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Lecture Notes to
Big Data Management and Analytics
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Text Processing and High-Dimensional Data

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DBS

Outline

- Text Processing
  - Motivation
  - Shingling of Documents
  - Similarity-Preserving Summaries of Sets
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  - Motivation
  - Principal Component Analysis
  - Singular Value Decomposition
  - CUR

Text Processing – Motivation

Given: Set of documents
Searching for patterns in large sets of document objects
→ Analyzing the similarity of objects
In many applications the documents are not identical, yet they share large portions of their text:

- Plagiarism
- Mirror Pages
- Articles from the same source

Problems in the field of Text Mining:

- Stop words (e.g. for, the, is, which ,…)
- Identify word stem
- High dimensional features (d > 10'000)
- Terms are not equally relevant within a document
- The frequency of terms are often $h_i = 0$ → very sparse feature space

→ We will focus on character-level similarity, not *‚similar meaning'*

Text Processing – Motivation

How to handle the relevance of a term?

TF-IDF (Term Frequency * Inverse Document Frequency)

- *Empirical probability of term t in document d:* $\boldsymbol{TF(t,d)} = \frac{n(t,d)}{max_{w \in d} n(w,d)}$

  frequency n(t,d) := number of occurrences of term (word) t in document d

- *Inverse probability of t regarding all documents:* $\mathbf{IDF(t)} = \frac{|DB|}{|\{d | d \in DB \wedge t \in d\}|}$

- *Feature vector is given by:* $r(d) = (TF(t_1, d) * IDF(t_1), \ldots, TF(t_n, d) * IDF(t_n)$

How to handle sparsity?

Term frequency often 0 => diversity of mutual Euclidean distances quite low → other distance measures required:

- ***Jaccard Coefficient:*** $d_{Jaccard}(D_1, D_2) = \frac{|D_1 \cap D_2|}{|D_1 \cup D_2|}$ (Documents → set of terms)
- ***Cosinus Coefficient:*** $d_{Cosinus}(D_1, D_2) = \frac{\langle D_1, D_2 \rangle}{\|D_1\| * \|D_2\|}$ (useful for high-dim. data)

Shingling of Documents

General Idea: construct a set of short strings that appear within a document

***K*- shingles**

Definition: A *k*-shingle is any substring of length *k* found within the document. (aka k-grams)

→ Associate with each document the set of *k*-shingles that appear n times within that document

Hashing Shingles:

Idea: pick hash function that maps strings of length *k* to some number of buckets and treat the resulting bucket number as the shingle

→ set representing document is then set of integers

Similarity-Preserving Summaries of Sets

Problem: Sets of shingles are large
→ replace large sets by much smaller representations called ‚*signatures*'

Matrix representation of Sets
Characteristic matrix:

- columns correspond to the sets (documents)
- rows correspond to elements of the universal set from which elements (shingles) of the columns are drawn

Example:

- universal set: {A,B,C,D,E},
- S1 = {A,D}, S2 = {C}, S3={B,D,E}, S4={A,C,D}

documents

shingles

Element	S1	S2	S3	S4
A	1	0	0	1
B	0	0	1	0
C	0	1	0	1
D	1	0	1	1
E	0	0	1	0

Similarity-Preserving Summaries of Sets

Minhashing

Idea: To minhash a set represented by a column c_i of the characteristic matrix, pick a permutation of the rows. The value of the minhash is the number of the first row, in the permutated order, with $h(c_i) = 1$

Example:
Suppose the order of rows ‚BEADC'

- h(S1) = A
- h(S2) = C
- h(S3) = B
- h(S4) = A

Element	S1	S2	S3	S4
B	0	0	1	0
E	0	0	1	0
A	1	0	0	1
D	1	0	1	1
C	0	1	0	1

Similarity-Preserving Summaries of Sets

Minhashing and Jaccard Similarity

The probability that the minhash function for a random permutation of rows produces the same value for two sets equals the Jaccard similarity of those sets.

Three different classes of similarity between sets (documents)

- Type X rows have 1 in both cols
- Type Y rows have 1 in one of the columns
- Type Z rows have 0 in both rows

Example

Considering the cols of S1 and S3:
The probability that h(S1) = h(S3) is given by:

$$SIM(S1, S3) = \frac{x}{(x+y)} = \frac{1}{4}$$

(Note that x is the size of $S1 \cap S2$ and (x+y) is the size of $S1 \cup S2$)

Element	S1	S2	S3	S4
B	0	0	1	0
E	0	0	1	0
A	1	0	0	1
D	1	0	1	1
C	0	1	0	1

Similarity-Preserving Summaries of Sets

Minhash Signatures

- Pick a random number n of permutations of the rows
- Vector $[h_1(S), h_2(S), \dots, h_n(S)]$ represents the minhash signature for S
- Put the specific vectors together in a matrix, forms the *signature matrix*
- Note that the *signature matrix* has the same number of columns as input matrix M but only n rows

How to compute minhash signatures:

1. Compute $h_1(S), h_2(S), \dots, h_n(S)$
2. For each row r: For each column c do the following:
   (a) if c has 0 in row r, do nothing
   (b) if c has 1 in row r then for each $i = 1, 2, \dots, n$ set
   $SIG(i, c) = \min(SIG(i, c), h_i(r))$

→ **Signature matrix allows to estimate the Jaccard similarities of the underlying sets!**

Similarity-Preserving Summaries of Sets

Minhash Signatures - Example

- Suppose two hash functions : $h_1(x) = (x + 1)\ mod\ 5$ and $h_2(x) = (3x + 1)\ mod\ 5$

Element	S1	S2	S3	S4	h1(x)	h2(x)
0	**1**	**0**	**0**	**1**	**1**	**1**
1	0	0	1	0	2	4
2	0	1	0	1	3	2
3	1	0	1	1	4	0
4	0	0	1	0	0	3

initialization

1.	s1	s2	s3	s4
h1	∞	∞	∞	∞
h2	∞	∞	∞	∞

2.	s1	s2	s3	s4
h1	1	∞	∞	1
h2	1	∞	∞	1

1st row

Check Sig for S1 and S4:

$SIG(i,c) = \min(SIG(i,c), h_i(r))$

S1: $\mathbf{min(\infty, 1) = 1}$

$\mathbf{min(\infty, 1) = 1}$

S4: $\boldsymbol{min(\infty, 1) = 1}$

$\boldsymbol{min(\infty, 1) = 1}$

Similarity-Preserving Summaries of Sets

Minhash Signatures - Example

- Suppose two hash functions : $h_1(x) = x + 1 \; mod \; 5$ and $h_2(x) = (3x + 1) \bmod 5$

Element	S1	S2	S3	S4	h1(x)	h2(x)
0	1	0	0	1	1	1
1	**0**	**0**	**1**	**0**	**2**	**4**
2	0	1	0	1	3	2
3	1	0	1	1	4	0
4	0	0	1	0	0	3

2nd row
Check Sig for S3:
$SIG(i,c) = \min(SIG(i,c), h_i(r))$

S3: $\mathbf{\min(\infty, 2) = 2}$
$\mathbf{\min(\infty, 4) = 4}$

initialization

1.	s1	s2	s3	s4
h1	∞	∞	∞	∞
h2	∞	∞	∞	∞

2.	s1	s2	s3	s4
h1	1	∞	∞	1
h2	1	∞	∞	1

3.	s1	s2	s3	s4
h1	1	∞	2	1
h2	1	∞	4	1

Similarity-Preserving Summaries of Sets

Minhash Signatures - Example

- Suppose two hash functions : $h_1(x) = x + 1 mod\ 5$ and $h_2(x) = (3x + 1) mod 5$

Element	S1	S2	S3	S4	h1(x)	h2(x)
0	1	0	0	1	1	1
1	0	0	1	0	2	4
2	**0**	**1**	**0**	**1**	**3**	**2**
3	1	0	1	1	4	0
4	0	0	1	0	0	3

3rd row

Check Sig for S2 and S4:

$SIG(i,c) = \min(SIG(i,c), h_i(r))$

S2: $\mathbf{\min(\infty, 3) = 3}$

$\mathbf{\min(\infty, 2) = 2}$

S4: $\min(1,3) = 1$

$\min(1,2) = 1$

initialization

1.	s1	s2	s3	s4
h1	∞	∞	∞	∞
h2	∞	∞	∞	∞

2.	s1	s2	s3	s4
h1	1	∞	∞	1
h2	1	∞	∞	1

3.	s1	s2	s3	s4
h1	1	∞	2	1
h2	1	∞	4	1

4.	s1	s2	s3	s4
h1	1	3	2	1
h2	1	2	4	1

Similarity-Preserving Summaries of Sets

Minhash Signatures - Example

- Suppose two hash functions : $h_1(x) = x + 1 mod\ 5$ and $h_2(x) = (3x + 1) mod 5$

Element	S1	S2	S3	S4	h1(x)	h2(x)
0	1	0	0	1	1	1
1	0	0	1	0	2	4
2	0	1	0	1	3	2
3	**1**	**0**	**1**	**1**	**4**	**0**
4	0	0	1	0	0	3

4th row

Check Sig for S1,S3,S4:

$SIG(i,c) = \min(SIG(i,c), h_i(r))$

S1: $\min(1,4) = 1$

$\boldsymbol{min(1,0) = 0}$

S3: $\min(2,4) = 2$

$\boldsymbol{min(4,0) = 0}$

S4: $\min(1,4) = 1$

$\boldsymbol{min(1,0) = 0}$

initialization

1.	s1	s2	s3	s4
h1	∞	∞	∞	∞
h2	∞	∞	∞	∞

2.	s1	s2	s3	s4
h1	1	∞	∞	1
h2	1	∞	∞	1

3.	s1	s2	s3	s4
h1	1	∞	2	1
h2	1	∞	4	1

4.	s1	s2	s3	s4
h1	1	3	2	1
h2	1	2	4	1

5.	s1	s2	s3	s4
h1	1	3	2	1
h2	0	2	0	0

Similarity-Preserving Summaries of Sets

Minhash Signatures - Example

- Suppose two hash functions : $h_1(x) = x + 1 mod\ 5$ and $h_2(x) = (3x + 1) mod 5$

Element	S1	S2	S3	S4	h1(x)	h2(x)
0	1	0	0	1	1	1
1	0	0	1	0	2	4
2	0	1	0	1	3	2
3	1	0	1	1	4	0
4	**0**	**0**	**1**	**0**	**0**	**3**

5th row

Check Sig for S3:

$SIG(i,c) = \min(SIG(i,c), h_i(r))$

S3: $\mathbf{min(2,0) = 0}$

$\min(0,3) = 0$

initialization

1.	s1	s2	s3	s4
h1	∞	∞	∞	∞
h2	∞	∞	∞	∞

2.	s1	s2	s3	s4
h1	1	∞	∞	1
h2	1	∞	∞	1

3.	s1	s2	s3	s4
h1	1	∞	2	1
h2	1	∞	4	1

4.	s1	s2	s3	s4
h1	1	3	2	1
h2	1	2	4	1

5.	s1	s2	s3	s4
h1	1	3	2	1
h2	0	2	0	1

6.	s1	s2	s3	s4
h1	1	3	0	1
h2	0	2	0	0

Jaccard(s_i, s_j)≈ #of h_l where $h_l(s_i)=h_l(s_j)$ /# of h's

Modeling data as matrices

Matrices often arise with data:

- $\boldsymbol{n}$ objects (documents, images, web pages, time series…)
- each with $\boldsymbol{m}$ features

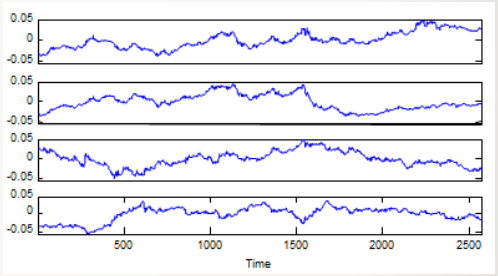
→ Can be represented by an $\boldsymbol{n}\ \boldsymbol{x}\ \boldsymbol{m}$ matrix

doc1	Two for wine and wine for two
doc2	Wine for me and wine for you
doc3	You for me and me for you

$$TDM \coloneqq \begin{pmatrix} 2 & 2 & 0 & 0 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & 2 & 2 \end{pmatrix} \begin{matrix} \text{Doc1} \\ \text{Doc2} \\ \text{Doc3} \end{matrix}$$

Two wine Me you

(filter ‚for', ‚and' as stopwords)



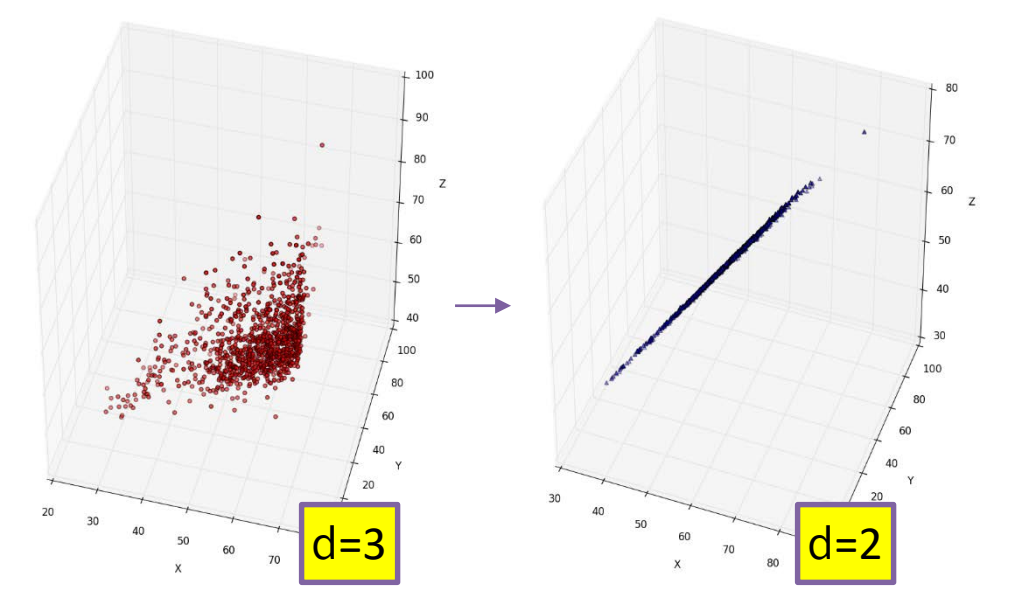
i-th series, $x^{(i)}$

$$X_{NxM} \coloneqq \begin{pmatrix} x_1^{(1)} & x_1^{(2)} & \cdots & x_1^{(M)} \\ x_2^{(1)} & x_2^{(2)} & \cdots & x_2^{(M)} \\ \vdots & \vdots & \ddots & \vdots \\ x_N^{(1)} & x_N^{(2)} & \cdots & x_N^{(M)} \end{pmatrix}$$

values at time t, x_t

Why reducing the dimensionality makes sense?

- discover hidden correlations
- remove redundant and noisy features
- interpretation and visualization
- easier storage and processing of the data
- transform a high-dimensional sparse matrix into a low-dimensional dense matrix



Axes of k-dimensional subspace are effective representation of the data

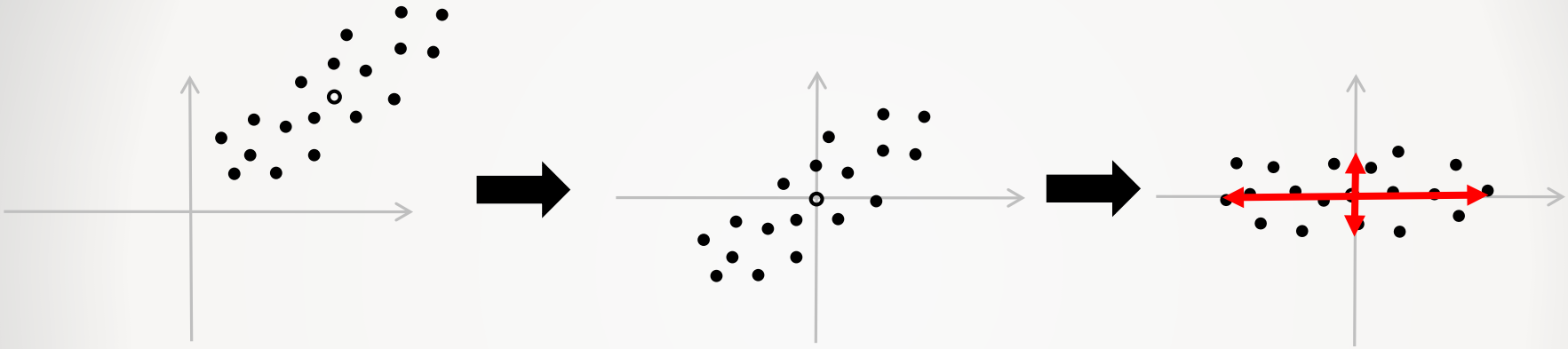
Principal Component Analysis (PCA)

- PCA computes the most meaningful basis to re-express noisy data
- Think of PCA as choosing a new coordinate system for the data, the principal components being the unit vectors along the axes
- PCA asks: *Is there another basis, which is a linear combination of the original basis, that best expresses our dataset?*
- General form: $PX=Y$

  where P is a linear transformation, X is the original dataset and Y the re-representation of this dataset.
  - P is a matrix that transforms X into Y
  - Geometrically, P is a *rotation* and a *scaling* which transforms X into Y
  - The eigenvectors are the rotations to the new axes
  - The eigenvalues are the amount of stretching that needs to be done
- The *p*'s are the principal components
  - Directions with the largest variance … those are the most important, most *principal*.

Principal Component Analysis (PCA)

Idea: Rotate the data space in a way that the principal components are placed along the main axis of the data space
=> Variance analysis based on principal components



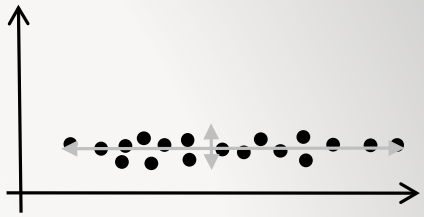
- Rotate the data space in a way that the direction with the largest variance is placed on an axis of the data space
- Rotation is equivalent to a basis transformation by an orthonormal basis
  - Mapping is equal of angle and preserves distances:

$$x \cdot B = x(b_{*,1},\ldots,b_{*,d}) = (\langle x, b_{*,1}\rangle,\ldots,\langle x, b_{*,d}\rangle) \quad mit \quad \forall_{i\neq j}\langle b_i, b_j\rangle = 0 \wedge \forall_{1\leq i\leq d}\|b_i\| = 1$$

- B is built from the largest variant direction which is orthogonal to all previously selected vectors in B.

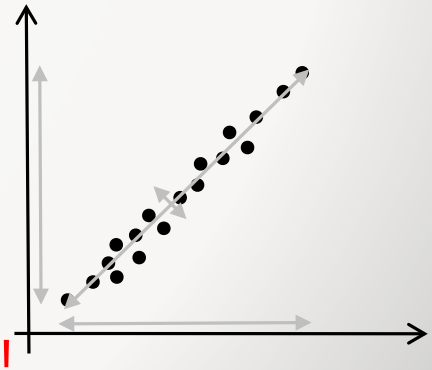
Variance Analysis for feature selection

- Which attributes are the most important to the distance ?
  => attributes with strongly varying value differences $|x_i - y_i|$
  => distance to the mean value is large $|x_i - \mu_i|$
  => variance is large: $\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_i)^2$



Idea: Variance Analysis (= unsupervised feature selection)

- Attributes with large variance allow strong distinction between objects
- Attributes with small variance: difference between objects are negligible
- Method:
  - Determine the variance between the values in each dimension
  - Sort all features w.r.t. to the variance
  - Select *k* features having the strongest variance



Beware: Even linear correlation can distribute one strong feature over arbitrarily many other dimensions!!!

Eigenvalue decomposition of the covariance matrix

- Applying the eigenvalue decomposition to the covariance matrix:

$$\Sigma_D = V \Lambda V^T = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_d \end{pmatrix} (v_1, \cdots, v_d)$$

- v_i: Orthogonal principal components (eigenvectors)
- λ_i: Variance along each direction (eigenvalues)

Beware: $\lambda_i = 0$ means that the corresponding direction is a linear combination of other principal components.

=> Depending on the algorithm completely redundant dimension cause problems

Workaround: Add a diagonal matrix with very small values δ_i to Σ_D.

PCA and Multivariate Gaussians

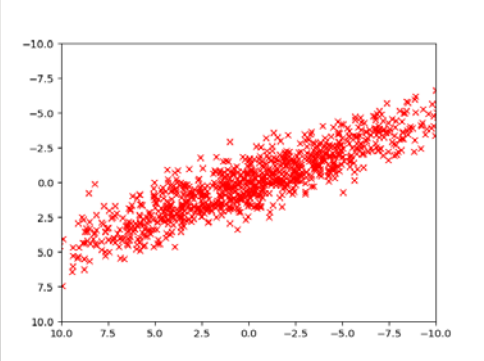
Multivariate Gaussian: $N(\mu, \Sigma) = \frac{1}{\sqrt{2 \cdot \pi \cdot det(\Sigma)}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$

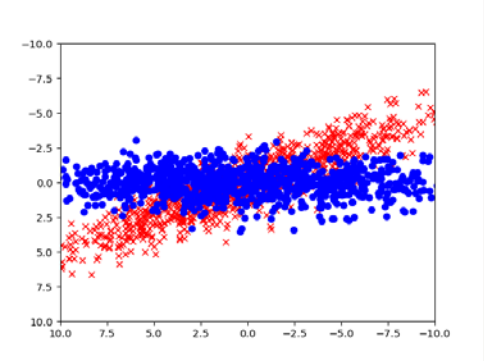
Center X and insert eigenvalue decomp. of Σ: $N(\mu, \Sigma) = \frac{1}{\sqrt{2 \cdot \pi \cdot det(\Sigma)}} e^{-\frac{1}{2} x^T (V \Lambda V^T)^{-1} x}$

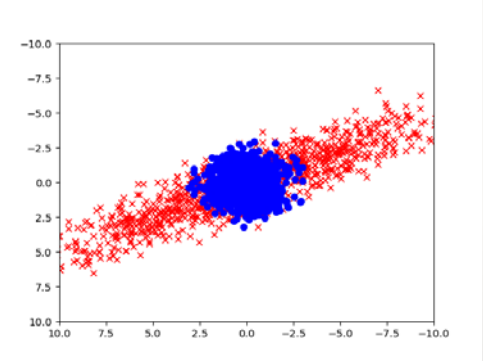
Substitute $x^T V$ by *u* rewrite det(Σ): $N(\mu, \Sigma) = \frac{1}{\sqrt{2 \cdot \pi \cdot \prod_{i=1} \lambda_i}} e^{-\frac{1}{2} \sum_{i=1}^{d} u_i^2 \lambda_i^{-1}}$

extract product : $N(\mu, \Sigma) = \prod_{i=1}^{d} \frac{1}{\sqrt{2 \cdot \pi \cdot \lambda_i}} e^{-\frac{u_i^2}{2 \cdot \lambda_i}}$

rescaling dimension i with $\sqrt{\frac{1}{\lambda_i}}$ leads to a standard Gaussian N(0,1).







PCA steps

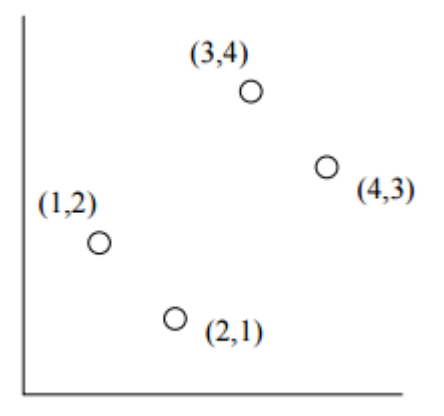
Feature reduction using PCA

1. Compute the covariance matrix Σ
2. Compute the eigenvalues and the corresponding eigenvectors of Σ
3. Select the *k* biggest eigenvalues and their eigenvectors (V‘)
4. The *k* selected eigenvectors represent an orthogonal basis
5. Transform the original $n \times d$ data matrix D with the $d \times k$ basis V‘:

$$D \cdot \mathrm{V}' = \begin{pmatrix} \mathrm{x}_1 \\ \vdots \\ \mathrm{x}_n \end{pmatrix} \left(v_1', \cdots, v_k' \right) = \begin{pmatrix} \left\langle \mathrm{x}_1, v_1' \right\rangle & \cdots & \left\langle \mathrm{x}_1, v_k' \right\rangle \\ \vdots & \ddots & \vdots \\ \left\langle \mathrm{x}_n, v_1' \right\rangle & \cdots & \left\langle \mathrm{x}_n, v_k' \right\rangle \end{pmatrix}$$

Example of transformation

- Original



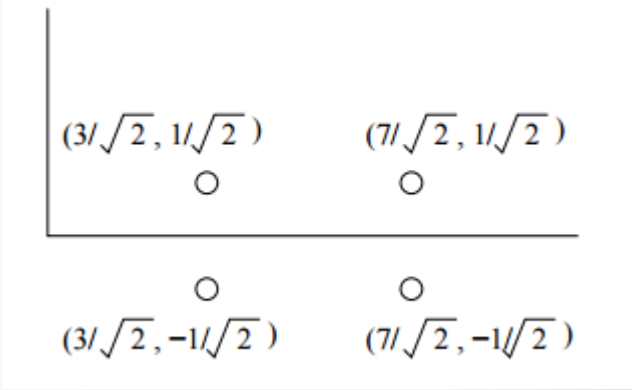
Eigenvectors

$$\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \qquad \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

In the rotated coordinate system

- Transformed data

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 3/\sqrt{2} & 1/\sqrt{2} \\ 3/\sqrt{2} & -1/\sqrt{2} \\ 7/\sqrt{2} & 1/\sqrt{2} \\ 7/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$



Source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

Percentage of variance explained by PCA

- Let *k* be the number of top eigenvalues out of *d* (*d* is the number of dimensions in our dataset)
- The percentage of variance in the dataset explained by the *k* selected eigenvalues is:

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

- Similarly, you can find the variance explained by each principal component
- Rule of thumb: keep enough to explain **85%** of the variation

PCA results interpretation

- Example: iris dataset (d=4), results from R
- 4 principal components

	PC1	PC2	PC3	PC4
Sepal.Length	0.5038236	-0.45499872	0.7088547	0.19147575
Sepal.Width	-0.3023682	-0.88914419	-0.3311628	-0.09125405
Petal.Length	0.5767881	-0.03378802	-0.2192793	-0.78618732
Petal.Width	0.5674952	-0.03545628	-0.5829003	0.58044745

Importance of components:

	PC1	PC2	PC3	PC4
Proportion of Variance	0.7331	0.2268	0.03325	0.00686
Cumulative Proportion	0.7331	0.9599	0.99314	1.00000

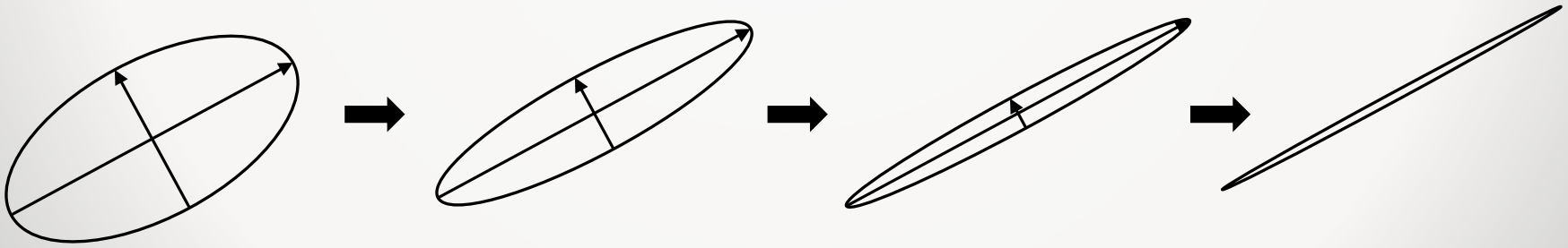
Computing PCA via Power Iteration

Problem:

- Computing the eigenvalues with standard algorithms is often expensive (many algorithm are well-known)
- Standard methods often involve matrix inversions ($O(n^3)$)
- For large matrixes more efficient methods are required:

Most prominent is the power iterations method ($O(n^2)$)

Intuition: Multiplying a matrix with itself increases the strongest direction relative to the other direction.



Power Iterations general idea

- **given**: data n×d matrix X and the corresponding covariance matrix Σ=1/n(X-μ(X)^T(X-μ(X)) where μ(X) is the mean vector of X.

- consider the eigenvalue decomposition of $\Sigma = V^T \Lambda V$ where $V = (v_1, .., v_d)$: is the column wise orthonormal eigenvector basis

$\Lambda = \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d \end{bmatrix}$: is the diagonal eigenvalue matrix

Note: $\Sigma^t = (V^T \Lambda V)^t = V^T \Lambda V \cdot V^T \Lambda V \cdot \ldots \cdot V^T \Lambda V = V^T \Lambda^t V$

$$= V^T \begin{bmatrix} \lambda_1^t & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d^t \end{bmatrix} V$$

What is the *i*th power of a diagonal matrix ?

- if PCA is well-defined all $\lambda >= 0$
- taking the i^{th} power: All values $\lambda > 1$ increase with the power and all λ values < 0 decrease exponentially fast.
- When normalizing the λ by $\sum_{i=1}^{d} \lambda_i$, we observe the following:

  for $\lambda_i \neq \lambda_j$ and $t \to \infty$: $\exists \lambda_{i*}: \frac{\lambda_{i*}^t}{\sum_{i=1}^{d} \lambda_i^t} \to 1 \; and \; \forall j \neq i*: \frac{\lambda_j^t}{\sum_{i=1}^{d} \lambda_i^t} \to 0$
- under normalization over all diagonal entries, only one component remains.
- Thus: the rank of Σ^t converges to 1 and the only component remaining is the strongest eigenvector.

Determining the Strongest Eigenvalue

The following algorithm computes the strongest eigenvalue of matrix M:

```
Input: d×d data matrix M
x_0 = random unit vector
M_0 = M
while || x_i/||x_i||- x_{i-1}/||x_{i-1}|| ||> ε do
        M_{i+1} = M^T_i M_i
        x_i = M_{i+1} x_0
        i=i+1
return x_i/||x_i||
```

Why does this work?

$$M^t x = [v_1, .., v_d] \begin{bmatrix} 0 & .. & 0 \\ .. & \lambda_j^t & .. \\ 0 & .. & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ : \\ v_d \end{bmatrix} x = [v_1, .., v_d] \begin{bmatrix} 0 & .. & 0 \\ .. & \lambda_j^t & .. \\ 0 & .. & 0 \end{bmatrix} \begin{bmatrix} \langle v_1, x \rangle \\ : \\ \langle v_d, x \rangle \end{bmatrix}$$

$$= [v_1, .., v_d] \begin{bmatrix} 0 \\ \lambda_j^t \langle v_j, x \rangle \\ 0 \end{bmatrix} = \begin{bmatrix} v_{1,1} \cdot 0 + .. + v_{1,j} \cdot \lambda_j^t \langle v_j, x \rangle + v_{1,d} \cdot 0 \\ : \\ v_{d,1} \cdot 0 + .. + v_{d,j} \cdot \lambda_j^t \langle v_j, x \rangle + v_{d,d} \cdot 0 \end{bmatrix} = v_j \cdot \lambda_j^t \langle v_j, x \rangle$$

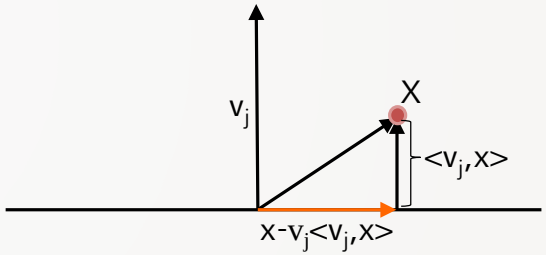
in other words the $M^T x$ has the same direction as the strongest eigenvector v_j.

Power Iterations: the complete method

- we now have a method to determine the strongest eigenvector
- to compute the k-strongest eigenvectors we proceed as follows:

```
For i=1 to k:
  determine the strongest eigenvector v_i
  reproject data X to the space being orthogonal to v_i:
  x' = x-v_i<v_i,x>
output the v_i
```

- explanation for the reprojection:



- if there are two equally strong eigenvalues $\lambda_i = \lambda_j$ then the algorithm returns an arbitrary vector from $span(v_i, v_j)$
- for $\lambda_i \approx \lambda_j$: the algorithm converges slower

Conclusion

- PCA is an important method for feature reduction
- general and complete methods for eigenvalue decomposition are often inefficient(compute the characteristic polynomial, using matrix inversion etc.)
- Power iterations are linear in the size of the matrix, i.e. quadratic in the dimension d.
- Power iterations compute only the k strongest eigenvalues but not all (stops when k strongest v are found)
- rely only on matrix multiplications

Singular Value Decomposition (SVD) – Generalization of the eigenvalue decomposition

Let $X_{n\times d}$ be a data matrix and let k be its rank. We can decompose X into matrices U, Σ, V as follows:

$$\underset{\boldsymbol{X}}{\begin{pmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{pmatrix}} = \underset{\boldsymbol{U}}{\begin{pmatrix} u_{1,1} & \cdots & u_{1,n} \\ \vdots & \ddots & \vdots \\ u_{n,1} & \cdots & u_{n,n} \end{pmatrix}} * \underset{\boldsymbol{\Sigma}}{\begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d \end{pmatrix}} * \underset{\boldsymbol{V^T}}{\begin{pmatrix} v_{1,1} & \cdots & v_{1,d} \\ \vdots & \ddots & \vdots \\ v_{d,1} & \cdots & v_{d,d} \end{pmatrix}}$$

- **X (Input data matrix)** is a $n\times d$ matrix (e.g. n customers, d products)
- **U (Left singular vectors)** is a $n\times n$ column-orthonormal matrix
- **Σ (Singular values)** is a diagonal $n\times d$ with the elements being the singular values of X
- **V (Right singular vectors)** is a $d\times d$ column-orthonormal matrix

Computing SVD of a Matrix

Connected to eingenvalues of matrices $X^T X$ and $X X^T$

$$X^T X = (U\,\Sigma\,V^T)^T U\,\Sigma\,V^T = (V^T)^T \Sigma^T U^T\, U\,\Sigma\,V^T = V\,\Sigma^2\,V^T$$

→ Multiplying each side with V:

$$(X^T X)\,V = V\,\Sigma^2$$

remember the eigenvalue problem:
$Av = \lambda v$

→ Same algorithm that computes the *eigenpairs* for $X^T X$ gives us matrix V for SVD

→ Square root of the eigenvalues of $X^T X$ gives us the singular values of X

→ U can be found by the same procedure as V, just with XX^T

Singular Value Decomposition (SVD)

How to reduce the dimensions?

Let X= $U\,\Sigma\,V^T$ (with rank(A) = r) and Y = $U\,S\,V^T$, with $S \in \mathbb{R}^{r\,x\,r}$ where $s_i = \lambda_i\ (i = 1\,, \ldots, k)$ else $s_i = 0$

$$\begin{pmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{pmatrix} = \begin{pmatrix} u_{1,1} & \cdots & u_{1,r} \\ \vdots & \ddots & \vdots \\ u_{n,1} & \cdots & u_{n,r} \end{pmatrix} \begin{pmatrix} u_{1,n} \\ \vdots \\ u_{n,n} \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & \cdots & \cdots \\ 0 & \ddots & \vdots & \vdots \\ \vdots & \cdots & \lambda_r & \vdots \\ \vdots & \ldots & \ldots & \lambda_d \end{pmatrix} \begin{pmatrix} v_{1,1} & \cdots & v_{1,d} \\ \vdots & \ddots & \vdots \\ v_{r,1} & \cdots & v_{r,d} \\ v_{d,1} & \cdots & v_{d,d} \end{pmatrix}$$

→ New matrix Y is a **best rank-k approximation to X**

Singular Value Decomposition (SVD) – Example

Ratings of movies by users

	Matrix	Alien	Star Wars	Cassablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	0	0	4	4
Jenny	0	0	0	5	5
Jane	0	0	0	2	2

Let A be a m$\times$n matrix, and let r be the rank of A

Here:

- a rank-2 matrix representing ratings of movies by users
- 2 underlying concepts: science-fiction + romance

Source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

Singular Value Decomposition (SVD) – Example

Ratings of movies by users - SVD

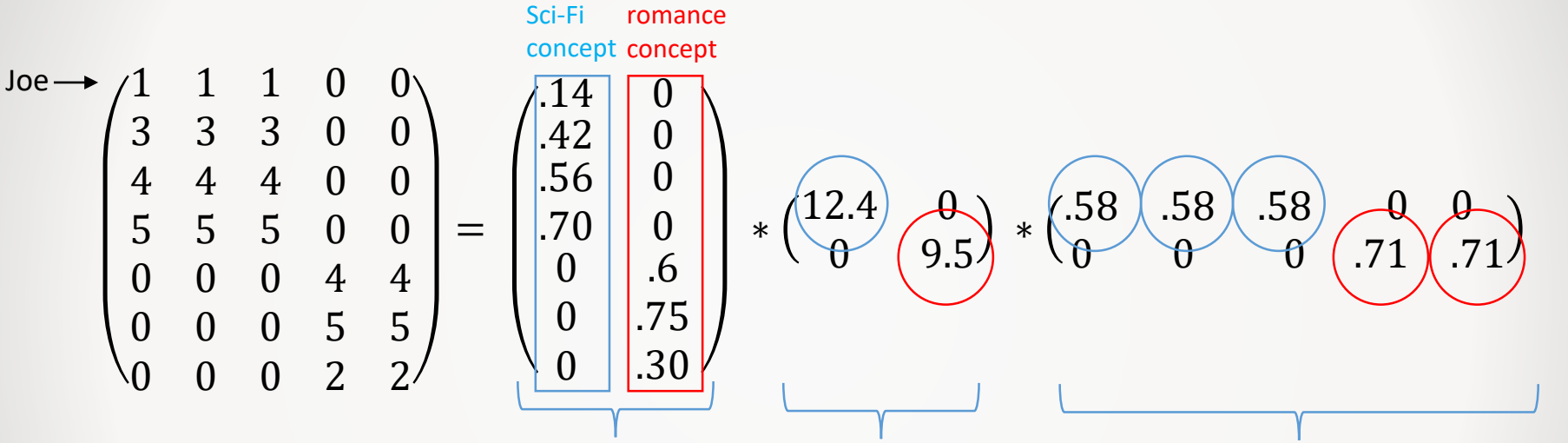
$$\begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 0 & 0 & 2 & 2 \end{pmatrix} = \begin{pmatrix} .14 & 0 \\ .42 & 0 \\ .56 & 0 \\ .70 & 0 \\ 0 & .6 \\ 0 & .75 \\ 0 & .30 \end{pmatrix} * \begin{pmatrix} 12.4 & 0 \\ 0 & 9.5 \end{pmatrix} * \begin{pmatrix} .58 & .58 & .58 & 0 & 0 \\ 0 & 0 & 0 & .71 & .71 \end{pmatrix}$$

$$X = U * \Sigma * V^T$$

- X: Raw data of user -movie-ratings
- U: Connects people to ‚concepts‘
- Σ: ‚strength‘ of each concept
- V^T: Relates movies to concepts

Singular Value Decomposition (SVD) – Example

Ratings of movies by users - SVD Interpretation



SVD and low-rank approximations

Summary

Basic SVD Theorem: Let A be an m x n matrix with rank p

- Matrix A can be expressed as $A = U\,\Sigma\,V^T$
- Truncate SVD of A yields 'best' rank-k approximation given by $A_k = U_k\,\Sigma_k V_k^T$,with $k < d$

Properties of truncated SVD:

- Often used in data analysis via PCA
- Problematic w.r.t sparsity, interpretability, etc.

Problems with SVD / Eigen-analysis

Problems: arise since structure in the data is not respected by mathematical operations on the data

Question: Is there a 'better' low-rank matrix approximations in the sense of …

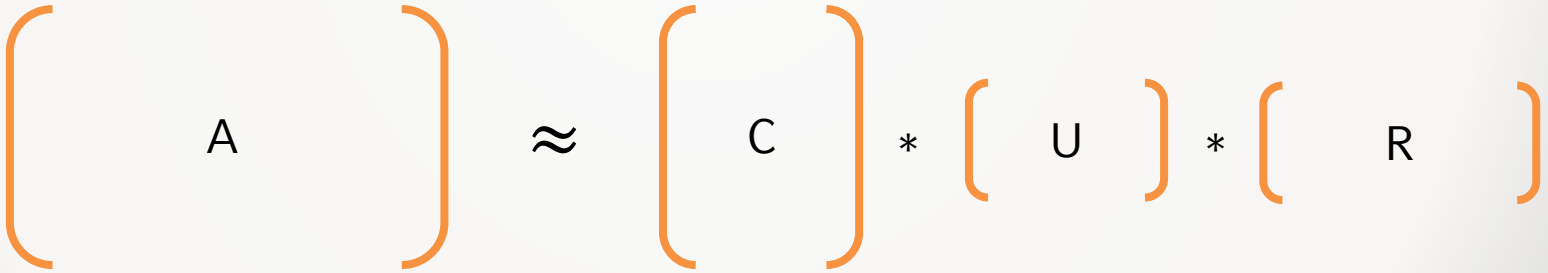
- … **structural properties** for certain application
- … respecting **relevant structure**
- … **interpretability** and **informing intuition**

→ **Alternative: CX and CUR matrix decompositions**

CX and CUR matrix decompositions

Definition CX : A CX decomposition is a low-rank approximation explicitly expressed in terms of a small number of *columns of A.*

Definition CUR : A CUR matrix decomposition is a low-rank approximation explicitly expressed in terms of a small number of ***c****olumns and* ***r****ows of A.*



CUR Decomposition

- *In large-data applications the raw data matrix M tends to be very sparse (e.g. matrix of customers/products , movie recommendation systems…)*
- *Problem with SVD :*
  - *Even if M is sparse, the SVD yields two dense matrices U and V*
- *Idea of CUR Decomposition:*
  - *By sampling a sparse Matrix M, we create two sparse matrices C ('columns') and R ('rows')*

CUR Definition

Input: let $\boldsymbol{M}$ *be a* $\boldsymbol{m \times n}$ ***matrix***

1.Step:

- *Choose a number* $\boldsymbol{r}$ *of 'concepts' (c.f. rank of matrix)*
  - *Perform biased Sampling of* $\boldsymbol{r}$ *cols from* $\boldsymbol{M}$ *and create a* $\boldsymbol{m \times r}$ ***matrix*** $\boldsymbol{C}$
  - *Perform biased Sampling of* $\boldsymbol{r}$ *rows from* $\boldsymbol{M}$ *and create a* $\boldsymbol{r \times n}$ ***matrix*** $\boldsymbol{R}$

2.Step:

- *Construct* $\boldsymbol{U}$ *from* $\boldsymbol{C}$ *and* $\boldsymbol{R}$*:*
  - *Create a* $\boldsymbol{r \times r}$ ***matrix*** $\boldsymbol{W}$ *by the intersection of the chosen cols from C and rows from R*
  - *Apply SVD on* $\boldsymbol{W = X \Sigma Y^t}$
  - *Compute* $\boldsymbol{\Sigma^+}$*, the moore-penrose pseudoinverse of* Σ
  - *Compute* $\boldsymbol{U = Y(\Sigma^+)^2 X^t}$

CUR – how to sample rows and cols from M?

Sample columns for C:

Input: matrix $M \in \mathbb{R}^{m\,x\,n}$, sample size r
Output: $C \in \mathbb{R}^{m\,x\,r}$

1. **For** x = 1 : n **do**
2. P(x) = $\sum_i (m_{i,x})^2$ / $\|M\|_F^2$
3. **For** y = 1 : r **do**
4. Pick $z \in 1{:}n$ based on Prob(x)
5. C(: , y) = M(: , z) / $\sqrt{r * P(z)}$

Frobenius-Norm:

$$\|M\|_F = \sqrt{\sum_i \sum_j (m_{i,j})^2}$$

(sampling of R for rows analogous)

CUR Definition

Example - Sampling

	Matrix	Alien	Star Wars	Cassablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	0	0	4	4
Jenny	0	0	0	5	5
Jane	0	0	0	2	2

Sample columns:

$$\sum_i m_{i,1} = \sum_i m_{i,2} = \sum_i m_{i,3} = 1^2 + 3^2 + 4^2 + 5^2 = 51$$

$$\sum_i m_{i,4} = \sum_i m_{i,5} = 4^2 + 5^2 + 2^2 = 45$$

$$FrobeniusNorm: \|M\|_F^2 = 243$$

➔ $P(x_1) = P(x_2) = P(x_3) = \frac{51}{243} = 0.210$

➔ $P(x_4) = P(x_5) = \frac{45}{243} = 0.185$

CUR Definition

Example - Sampling

	Matrix	Alien	Star Wars	Cassablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	0	0	4	4
Jenny	0	0	0	5	5
Jane	0	0	0	2	2

Sample columns:

- Let r = 2
- Randomly choosen columns, e.g. Star Wars + Cassablanca

$$[1,3,4,5,0,0,0]^T \frac{1}{\sqrt{r * P(x_3)}} = [1,3,4,5,0,0,0]^T \frac{1}{\sqrt{2 * 0.210}}$$
$$= [1.54, 4.63, 6.17, 7.72, 0, 0, 0]^T$$

$$[0,0,0,0,4,5,2]^T \frac{1}{\sqrt{r * P(x_4)}} = [0,0,0,0,4,5,2]^T \frac{1}{\sqrt{2 * 0.185}}$$
$$= [0, 0, 0, 0, 6.58, 8.22, 3.29]^T$$

$$\Rightarrow C = \begin{pmatrix} 1.54 & 0 \\ 4.63 & 0 \\ 6.17 & 0 \\ 7.72 & 0 \\ 0 & 6.58 \\ 0 & 8.22 \\ 0 & 3.29 \end{pmatrix}$$

R is constructed analogous

CUR Definition

Input: let $\boldsymbol{M}$ *be a* $\boldsymbol{m\ x\ n}$ ***matrix***

1.Step:

- *Choose a number* $\boldsymbol{r}$ *of 'concepts' (c.f. rank of matrix)*
  - *Perform biased Sampling of* $\boldsymbol{r}$ *cols from* $\boldsymbol{M}$ *and create a* $\boldsymbol{m\ x\ r}$ ***matrix*** $\boldsymbol{C}$
  - *Perform biased Sampling of* $\boldsymbol{r}$ *rows from* $\boldsymbol{M}$ *and create a* $\boldsymbol{r\ x\ n}$ ***matrix*** $\boldsymbol{R}$

2.Step:

- *Construct* $\boldsymbol{U}$ *from* $\boldsymbol{C}$ *and* $\boldsymbol{R}$*:*
  - *Create a* $\boldsymbol{r\ x\ r}$ ***matrix*** $\boldsymbol{W}$ *by the intersection of the chosen cols from* C *and rows from* R
  - *Apply SVD on* $\boldsymbol{W = X\ \Sigma\ Y^T}$
  - *Compute* $\boldsymbol{\Sigma^+}$*, the moore-penrose pseudoinverse of* Σ
  - *Compute* $\boldsymbol{U = Y(\Sigma^+)^2\ X^T}$

CUR Definition

Example – Calculating U

	Matrix	Alien	Star Wars	Cassablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	0	0	4	4
Jenny	0	0	0	5	5
Jane	0	0	0	2	2

Suppose C (Star Wars, Cassablance) and R (Jenny, Jack)

→ W as intersection of cols from C and rows from R:

$$W = \begin{pmatrix} 0 & 5 \\ 5 & 0 \end{pmatrix}$$

Ensure the correct order!

→ SVD applied on W:

$$W = \begin{pmatrix} 0 & 5 \\ 5 & 0 \end{pmatrix} = X\,\Sigma\,Y^T = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix}\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

→ Pseudo-Inverse of Σ

(replace diagonal entries with their numerical inverse)

$$\Sigma^+ = \begin{pmatrix} 1/5 & 0 \\ 0 & 1/5 \end{pmatrix}$$

→ Compute U

$$U = Y\,(\Sigma^+)^2 X^T = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1/5 & 0 \\ 0 & 1/5 \end{pmatrix}^2\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 1/25 \\ 1/25 & 0 \end{pmatrix}$$

High Dimensionality Data

[1] Less is More: Compact Matrix Decomposition for Large Sparse Graphs, Jimeng Sun, Yinglian Xie, Hui Zhang, and Christos Faloutsos, Proceedings of the 2007 SIAM International Conference on Data Mining. 2007, 366-377

[2] Rajaraman, A.; Leskovec, J. & Ullman, J. D. (2014), *Mining Massive Datasets* .