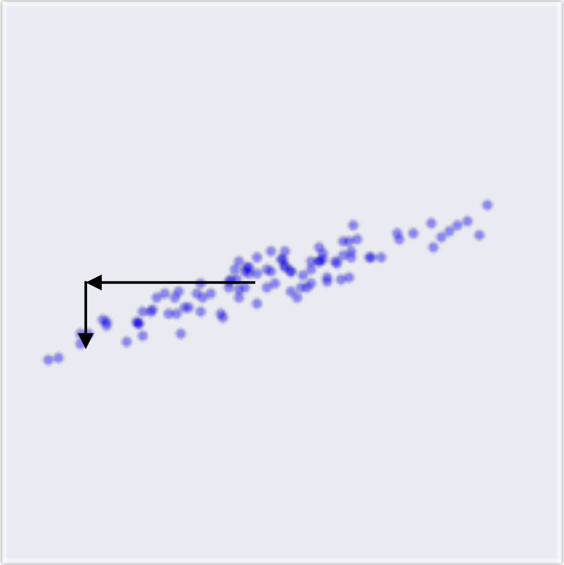

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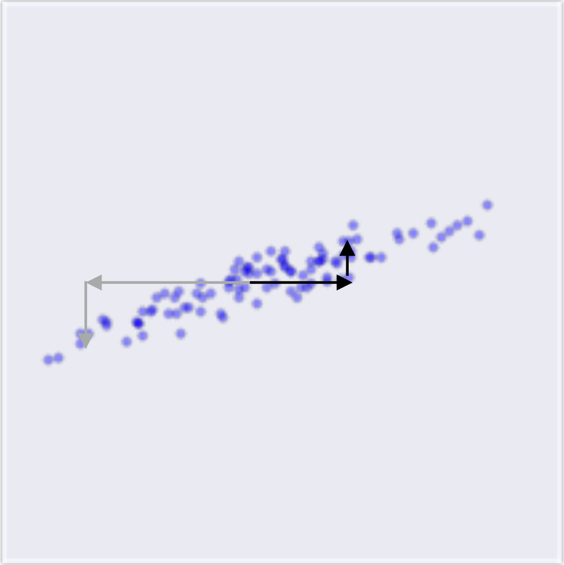

*The **variance** measures how far a set of numbers is spread out*

*The **covariance** measures how much two variables change together*

The **covariance matrix** *of a feature matrix* ***X*** *measures how much each pair of features change together*

$$
\mathrm{C} = \begin{bmatrix}
\mathrm{E}[(X_1-\mu_1)(X_1-\mu_1)] & \mathrm{E}[(X_1-\mu_1)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_1-\mu_1)(X_n-\mu_n)] \\
\mathrm{E}[(X_2-\mu_2)(X_1-\mu_1)] & \mathrm{E}[(X_2-\mu_2)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_2-\mu_2)(X_n-\mu_n)] \\
\vdots & \vdots & \ddots & \vdots \\
\mathrm{E}[(X_n-\mu_n)(X_1-\mu_1)] & \mathrm{E}[(X_n-\mu_n)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_n-\mu_n)(X_n-\mu_n)]
\end{bmatrix}
$$

The **covariance matrix** *is always square*

- *diagonal elements c_{ii} give the variance of X_i*
- *off-diagonal elements c_{ij} give the covariance between X_i and X_j $(i \neq j)$*

$$C = \begin{bmatrix} E[(X_1-\mu_1)(X_1-\mu_1)] & E[(X_1-\mu_1)(X_2-\mu_2)] & \cdots & E[(X_1-\mu_1)(X_n-\mu_n)] \\ E[(X_2-\mu_2)(X_1-\mu_1)] & E[(X_2-\mu_2)(X_2-\mu_2)] & \cdots & E[(X_2-\mu_2)(X_n-\mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ E[(X_n-\mu_n)(X_1-\mu_1)] & E[(X_n-\mu_n)(X_2-\mu_2)] & \cdots & E[(X_n-\mu_n)(X_n-\mu_n)] \end{bmatrix}$$

Note that, if all features are scaled, i.e.,

when the mean of each feature $\boldsymbol{\mu} = E[\boldsymbol{X}]$ is equal to 0,

that we can write the covariance matrix as

$$\boldsymbol{C} = \boldsymbol{X}\,\boldsymbol{X}^T$$

Now write the **eigenvalue decomposition** *of the covariance matrix*

$$C = Q \Lambda Q^{-1}$$

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Recall, for an eigenvector v *of* C *and its eigenvalue* λ*, we have:*

$$Cv = \lambda v$$

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$$C = Q \Lambda Q^{-1}$$

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We can write $C = Q \Lambda Q^{-1}$ where

- *The columns of Q are its eigenvalues, and*
- *The matrix Λ is a diagonal matrix containing its eigenvalues*

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$$C = Q\Lambda Q^{-1}$$

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$$Cv = \lambda v$$

We can write $C = Q\Lambda Q^{-1}$ where

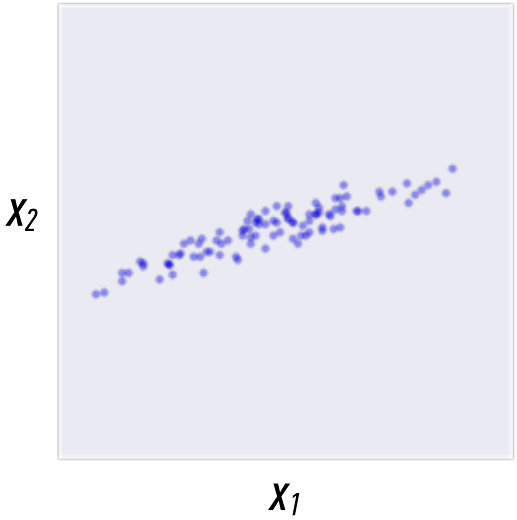
- *The columns of Q are its eigenvalues, and*
- *The matrix Λ is a diagonal matrix containing its eigenvalues*

NOTE

You can think of this as a change of **coordinate systems**. With these new coordinates, the matrix C simply scales vectors along the axes (i.e. no rotations)

BACK TO PCA

- *Principal Component Analysis (PCA) seeks the dimensions in which the most variance occurs*



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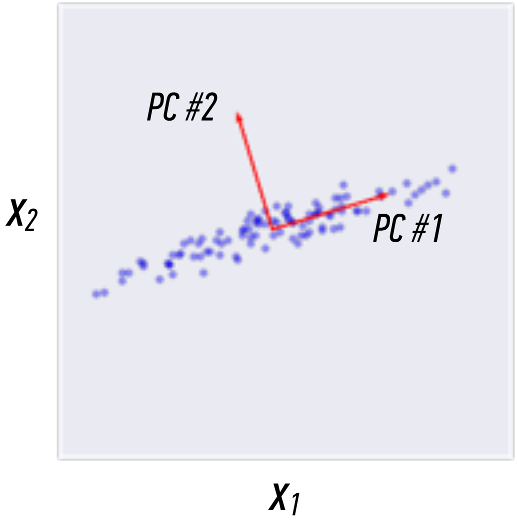
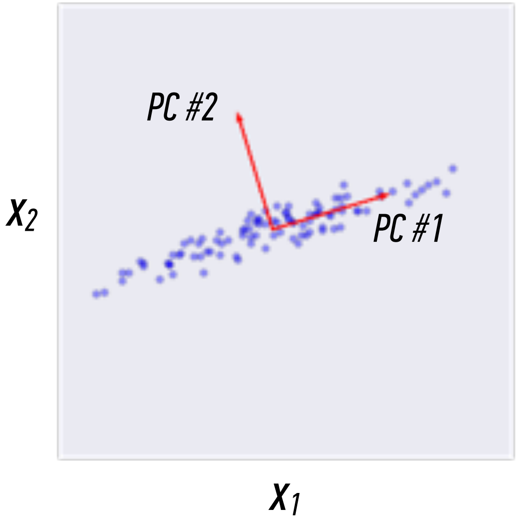
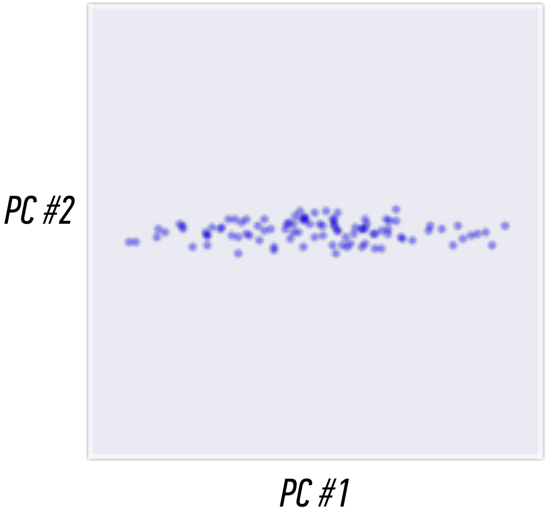
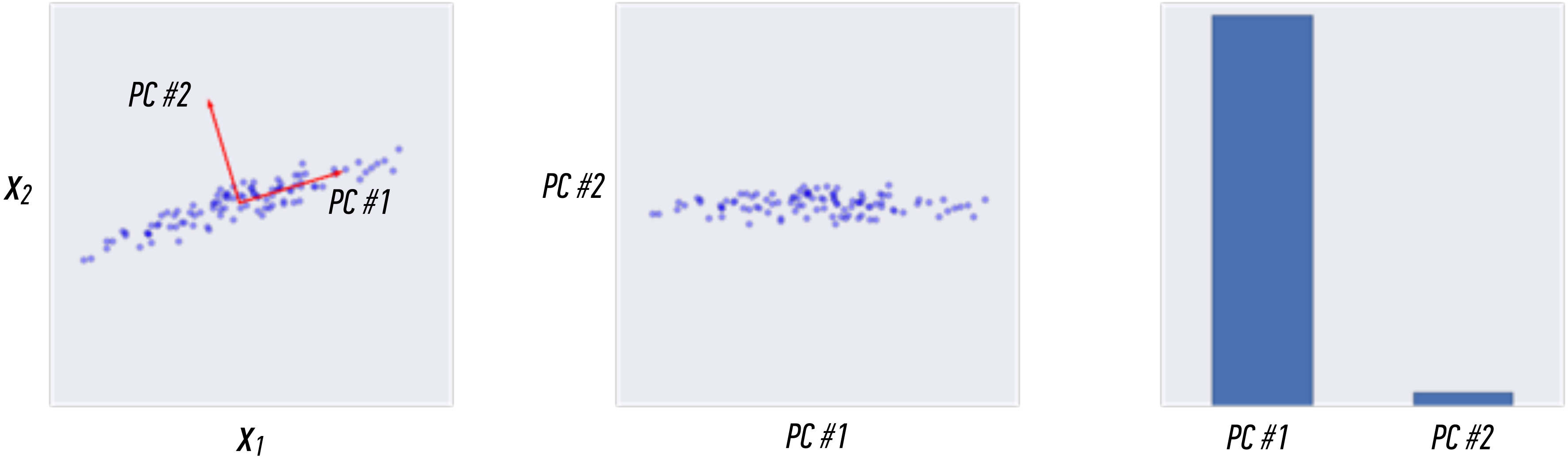


- *Principal Component Analysis (PCA) seeks the dimensions in which the most variance occurs*
- *It can be seen as a transformation to a new orthogonal basis*

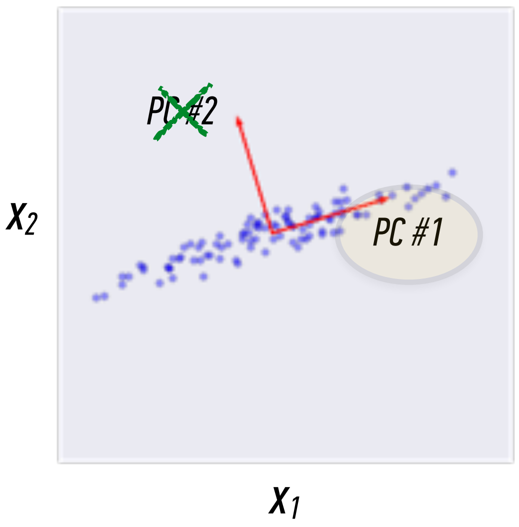


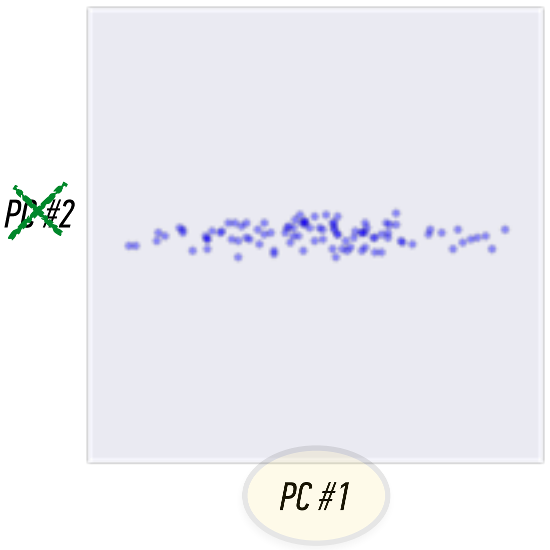


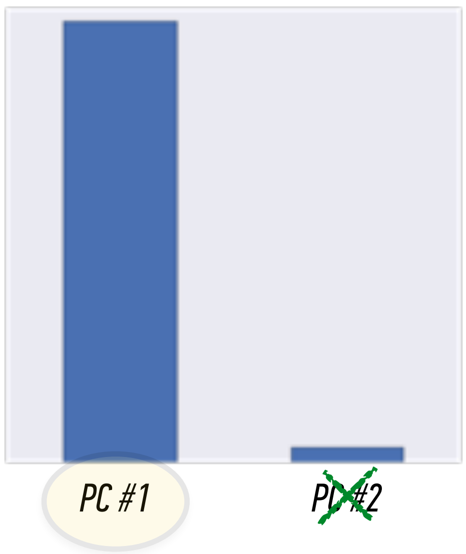
- *Principal Component Analysis (PCA) seeks the dimensions in which the most variance occurs*
- *It can be seen as a transformation to a new orthogonal basis*
- *The principal components are ordered by the size of their variance*



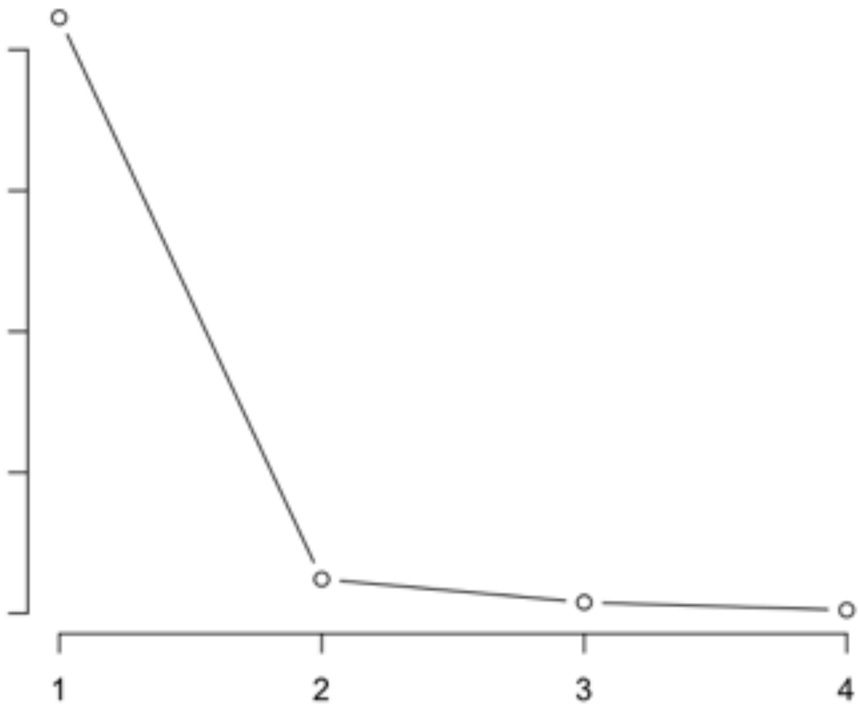
We can now **reduce the dimension** *by only looking at the first few principal components that explain the most variance*



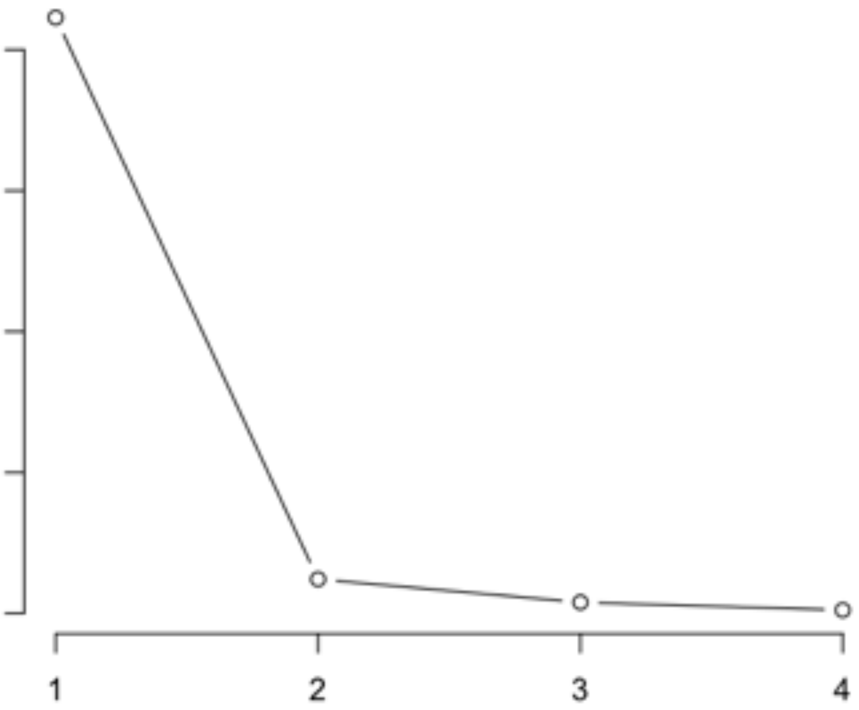




Principal components of Iris dataset



Principal components of Iris dataset



NOTE

Looking at this plot also gives you an idea of how many principal components to keep.

Apply the ***elbow*** *test*: keep only those pc's that appear to the left of the elbow in the graph.

RELATION TO SVD

What is the relationship between PCA and SVD?

$$A = U\Sigma V^T$$

singular value decomposition of A

$$A = U\Sigma V^T$$

singular value decomposition of A

$$AA^T$$

covariance matrix of A
(assuming features are scaled)

$$A = U\Sigma V^T$$

singular value decomposition of A

$$AA^T = (U\Sigma V^T)(V\Sigma U^T)$$

covariance matrix of A
(assuming features are scaled)

$$A = U\Sigma V^T$$

singular value decomposition of A

$$AA^T = (U\Sigma V^T)(V\Sigma U^T)$$

covariance matrix of A
(assuming features are scaled)

$$= U\Sigma^2 U^T$$

Using $AA^T = \mathbf{1}$

$$A = U\Sigma V^T$$

singular value decomposition of A

$$AA^T = (U\Sigma V^T)(V\Sigma U^T)$$

covariance matrix of A
(assuming features are scaled)

$$= U\Sigma^2 U^T$$

eigenvalue decomposition of AA^T

$$A = U\Sigma V^T$$

singular value decomposition of A

$$AA^T = (U\Sigma V^T)(V\Sigma U^T)$$

covariance matrix of A
(assuming features are scaled)

$$= U\Sigma^2 U^T$$

eigenvalue decomposition of AA^T

eigenvectors of AA^T
(base transformation)

$$A = U\Sigma V^T$$

singular value decomposition of A

$$AA^T = (U\Sigma V^T)(V\Sigma U^T)$$

covariance matrix of A
(assuming features are scaled)

$$= U\Sigma^2 U^T$$

eigenvalue decomposition of AA^T

eigenvectors of AA^T
(base transformation)

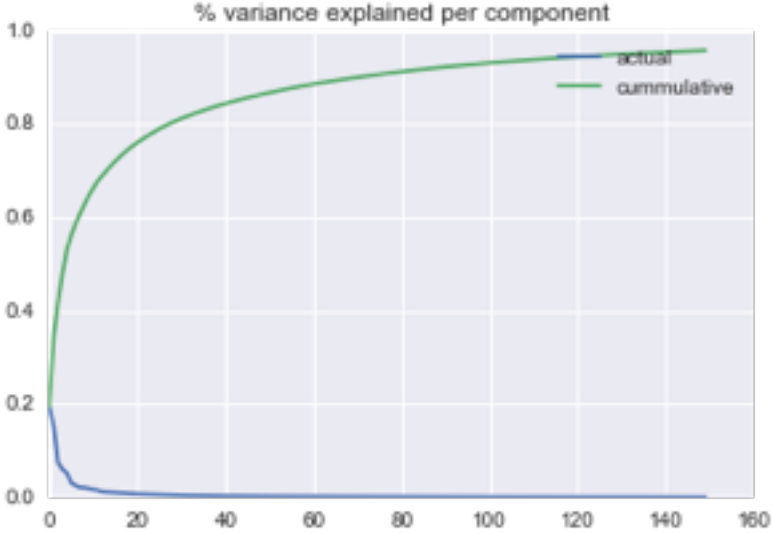
eigenvalues of AA^T
(variance of dimension)

EIGENFACES

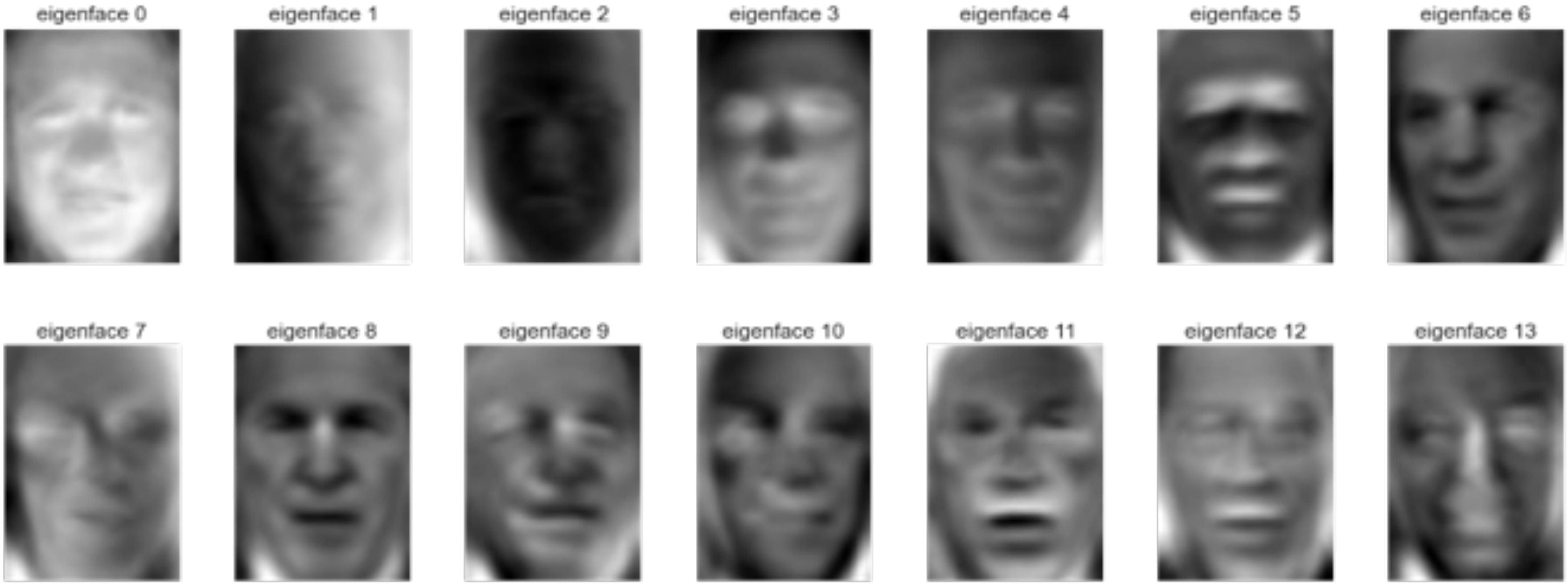

Ariel Sharon
77 images (5%)
Colin Powell
236 images (18%)
Donald Rumsfeld
121 images (9%)
George W Bush
530 images (41%)
Gerhard Schroeder
109 images (8%)
Hugo Chavez
71 images (5%)
Tony Blair
144 images (11%)

Average face

Average face



EIGENFACES


eigenface 0
eigenface 1
eigenface 2
eigenface 3
eigenface 4
eigenface 5
eigenface 6
eigenface 7
eigenface 8
eigenface 9
eigenface 10
eigenface 11
eigenface 12
eigenface 13

Average face

Average face

EIGENFACES

Average face

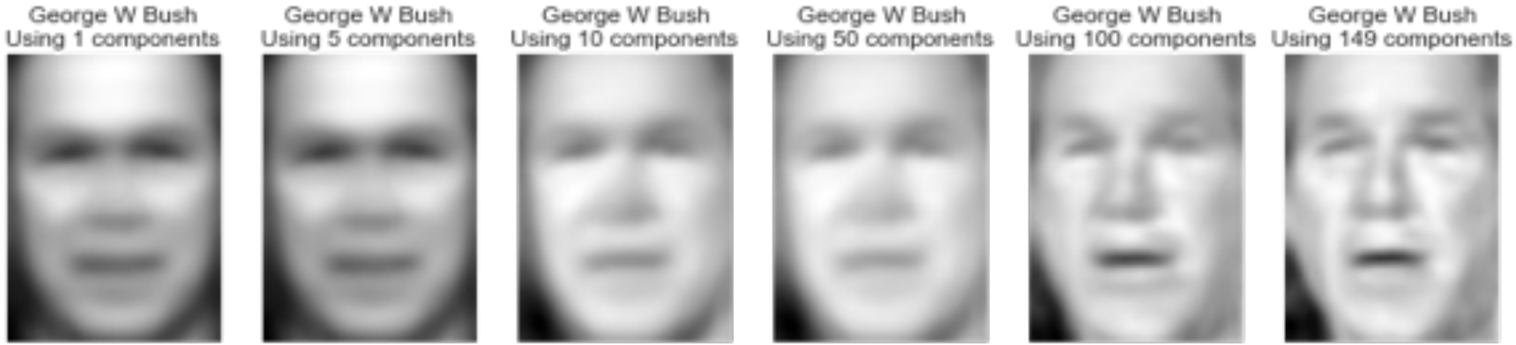
George W Bush
Using 1 components

George W Bush
Using 5 components

George W Bush
Using 10 components

EIGENFACES

Average face



DISCUSSION