Data Preprocessing & Dimensionality reduction

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Outline

Distance Measures

Data Exploration and Preprocessing

Dimensionality Reduction

Distance Measures

Machine Learning algorithms capitalize on similarity or distance measures between objects.

Similarity or distance between data points can be expressed as:

- Explicit similarity for each pair of objects
- Similarity obtained indirectly based on data vector attributes.

A distance $d(i,j)$ is a metric iff

1. $d(i,j) \geq 0$ for all i, j and $d(i,j)=0$ iff $i=j$
2. $d(i,j)=d(j,i)$ for all i and j
3. $d(i,j) \leq d(i,k)+d(k,j)$ for all i,j and k

It has to have the *shuffling invariant property*

Distance

- Notation: n objects with p attributes

$$x(i) = (x_1(i), x_2(i), \ldots x_p(i))$$

- Most common distance metric is *Euclidean* distance:

$$d_E(i,j) = \left(\sum (x_k(i) - x_k(j))^2\right)^{1/2}$$

- Makes sense in the case where the different measurements are are proportional; each variable measured in the same units.
- If the measurements are different, length and weight, it is not clear – need for standardization

Weighted Euclidean distance

Finally, if we have some idea of the relative importance of each variable, we can weight them:

$$d_E(i,j) = (\sum w_k (x_k(i) - x_k(j))^2)^{1/2}$$

Other Distance Metrics

Minkowski or L_p metric:

$$d_E(i,j) = (\sum_{k=1}^{p} (x_k(i) - x_k(j))^{\lambda})^{1/\lambda}$$

Manhattan, city block or L_1 metric:

$$d_E(i,j) = \sum_{k=1}^{p} |x_k(i) - x_k(j)|$$

Chebyshev L_∞

$$d_E(i,j) = max_k |x_k(i) - x_k(j)|$$

Variants of the L_1 family

Sorensen $$d_{sor}(i,j) = \frac{\sum_{k=1}^{p} |x_k(i) - x_k(j)|}{\sum_{i=1} |x_k(i) + x_k(j)|}$$

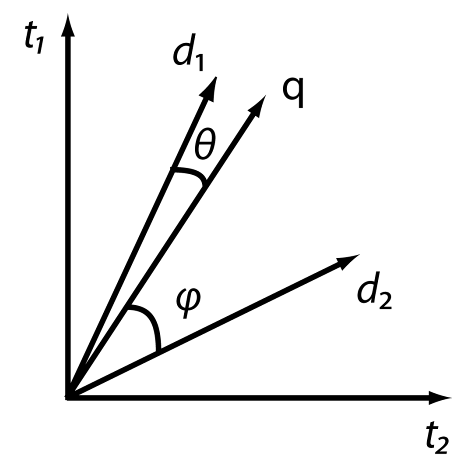
Gowers $$d_{gow}(i,j) = 1/p \sum_{k=1}^{p} |x_k(i) - x_k(j)|$$

Lorentzian $$d_{Lor}(i,j) = \sum_{k=1}^{p} ln(1 + |x_k(i) - x_k(j)|)$$

Inner product family

Inner product $$s_{IP}(i,j) = \sum_{k=1}^{p} x_k(i)x_k(j)$$

Harmonic Mean $$s_{HM}(i,j) = 2\sum_{k=1}^{p} \frac{x_k(i)x_k(j)}{x_k(i)+x_k(j)}$$



Cosine based similarity

$$sim(q,d) = \frac{q \cdot d}{|q||d|} = \frac{\sum_{k=1}^{p} w_{k,q} \cdot w_{k,d}}{\sqrt{\sum_{k=1}^{p} w_{k,q}^2} \cdot \sqrt{\sum_{k=1}^{p} w_{k,d}^2}}$$

Intersection family

Intersection
$$s_{IS}(i,j) = \sum_{k=1}^{p} min((x_k(i), x_k(j))$$

Czekanowski
$$s_{Cze}(i,j) = \frac{2\sum_{k=1}^{p} min(x_k(i), x_k(j))}{\sum_{k=1}^{p}(x_k(i) + x_k(j))}$$

Jaccard
$$s_{Jac}(i,j) = \frac{\sum_{k=1}^{p} x_k(i)x_k(j)}{\sum_{k=1}^{p} x_k(i)^2 + \sum_{k=1}^{p} x_k(j)^2 - \sum_{k=1}^{p} x_k(i)x_k(j)}$$

Dice
$$s_{Dice}(i,j) = \frac{2\sum_{k=1}^{p} x_k(i)x_k(j)}{\sum_{k=1}^{p} x_k(i)^2 + \sum_{k=1}^{p} x_k(j)^2}$$

Comprehensive Survey on Distance/Similarity Measures between Probability Density Functions
Sung-Hyuk Cha, INT. J. OF MATHEMATICAL MODELS AND METHODS IN APPLIED SCIENCES

Squared L2 family

Squared Euclidean

$$d_{sqe}(i,j) = \sum_{k=1}^{p} (x_k(i) - x_k(j))^2$$

Pearson x^2

$$d_{pre}(i,j) = \frac{\sum_{k=1}^{p} (x_k(i) - x_k(j))^2}{x_k(j)}$$

Divergence

$$d_{DIV}(i,j) = 2\sum_{k=1}^{p} \frac{(x_k(i) - x_k(j))^2}{(x_k(i) + x_k(j))^2}$$

Shannon's entropy family

Kullback Leibler $$d_{KL}(i,j) = \sum_{k=1}^{p} x_k(i) ln \frac{x_k(i)}{x_k(j)}$$

Jeffreys $$d_{JF}(i,j) = \sum_{k=1}^{p} (x_k(i) - x_k(j)) ln \frac{x_k(i)}{x_k(j)}$$

K- divergence $$d_{kids}(i,j) = \sum_{k=1}^{p} x_k(i) ln \frac{2x_k(i)}{x_k(i) + x_k(j)}$$

Jensen Shannon

$$d_{JS}(i,j) = 1/2[\sum_{k=1}^{p} x_k(i) ln \frac{2x_k(i)}{x_k(i) + x_k(j)} + \sum_{k=1}^{p} x_k(j) ln \frac{2x_k(j)}{x_k(i) + x_k(j)}]$$

Distance metrics – Nominal values / text

Nominal variables

Number of matches divided by number of dimensions

A	A	B	B	C	B	B	C	C	A
A	B	B	A	C	B	B	C	C	C

7/10

- Edit (Levenshtein) distance

kitten → **s**itten (substitution of "s" for "k")

sitt**e**n → sitt**i**n (substitution of "i" for "e")

sittin → sittin**g** (insertion of "g" at the end)”

Exploratory Data Analysis

Methods not including formal statistical modeling and inference

- Detection of mistakes
- Checking of assumptions
- Preliminary selection of appropriate models
- Determining relationships among the explanatory variables, and
- Assessing the direction and rough size of relationships between explanatory and outcome variables (i.e. demographics – purchase)

Useful information about the data

- Min and Max values
- Mean Value
- Standard Deviation
- Number of instances per value (for nominal data)
- Percentage of missing values
- Data distribution

Data Quality

Random noise in individual measurements

- Variance (precision)
- Bias
- Random data entry errors
- Noise in label assignment (e.g., class labels in medical data sets)

Systematic errors

- E.g., all ages > 99 recorded as 99
- More individuals aged 20, 30, 40, etc than expected

Missing information

- Missing at random
  - Questions on a questionnaire that people randomly forget to fill in
- Missing systematically
  - Questions that people don't want to answer
  - Patients who are too ill for a certain test

Data Quality

- Ideal case = random sample from population of interest
- Real case = often a biased sample of some sort
- Key point: patterns or models from training data are valid on future (test) data only if they are *generated from the same probability distribution*

Examples of non-randomly sampled data

- Medical study where subjects are all students
- Geographic dependencies
- Temporal dependencies
- Stratified samples
  - E.g., 50% healthy, 50% ill
- Hidden systematic effects
  - E.g., market basket data the weekend of a large sale in the store
  - E.g., Web log data during finals week

Standardization

0-1 scaling:

- each variable V is recomputed as

$$(V - min\ V)/(max\ V - min\ V)$$

- allows variables to have differing means and standard deviations but equal ranges.
- at least one value at the 0 and 1 endpoints.

Dividing each value by the range:

- each variable V is recomputed as

$$V/(max\ V - min\ V).$$

- means, variances, and ranges of the variables are still different
- ranges are likely to be more similar.

Standardization

Z-score scaling:

- each variable V is recomputed as $(V - mean\ of\ V)/s$, s standard deviation.
- all variables have equal means (0) and standard deviations (1) but different ranges.

Dividing each value by the standard deviation.

- transformed variables with variances of 1
- different means and ranges.

Dependence among Variables

Covariance and correlation measure linear dependence

Assume variables X and Y and n objects taking on values

$x(1), \ldots, x(n)$ and $y(1), \ldots, y(n)$.

Sample covariance of X and Y is:

$$Cos(X,Y) = \frac{1}{N}\sum_{1}^{n}(x(i) - \overline{x})(y(i) - \overline{y})$$

The covariance is a measure of how X and Y vary together.

large and positive if large values of X are associated with large values of Y, and small $X \Rightarrow$ small Y

Sample correlation coefficient

- Covariance depends on ranges of X and Y
- Standardize dividing with standard deviation

Sample correlation coefficient

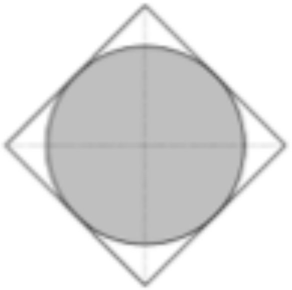
$$\rho(X,Y) = \frac{\sum_{i=1}^{n}(x(i)-\bar{x})(y(i)-\bar{y})}{\left(\sum_{i=1}^{n}(x(i)-\bar{x})^2 \sum_{i=1}^{n} (y(i)-\bar{y})^2\right)^{\frac{1}{2}}}$$

Dimensionality Reduction

Curse of Dimensionality

- Some coordinates do not contribute to the data representation.
- Subsets of the dimensions may be highly correlated.
- Nearest neighbor is distorted in a high dimensional space
- Low dimension intuitions do not apply to high dimensions
- Empty space phenomenon

Empty space phenomenon



Hyper sphere within a hyper rectangle

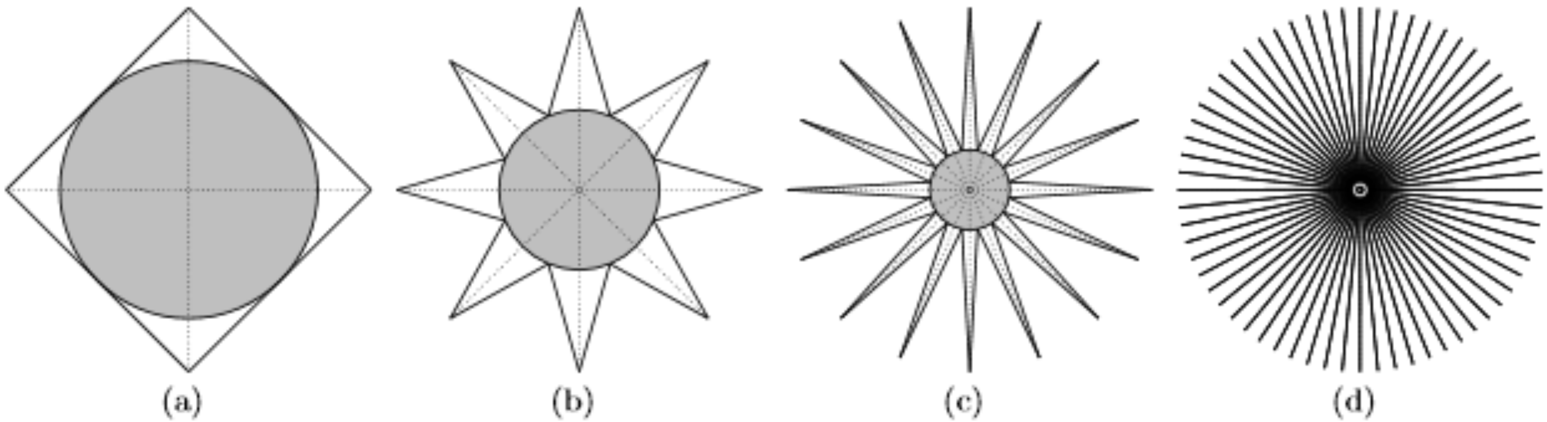
Respective volumes: $\mathbf{V}(\boldsymbol{S}) = {2r^d\pi^{\frac{d}{2}}}\Big/{d\Gamma(d/2)}, \boldsymbol{V}(\boldsymbol{R}) = (\mathbf{2}\boldsymbol{r})^{\boldsymbol{d}}$

The fraction of the sphere within the rectangle becomes insignificant with d increasing:

$$\lim_{d\to\infty}\left({\pi^{\frac{d}{2}}}\Big/{d2^{d-1}\Gamma(d/2)}\right) = 0$$

- the normal distribution in high dimensions
- longest/shortest distances converge.
- clustering becomes infeasible

Inscription of hyper sphere in a hypercube



The radius of the inscribed circle accurately reflects the difference between the volume of the hypercube and the inscribed hypersphere in d-dimensions.

http://www.cs.rpi.edu/~zaki/www-new/uploads/Dmcourse/Main/chap6.pdf

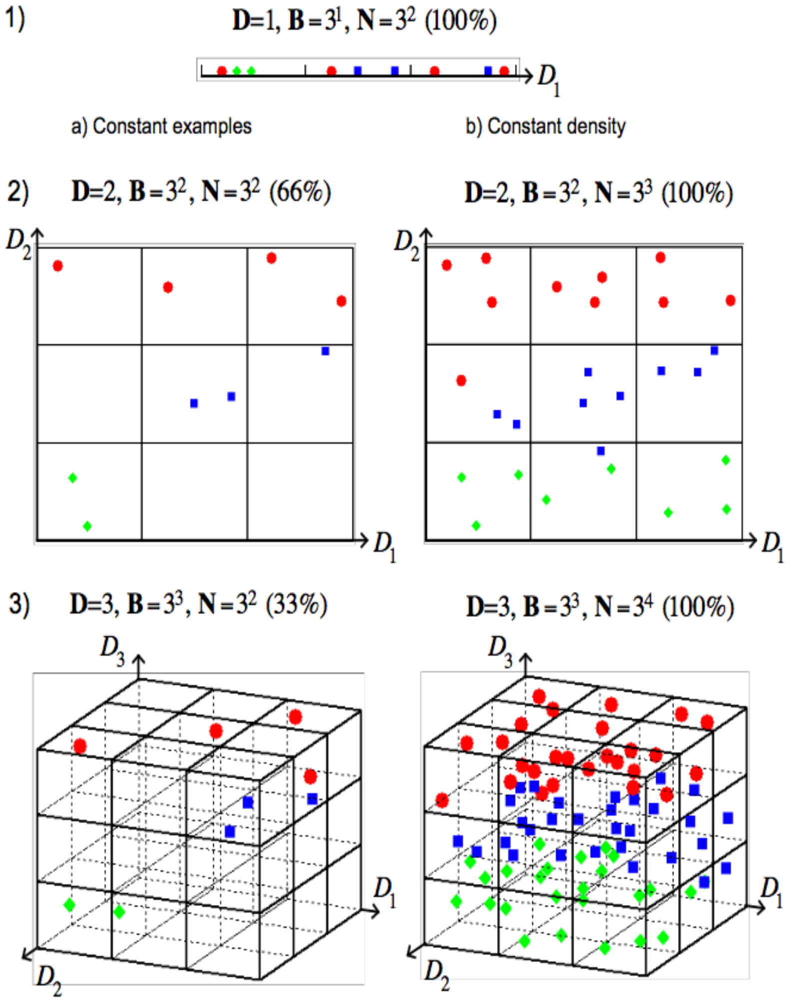
Curse of Dimensionality [Belmann 1961]

- Some coordinates do not contribute to the data representation.
- Subsets of the dimensions may be highly correlated.
- Nearest neighbor is distorted in a high dimensional space
- Low dimension intuitions do not apply to high dimensions

Curse of Dimensionality

Assuming 3 classes (colors)

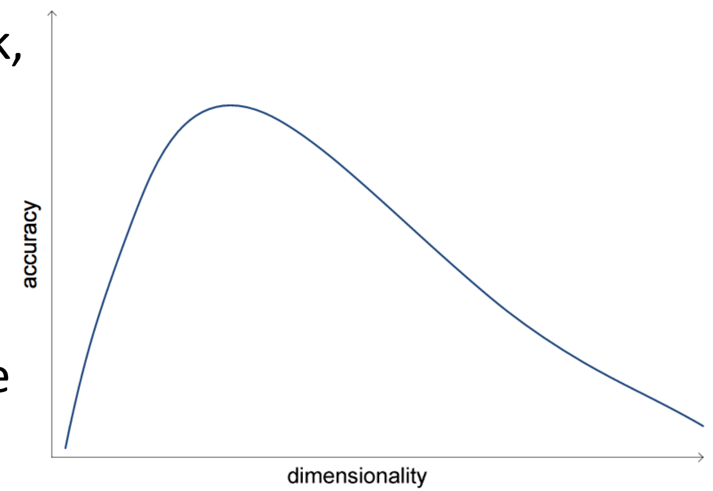
- same number of points embedded in higher dimensions (sparsity)
- need exponentially more points to maintain density in higher dimensions (curse of dimensionality)
- Data tend to gather in extremes of small areas of the multidimensional space (empty space phenomenon)



Curse of Dimesionality

Point queries

- “contrast in distances to different data points becomes nonexistent” - “When Is “Nearest Neighbor” Meaningful? “ - Beyer et al., [1999]
- Increasing dimensionality may decrease of overall accuracy of system according to statistical learning theory approach [Vapnik, 1998].
- for a given dataset, there is a maximum number of dimensions above which the quality of data analysis degrades when the number of training samples is small relative to dimensionality



Deterministic dimensionality reduction

- methods optimise an objective function
- does not contain any local optima - the solution space is convex [Boyd and Vandenberghe, 2004].
- has usually the form of a (generalised) Rayleigh-Ritz and therefore is optimized by solving the (generalized) eigenvalue problem.
- final embedded space formed by eigenvectors which correspond to smallest or largest eigenvalues.

Deterministic methods classification

- *Global methods:* eigen-decomposition of a dense cost matrix
  - Methods: Principal Component Analysis, Multidimensional Scaling, Kernel Principal Component Analysis, Isomap, Maximum Variance Unfolding
- *Local methods:* eigen-decomposition of a sparse cost matrix
  - Methods: Locally Linear Embedding, Laplacian Eigenmaps).

Dim. Reduction – Linear Algorithms

Matrix Factorization methods

- Principal Components Analysis (PCA)
- Singular Value Decomposition (SVD)
- Multidimensional Scaling (MDS)
- Non negative Matrix Factorization (NMF)
- Latent Semantic Indexing (LSI)

Low Rank Approximation

Data: $\boldsymbol{X} = \{\boldsymbol{x_i} \in \boldsymbol{R^{mxn}} | \boldsymbol{x_i}$ **columns of** $\boldsymbol{X}\}$

Goal: approximate $\boldsymbol{X} = \boldsymbol{UV^T}$,

$\boldsymbol{U} \in \boldsymbol{R^{mxr}}$, $\boldsymbol{V} \in \boldsymbol{R^{nxr}}$, , $\boldsymbol{r<<n}$

- each data vector $\boldsymbol{x_i}$: $\boldsymbol{x_i} \sim \mathrm{U}\boldsymbol{v_i}^T$, $\boldsymbol{v_i}$ is the i-th column of $\boldsymbol{V}$.

Geometric interpretation:

- each data vector $\boldsymbol{x_i} \in \boldsymbol{R^m}$, $_i\sim \mathrm{U}\boldsymbol{v_i}^T$, is approximated by its projection to an r-dimesional space spanned by the column vectors of U
- $\boldsymbol{Y} = \boldsymbol{U}\,\boldsymbol{V^T}$ the approximation matrix, max rank r

Evaluating the approximation

- Assuming a matrix A_{mxn} we need to define their similarity/distance.
- A popular matrix norm is the Frobenius (L_2 norm treated as a vector)

$$|A|_F = \sum_{i=1}^{m}\sum_{j=1}^{n} \alpha_{ij}^2 = \sum_{i=1}^{min(m,n)} \sigma_i^2$$

- So assuming: $X = UV^T$

- the error approximation will be: $|X - UV^T|_2$

SOME CONTRIBUTIONS TO DIMENSIONALITY REDUCTION, Wei Tong, Ph.D. thesis, 2010, Michigan State University
http://www.ece.uprm.edu/~domingo/teaching/ciic8996/SOME%20CONTRIBUTIONS%20TO%20DIMENSIONALITY%20REDUCTION.pdf

Dim. Reduction–Eigenvectors

A nxn matrix

- eigenvalues λ: $|A-\lambda I|=0$
- Eigenvectors $x : Ax=\lambda x$
- Matrix rank: # linearly independent rows or columns
- A real symmetric table A nxn can be expressed as: $A=U\Lambda U^T$
- U's columns are A's eigenvectors
- Λ' s diagonal contains A's eigenvalues
- $A=U\Lambda U^T=\lambda_1 x_1 x^T{}_1+\lambda_2 x_2 x^T{}_2+\ldots+\lambda_n x_n x^T{}_n$
- $x_1 x^T{}_1$ represents projection via x_1 (λ_i eigenvalue, x_i eigenvector)
- Interpretations: xx^T vs. x^Tx

Singular Value Decomposition (SVD)

Eigen values and eigenvectors decomposition is applied to square matrices. For non square matrices we apply ***Singular Value Decomposition.***

Let **X** a **mxn table**, $X = U\Sigma V^T$

U : orthogonal mxm, its columns are the eigenvectors of XX^T.

U,V define orthogonal basis: $U^TU = VV^T = 1$

Σ: mxn contains A's singular values (square roots of XX^T eigenvalues)

V : nxn, its columns are the eigenvectors of X^TX

Singular Value Decomposition (SVD) - I

Proof:

$X = U\Sigma V^T$, $X^T = V\Sigma^T U^T$ =>

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

Similarly: $X^T X = V\Sigma^T\Sigma V^T$

Therefore: U: eigenvectors of XX^{T} (V: eigenvectors of $X^T X$)

Σ: sqrt of the eigenvalues of XX^T

X k-dimensional representation: $\boldsymbol{X_k = U_k \Sigma_k V_k{}^T}$

Singular Value Decomposition (SVD) - II

Matrix approximation $X_k = U_k \Sigma_k {V_k}^T$

The best rank κ approximation Y' of a matrix X. (minimizing the Frobenius norm)

$$||X||_F = \sqrt{\sum_1^m \sum_1^n x_{ij}^2} = \sqrt{trace(X^T X)} = \sqrt{\sum_{i=1}^{min(m,n)} \sigma_I^2(X)}$$

Where X^T transpose of A, σi are the singular values of X, and the trace function is used.

Multidimensional Scaling (MDS)

- Decomposition of the data similarity matrix: XX^T
- Aim to minimize the stress:

$$stress = \frac{\sum_{ij}(d(i,j) - d'(i,j))^2}{\sum_{ij}(d(i,j))^2}$$

  Complexity $O(N^3)$ (N: number of vectors)

- Result:
  - A new representation of the data in a lower dimensional space.
- Implement usually by:
  - Eigen decomposition of the inner product matrix
  - projection on the k eigenvectors corresponding to the k largest eigenvalues.

Multidimensional Scaling

- **Data is given as rows in X**
  - $C=XX^T$ (inner product of x_i with x_j)
  - Eigen decomposition of $C' = ULU^{-1}$
  - Eventually $X' = U_k L_k^{1/2}$, where k is the projection dimension

$$X=\begin{bmatrix} 2 & 3 & 4 & 5 \\ 6 & 4 & 2 & 6 \\ 1 & 5 & 6 & 8 \\ 1 & 4 & 4 & 6 \\ 3 & 4 & 9 & 5 \end{bmatrix}$$

$\downarrow XX^T$

$$C=\begin{bmatrix} 54. & 62. & 81. & 60. & 79. \\ 62. & 92. & 86. & 66. & 82. \\ 81. & 86. & 126. & 93. & 117. \\ 60. & 66. & 93. & 69. & 85. \\ 79. & 82. & 117. & 85. & 131. \end{bmatrix}$$

EVD

$$U=\begin{bmatrix} -0.3540571 & -0.0266618 & -0.0427173 & 0.7674171 & -0.5321456 \\ -0.4041785 & -0.8612673 & 0.2512931 & -0.1004458 & 0.1470402 \\ -0.5309769 & 0.1813750 & -0.5293206 & 0.1591309 & 0.6161685 \\ -0.3931327 & 0.0342107 & -0.4240133 & -0.5922139 & -0.5601532 \\ -0.5242075 & 0.4726950 & 0.6892456 & -0.1579292 & 0.0420115 \end{bmatrix}$$

$$L=\begin{bmatrix} 429.83919 & 28.182284 & 13.857017 & 0.1215106 & 1.380D-14 \end{bmatrix}$$

$$X'=U_2L_2^{1/2}=\begin{bmatrix} -152.18764 & -0.7513907 \\ -173.73175 & -24.27248 \\ -228.23469 & 5.1115622 \\ -168.98385 & 0.9641354 \\ -225.32491 & 13.321624 \end{bmatrix}$$

Principal Components Analysis

The main concept behind *Principal Components Analysis* is dimensionality reduction, maintaining as much as possible data's variance.

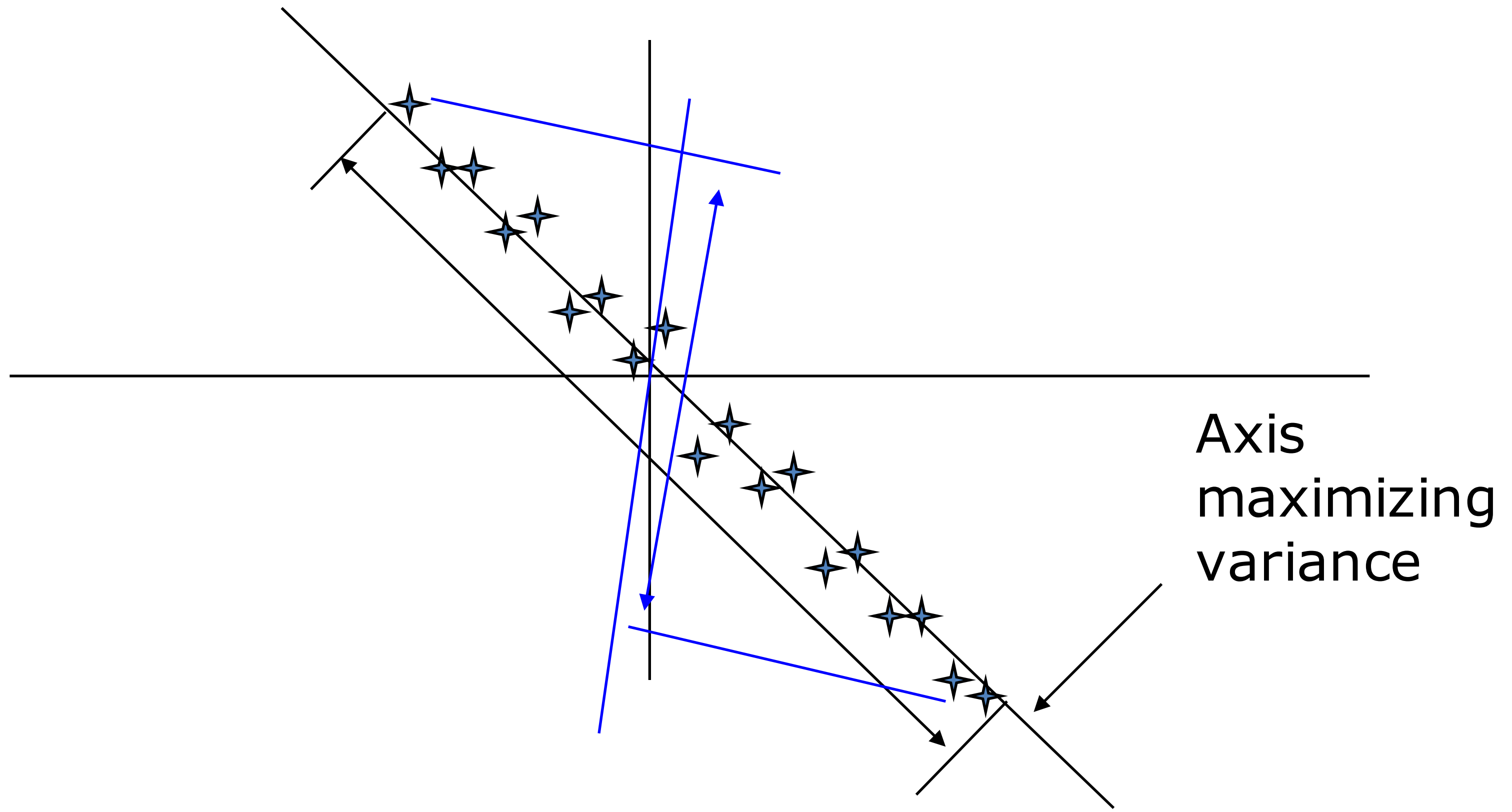
variance: $V(X)=\sigma^2=E[(X-\mu)^2]$

Let *N* objects, with mean value, *m*, it is approximated as:

$$\frac{1}{N}\sum_{i=1}^{N}(x_i-m)^2,$$

Sample of *N* objects with unknown mean value: $\frac{1}{N-1}\sum_{i=1}^{N}(x_i-\overline{x})^2,$

Dimensionality reduction based on variance maintenance



Covariance Matrix

Let Matrix $X = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix}$ ere Xi vectors

covariance matrix Σ is the matrix whose (i, j) entry is the covariance

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

Also: $cov(X) = X'^T X'$, where $X' = X\text{-}M$

Principal Components Analysis (PCA)

- **PCA intuition: maximization of the covariance.**
  - Variance: Depicts the maximum deviation of a random variable from the mean.

$$\sigma^2 = \sum_{i=1}^{n} (x_i - \mu_i)^2 / n$$

- **Method:**
  - Assumption: Data is described by p variables and contained as rows in matrix X_{pxn}
  - We subtract mean values from columns. $X' = (X - M)$
  - Calculate covariance matrix $W = X'^T X'$

Principal Components Analysis (PCA) – (2)

- Calculation of covariance matrix (W)
  - A matrix nxn, in each cell of which (i,j) we have the covariance of X_i, X_j.
- Calculate eigenvalues and eigenvectors of

$$W = U\Lambda U^T$$

- Retain k largest eigenvalues and eigenvectors
  - k is an input parameter
  - k is estimated by $\sum^{p}{}_{j=k+1}\lambda_j / \sum^{p}{}_{j=1}\lambda_j > 85\%$

- Projection : $A'Xk$

Principal Components Analysis

$X=$

x_1	2	3	4	5
x_2	6	4	2	6
x_3	1	5	6	8
x_4	1	4	4	6
x_5	3	4	9	5

15 20 25 30

$\Sigma_{j=1}^{5} x_{ij}$

$\text{sum}_j/5$

3 4 5 6

$x_{ij} - m_j$

$X'=$

x_1	-1	-1	-1	-1
x_2	3	0	-3	0
x_3	1	1	1	2
x_4	-2	-1	-1	1
x_5	0	0	0	-1

$X'^T X'$

$(\Sigma_{f=1}^{5}(x_{if}-m_i)(x_{jf}-m_j))/4$

Cov=

3.70	1.05	-1.05	0.2
1.05	0.7	0.55	0.55
-1.05	0.55	2.20	0.70
0.2	0.55	0.70	1.70

$Cov = ULU^T$

U=

-0.90	-0.18	-0.19	0.34
-0.20	-0.40	-0.20	-0.86
0.38	-0.66	-0.54	0.34
-0.01	-0.60	0.78	0.09

L=

4.38	2.89	1.02	0.004

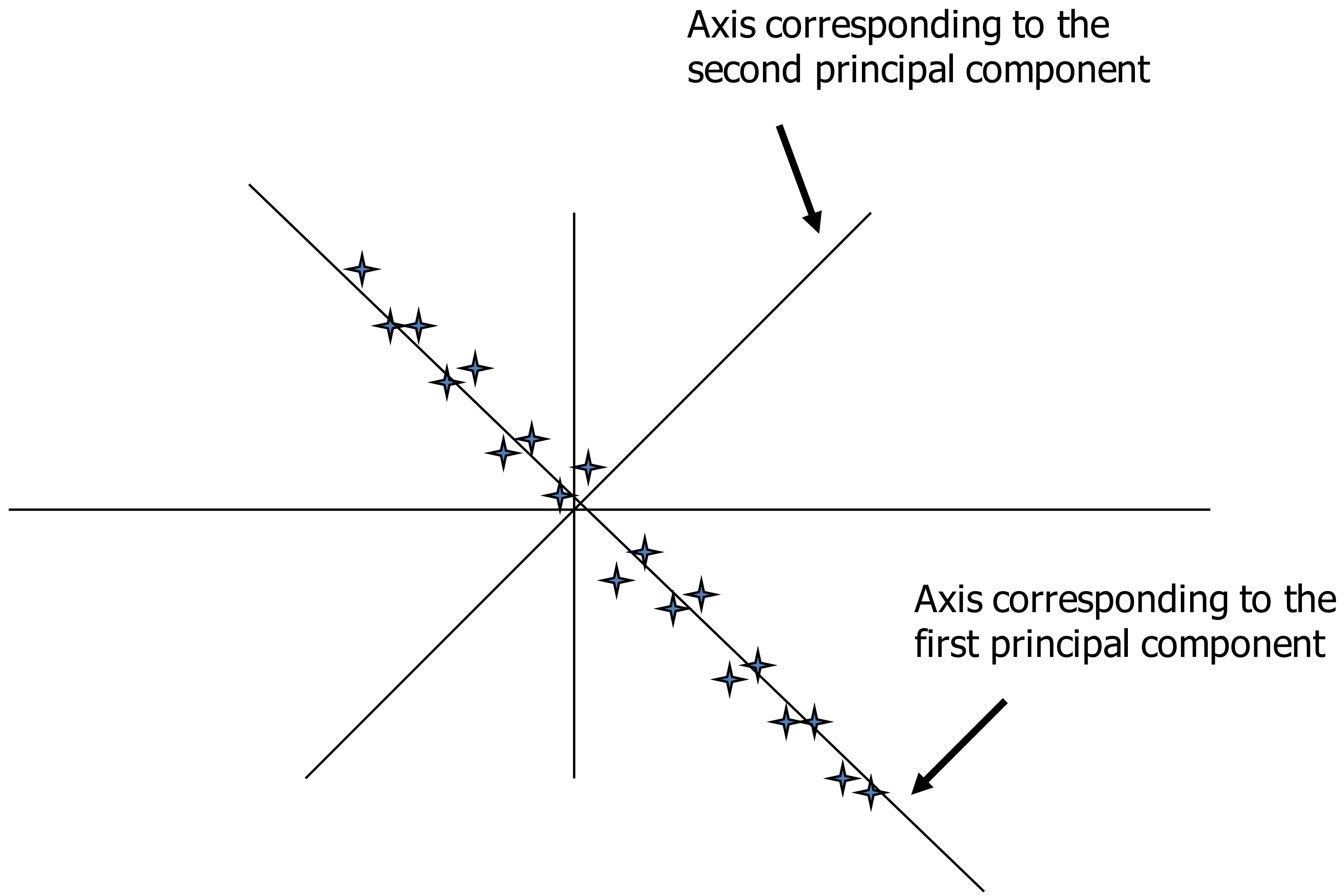
k=2

-0.90	**-0.18**
-0.20	**-0.40**
-0.38	**-0.66**
-0.01	**-0.60**

$X'U_k$

2.2	1.16
0	0
-2.4	-1.56
2.7	0.54
0.2	0.4

PCA, example


Axis corresponding to the
second principal component
Axis corresponding to the
first principal component

PCA Synopsis & Applications

- Preprocessing step preceding the application of data mining algorithms (such as clustering).
- Data Visualization & Noise reduction.

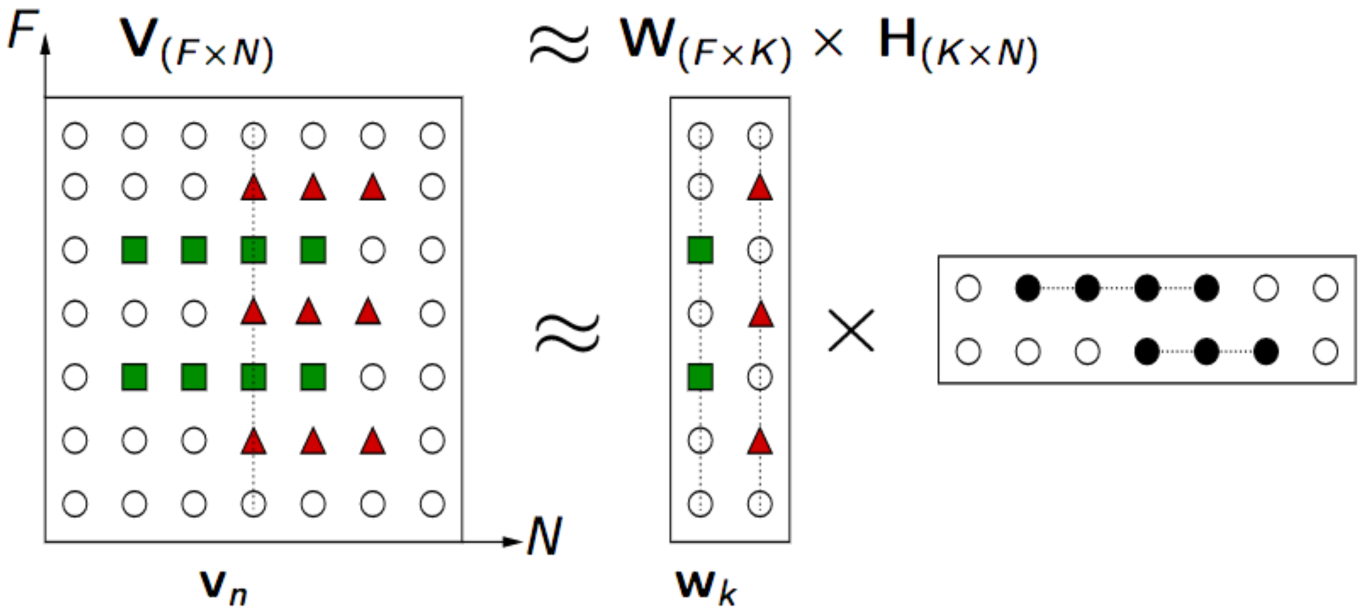
- It is a dimensionality reduction method
- Nominal complexity $O(np^2+p^3)$

  n: number of data points

  p: number of initial space dimensions

- The new space maintains sufficiently the data variance.

Explaining data by factorization



data matrix

"explanatory variables"
"basis", "dictionary",
"patterns", "topics"

"regressors",
"activation coefficients",
"expansion coefficients"

Illustration by C. Févotte

Non Negative Matrix factorization (NMF)

- Data is often nonnegative by nature
    - pixel intensities; occurrence counts; food or energy consumption; user scores; stock market values;
- Interpretability of the results, optimal processing of nonnegative data may call for processing under Nonnegativity constraints

.

- Applying SVD results in factorized matrices with positive and negative elements may contradict the physical meaning of the result.

  - *Nonnegative matrix factorization (NMF)*

  find the reduced rank *nonnegative factors* to approximate a given nonnegative data matrix.

NMF model

$V \simeq WH$

- $W = [w_{fk}],\ w_{fk} >= 0$
- $H = [h_{kn}],\ h_{kn} >= 0$
- $k << f, n$

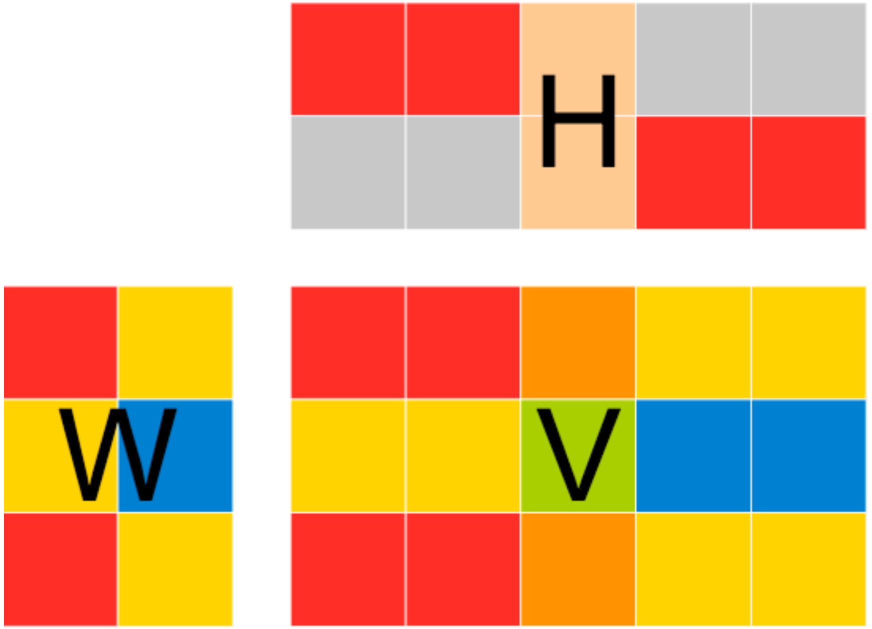


Illustration by N. Seichepine

NMF

Assume X (mxn) data matrix and r<< m,n

NMF aims to find non negative matrices

$$U \in R^{mxr}, V \in R^{rxn} : X \approx UV^T$$

To find U.V, optimization problem:

$$min_{(U,V)} ||X - UV^T||_2$$

Alternative error function:

$$\min_{U,V} \quad f(U,V) = \sum_{i=1}^{m} \sum_{j=1}^{n} \left(X_{ij} \log \frac{X_{ij}}{(UV^\top)_{ij}} - X_{ij} + (UV^\top)_{ij} \right)$$
$$\text{s. t.} \quad U_{ia} \geq 0, V_{jb} \geq 0, \forall i, a, b, j.$$

Alternating Least squares

1. Suppose we know U, $with\ V$ unknown.

for each j we could minimize $||X_{.j} - UV_{.j}^T||_2$

- find $V_{\cdot j}$ that minimizes with $X_{\cdot j}$ and U known.
- Frobenius norm: sum of squares,
  - minimization is a least-squares problem, i.e. linear regression
  - "predicting" $X.j$ from W.

$$V_{.j} = (U^T U)^{-1} U^T X.j$$

- repeat for all columns $V_{\cdot j}$

2. assume V, $with\ U$ unknown: $X^T = VU^T$
   - Interchange roles of U, V in the above optimization
   - Compute a row of U, repeat for all rows

Alternating Least squares

Putting all this together

- first choose initial guesses, random numbers,for U and V
- alternate:
  - Compute U assuming V known
  - Compute V based on that new U
  - …
- may generate negative values: truncate to 0

Other NMF Algorithms

Multiplicative: updating solutions U and V

$$V_{bj}^{\top} \leftarrow V_{bj}^{\top} \frac{\left(U^{\top} X\right)_{bj}}{\left(U^{\top} U V^{\top}\right)_{bj}} \qquad U_{ia} \leftarrow U_{ia} \frac{(XV)_{ia}}{(UV^{\top}V)_{ia}}$$

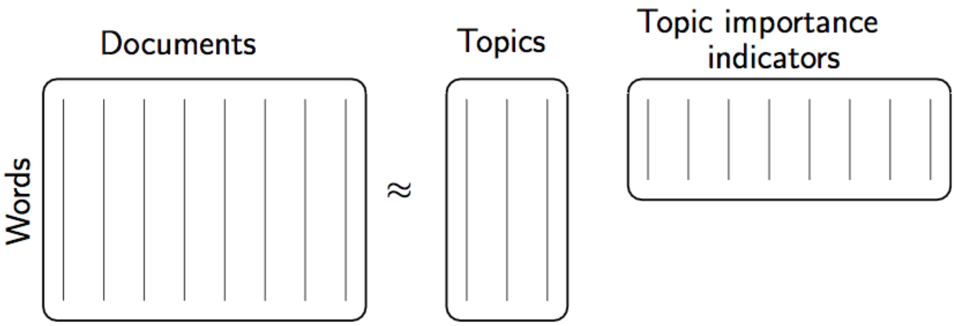
Gradient descent algorithms

$$V_{bj}^{\top} \leftarrow V_{bj}^{\top} - \epsilon_V \frac{\partial f}{\partial V_{bj}^{\top}} \qquad U_{ia} \leftarrow U_{ia} - \epsilon_U \frac{\partial f}{\partial U_{ia}}$$

ε_V and ε_U are the step sizes.

NMF issues, applications

- Uniqueness and Convergence
- U_{mxr} , r (rank) choice: via SVD…
- Applications
  - Topic detection
  - Source separation (music , speech)
  - Clustering
  - Recommendations



SVD application - Latent Structure in documents

- Documents are represented based on the Vector Space Model
- Vector space model consists of the keywords contained in a document.
- In many cases baseline keyword based performs poorly – not able to detect synonyms.
- Therefore document clustering is problematic
- Example where of keyword matching with the query: “IDF in computer-based information look-up”

	access	document	retrieval	information	theory	database	indexing	computer
Doc1	x	x	x			x	x	
Doc2				x	x			x
Doc3			x	x				x

Indexing by Latent Semantic Analysis (1990) Scott Deerwester, Susan T. Dumais, George W. Furnas, Thomas K. Landauer, Richard Harshman, Journal of the American Society of Information Science

Latent Semantic Indexing (LSI) -I

- Finding similarity with exact keyword matching is problematic.
- Using SVD we process the initial document-term document.
- Then we choose the k larger singular values. The resulting matrix is of order k and is the most similar to the original one based on the Frobenius norm than any other k-order matrix.

Latent Semantic Indexing (LSI) - II

- The initial matrix is SVD decomposed as: $A=ULV^T$
- Choosing the top-k singular values from L we have:

$$A_k=U_kL_kV_k^T \ ,$$

- L_k is square kxk containing the top-k singular values of the diagonal in matrix L,
- $U_{k,}$ the mxk matrix containing the first k columns in U (left singular vectors)
- $V_k^{T,}$ the kxn matrix containing the first k lines of V^T (right singular vectors)

Typical values for κ~200-300 (empirically chosen based on experiments appearing in the bibliography)

LSI capabilities

- Term to term similarity: $A_k A_k^T = U_k L_k^2 U_k^T$

  $A_k = U_k L_k V_t$

- Document-document similarity: $A_k^T A_k = V_k L_k^2 V_k^T$

- Term document similarity (as an element of the transformed – document matrix)

- Extended query capabilities transforming initial query q to q_n : $q_n = q^T U_k L_k^{-1}$

- Thus q_n can be regarded a line in matrix V_k

LSI – an example

LSI application on a term – document matrix

C1: Human machine Interface for Lab ABC computer application

C2: A survey of user opinion of computer system response time

C3: The EPS user interface management system

C4: System and human system engineering testing of EPS

C5: Relation of user-perceived response time to error measurements

M1: The generation of random, binary unordered trees

M2: The intersection graph of path in trees

M3: Graph minors IV: Widths of trees and well-quasi-ordering

M4: Graph minors: A survey

- The dataset consists of 2 classes, 1st: “human – computer interaction” (c1-c5) 2nd: related to graph (m1-m4). After feature extraction the titles are represented as follows.

Indexing by Latent Semantic Analysis (1990) Scott Deerwester, Susan T. Dumais, George W. Furnas, Thomas K. Landauer, Richard Harshman, Journal of the American Society of Information Science

LSI – an example

	C1	C2	C3	C4	C5	M1	M2	M3	M4
human	1	0	0	1	0	0	0	0	0
Interface	1	0	1	0	0	0	0	0	0
computer	1	1	0	0	0	0	0	0	0
User	0	1	1	0	1	0	0	0	0
System	0	1	1	2	0	0	0	0	0
Response	0	1	0	0	1	0	0	0	0
Time	0	1	0	0	1	0	0	0	0
EPS	0	0	1	1	0	0	0	0	0
Survey	0	1	0	0	0	0	0	0	1
Trees	0	0	0	0	0	1	1	1	0
Graph	0	0	0	0	0	0	1	1	1
Minors	0	0	0	0	0	0	0	1	1

LSI – an example

$A=ULV^T$

A=

1	0	0	1	0	0	0	0	0
1	0	1	0	0	0	0	0	0
1	1	0	0	0	0	0	0	0
0	1	1	0	1	0	0	0	0
0	1	1	2	0	0	0	0	0
0	1	0	0	1	0	0	0	0
0	1	0	0	1	0	0	0	0
0	0	1	1	0	0	0	0	0
0	1	0	0	0	0	0	0	1
0	0	0	0	0	1	1	1	0
0	0	0	0	0	0	1	1	1
0	0	0	0	0	0	0	1	1

LSI – an example

$A=ULV^T$

U=

0.22	-0.11	0.29	-0.41	-0.11	-0.34	0.52	-0.06	-0.41	0	0	0
0.20	-0.07	0.14	-0.55	0.28	0.50	-0.07	-0.01	-0.11	0	0	0
0.24	0.04	-0.16	-0.59	-0.11	-0.25	-0.30	0.06	0.49	0	0	0
0.40	0.06	-0.34	0.10	0.33	0.38	0.00	0.00	0.01	0	0	0
0.64	-0.17	0.36	0.33	-0.16	-0.21	-0.17	0.03	0.27	0	0	0
0.27	0.11	-0.43	0.07	0.08	-0.17	0.28	-0.02	-0.05	0	0	0
0.27	0.11	-0.43	0.07	0.08	-0.17	0.28	-0.02	-0.05	0	0	0
0.30	-0.14	0.33	0.19	0.11	0.27	0.03	-0.02	-0.17	0	0	0
0.21	0.27	-0.18	-0.03	-0.54	0.08	-0.47	-0.04	-0.58	0	0	0
0.01	0.49	0.23	0.03	0.59	-0.39	-0.29	0.25	-0.23	0	0	0
0.04	0.62	0.22	0.00	-0.07	0.11	0.16	-0.68	0.23	0	0	0
0.03	0.45	0.14	-0.01	-0.30	0.28	0.34	0.68	0.18	0	0	0

LSI – an example

$A = ULV^T$

L=

3.34	0	0	0	0	0	0	0	0
0	2.54	0	0	0	0	0	0	0
0	0	2.35	0	0	0	0	0	0
0	0	0	1.64	0	0	0	0	0
0	0	0	0	1.50	0	0	0	0
0	0	0	0	0	1.31	0	0	0
0	0	0	0	0	0	0.85	0	0
0	0	0	0	0	0	0	0.56	0
0	0	0	0	0	0	0	0	0.36
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0

LSI – an example

$A = ULV^T$

$V=$

0.20	-0.06	0.11	-0.95	0.05	-0.08	0.18	-0.01	-0.06
0.61	0.17	-0.50	-0.03	-0.21	-0.26	-0.43	0.05	0.24
0.46	-0.13	0.21	0.04	0.38	0.72	-0.24	0.01	0.02
0.54	-0.23	0.57	0.27	-0.21	-0.37	0.26	-0.02	-0.08
0.28	0.11	-0.51	0.15	0.33	0.03	0.67	-0.06	-0.26
0.00	0.19	0.10	0.02	0.39	-0.30	-0.34	0.45	-0.62
0.01	0.44	0.19	0.02	0.35	-0.21	-0.15	-0.76	0.02
0.02	0.62	0.25	0.01	0.15	0.00	0.25	0.45	0.52
0.08	0.53	0.08	-0.03	-0.60	0.36	0.04	-0.07	-0.45

LSI – an example

Choosing the 2 largest singular values we have

U_k=

0.22	-0.11
0.20	-0.07
0.24	0.04
0.40	0.06
0.64	-0.17
0.27	0.11
0.27	0.11
0.30	-0.14
0.21	0.27
0.01	0.49
0.04	0.62
0.03	0.45

L_k=

3.34	0
0	2.54

V_k^T=

0.20	0.6 1	0.46	0.54	0.28	0.00	0.02	0.02	0.08
- 0.06	0.1 7	-0.13	-0.23	0.11	0.19	0.44	0.62	0.53

LSI (2 singular values)

$A_k =$

	C1	C2	C3	C4	C5	M1	M2	M3	M4
human	0.16	0.40	0.38	0.47	0.18	-0.05	-0.12	-0.16	-0.09
Interface	0.14	0.37	0.33	0.40	0.16	-0.03	-0.07	-0.10	-0.04
Computer	0.15	0.51	0.36	0.41	0.24	0.02	0.06	0.09	0.12
User	0.26	0.84	0.61	0.70	0.39	0.03	0.08	0.12	0.19
System	0.45	1.23	1.05	1.27	0.56	-0.07	-0.15	-0.21	-0.05
Response	0.16	0.58	0.38	0.42	0.28	0.06	0.13	0.19	0.22
Time	0.16	0.58	0.38	0.42	0.28	0.06	0.13	0.19	0.22
EPS	0.22	0.55	0.51	0.63	0.24	-0.07	-0.14	-0.20	-0.11
Survey	0.10	0.53	0.23	0.21	0.27	0.14	0.31	0.44	0.42
Trees	-0.06	0.23	-0.14	-0.27	0.14	0.24	0.55	0.77	0.66
Graph	-0.06	0.34	-0.15	-0.30	0.20	0.31	0.69	0.98	0.85
Minors	-0.04	0.25	-0.10	-0.21	0.15	0.22	0.50	0.71	0.62

LSI Example

- Query: "human computer interaction" retrieves documents: c_1,c_2, c_4 but *not* c_3 and c_5.
- If we submit the same query (based on the transformation shown before) to the transformed matrix we retrieve (using cosine similarity) all c_1-c_5 even if c_3 and c_5 have no common keyword to the query.
- According to the transformation for the queries we have:

Query transformation

	query
human	1
Interface	0
computer	1
User	0
System	0
Response	0
Time	0
EPS	0
Survey	0
Trees	0
Graph	0
Minors	0

$$q = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Query transformation

$q^T=$

1	0	1	0	0	0	0	0	0	0	0	0

$U_k=$

0.22	-0.11
0.20	-0.07
0.24	0.04
0.40	0.06
0.64	-0.17
0.27	0.11
0.27	0.11
0.30	-0.14
0.21	0.27
0.01	0.49
0.04	0.62
0.03	0.45

$L_k=$

0.3	0
0	0.39

$q_n=q^TU_kL_k=$

0.138	-0.0273

Query transformation

Map docs to the 2 dim space $V_k L_k =$

0.20	-0.06
0.61	0.17
0.46	-0.13
0.54	-0.23
0.28	0.11
0.00	0.19
0.01	0.44
0.02	0.62
0.08	0.53

3.34	0
0	2.54

=

0.67	-0.15
2.04	0.43
1.54	-0.33
1.80	-0.58
0.94	0.28
0.00	0.48
0.03	1.12
0.07	1.57
0.27	1.35

$q_n L_k =$

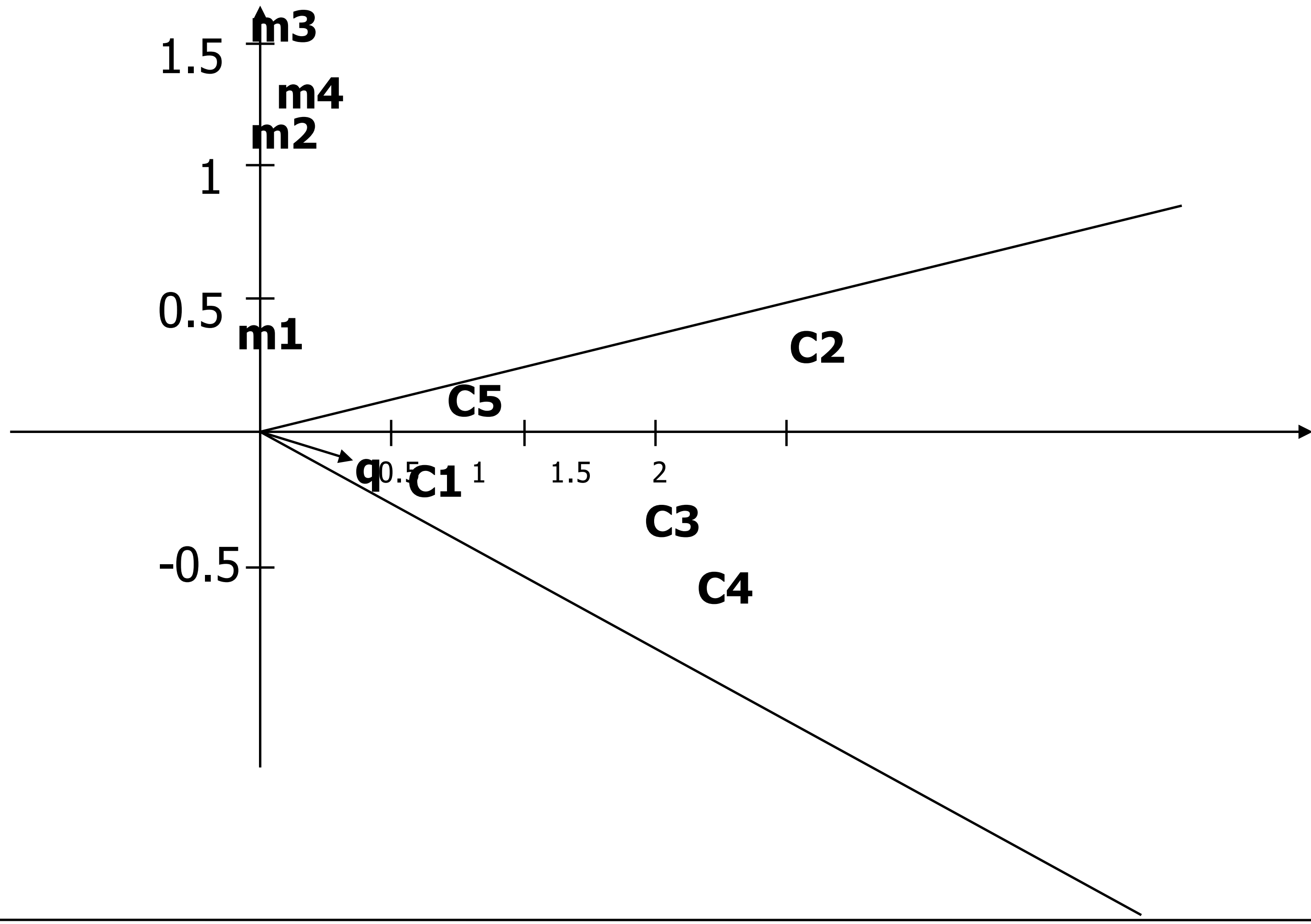
0.138	-0.0273

3.34	0
0	2.54

=

0.46	-0.069

Query transformation



Query transformation

- Comparison of the transformed query to the new document vectors based on cosine similarity, where the similarity is computed as:

$$Cos(x,y)=<x,y>/||x||.||y||$$

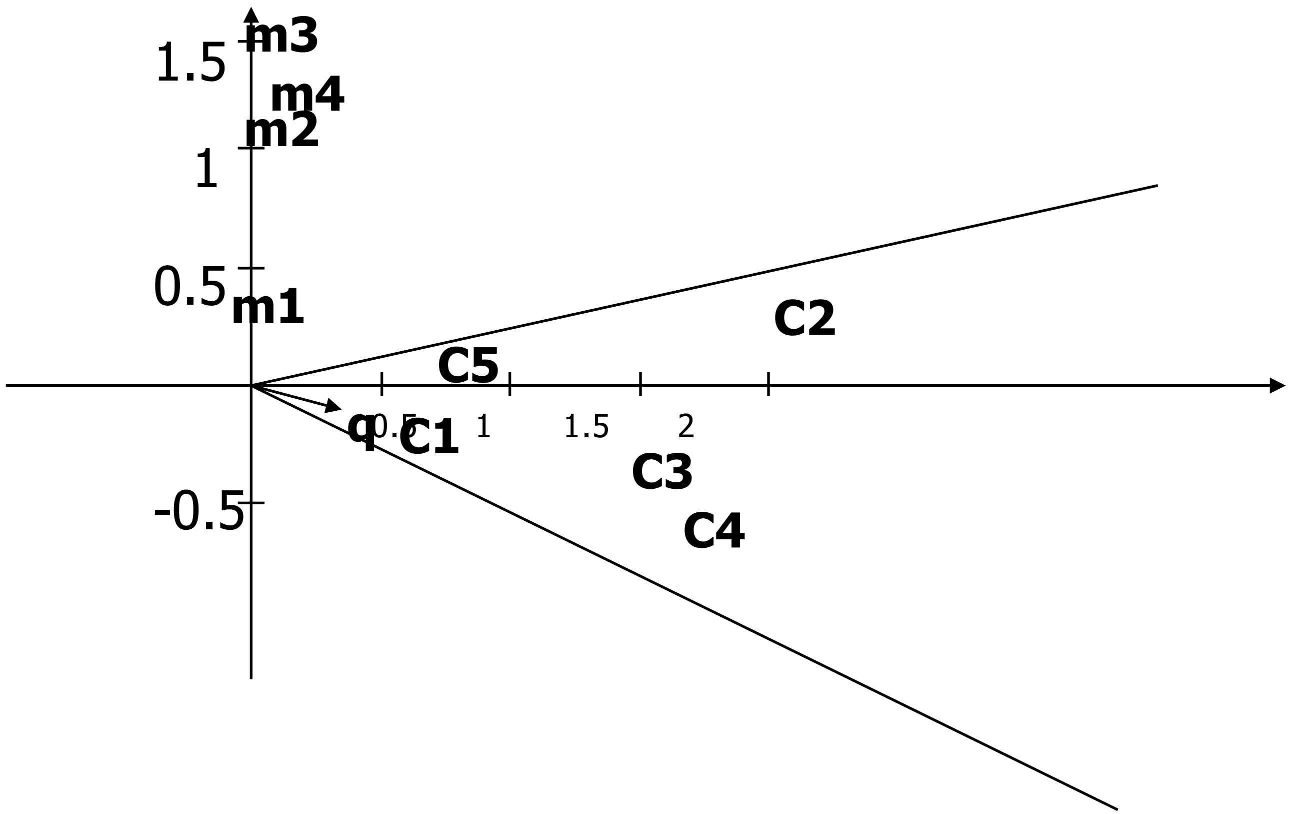
Where $x=(x_1,\ldots,x_n)$, $y=(y_1,\ldots,y_n)$

$$<x,y>=x_1*y_1+\ldots+x_n*y_n$$

Query transformation

- The cosine similarity matrix of query vector to the documents is:

	query
C1	0.99
C2	0.94
C3	0.99
C4	0.99
C5	0.90
M1	-0.14
M2	-0.13
M3	-0.11
M4	0.05



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