COMP30120

Dimension Reduction

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Overview

- Feature Transformation v Selection
- Feature Transformation Methods
 - Principal Component Analysis (PCA)
 - Linear Discriminant Analysis (LDA)
 - Latent Semantic Indexing (LSI)

Feature Transformation v Selection

Feature Selection

 Tries to find a minimum subset of the original features that optimises one or more criteria, rather than producing an entirely new set of dimensions for the data.

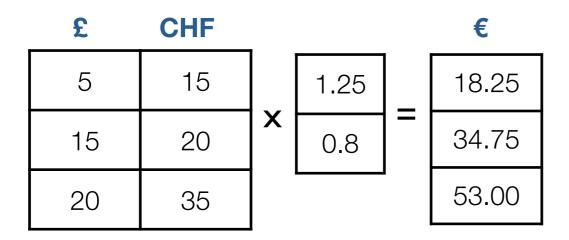
Feature Transformation (Feature Extraction)

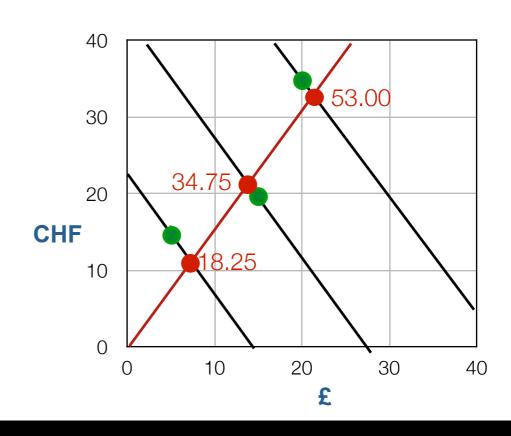
- A popular alternative strategy in data pre-processing is to transform the data into an entirely different format.
- Examples represented by one set of features are transformed to another new set of features.
- Resulting features can be more compact and less noisy, resulting in more accurate predictions.
- Typically involve a linear transformation of the original data.

Linear Transformations

- In a linear transformation, the new variables are linear functions of the old variables.
- Simple example: Bill owes Mary £5 and CHF15 after a holiday.
 - Current exchange rates:

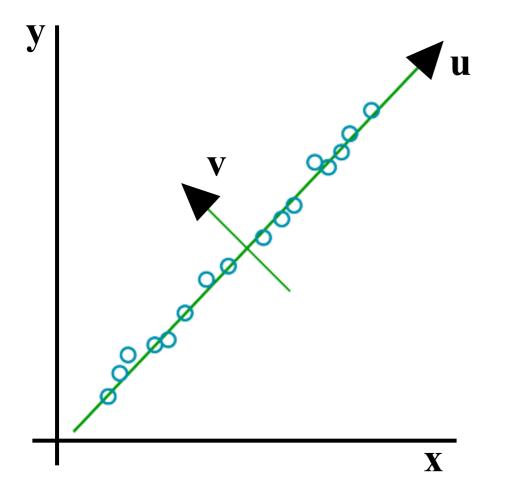
- Based on rates, Bill owes €(1.25 x 5 + 0.8 x 15) = €18.25
- We can view this as a linear transformation...





Principle Component Analysis (PCA)

- Projection methods find a mapping from the original d-dimensional space to a new (k < d)-dimensional space, with minimum loss of information.
- "Good" spaces for projections are characterised by preserving most of the useful information in the data.
- PCA: An unsupervised method which performs dimensionality reduction while keeping as much of the variance in the original space as possible.
 Allows us to find the direction in which the data varies.



Given data in terms of dimensions (x,y), the principal direction in which the data varies is along the u axis.

Very little variation in the data in the direction of *v*.

→ We could represent the data using the *u* dimension, and discard *v*.

Eigenvectors and Eigenvalues

 Given an input matrix X, an eigenvector of the matrix is a nonzero vector v that satisfies the equation:

$$\mathbf{X}v = \lambda v$$

where the corresponding number λ is called an eigenvalue.

 Eigendecomposition is the factorization of a matrix into its eigenvalues and eigenvectors.

$$\mathbf{X} = \begin{pmatrix} 1.0000 & 0.5000 & 0.3330 & 0.2500 \\ 0.5000 & 1.0000 & 0.6667 & 0.5000 \\ 0.3333 & 0.6667 & 1.0000 & 0.7500 \\ 0.2500 & 0.5000 & 0.7500 & 1.0000 \end{pmatrix}$$

4 x 4 matrix

$$\mathbf{\Lambda} = \begin{pmatrix} 2.5361 & 0 & 0 & 0\\ 0 & 0.8483 & 0 & 0\\ 0 & 0 & 0.4078 & 0\\ 0 & 0 & 0 & 0.2077 \end{pmatrix}$$

4 eigenvalues

$$\mathbf{V} = \begin{pmatrix} -0.37775 & -0.81052 & -0.44217 & -0.06988 \\ -0.53223 & -0.18762 & 0.74199 & 0.36221 \\ -0.56139 & 0.30099 & 0.04872 & -0.76926 \\ -0.50881 & 0.46611 & -0.50155 & 0.52169 \end{pmatrix}$$

4 eigenvectors

Principle Component Analysis (PCA)

- Principal Components (PCs): New features constructed as linear combinations of the original features, which are uncorrelated with one another.
- First PC accounts for the most variability in the data. Next PC has the highest variance possible under the constraint that it is orthogonal to (uncorrelated with) the first PC, and so on...

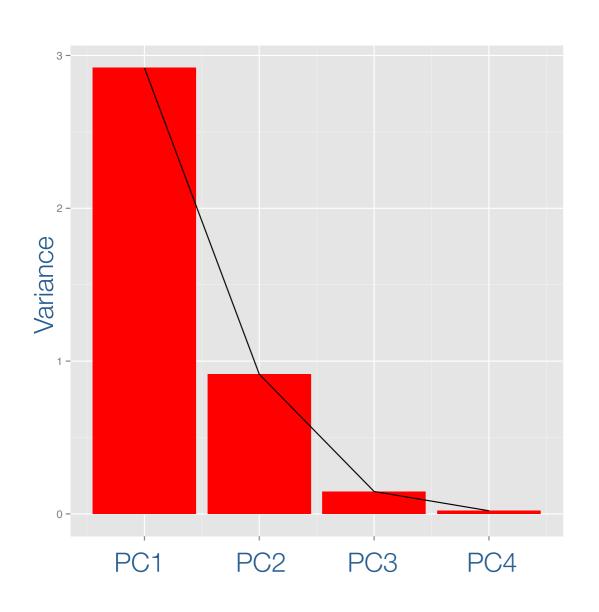
Applying PCA:

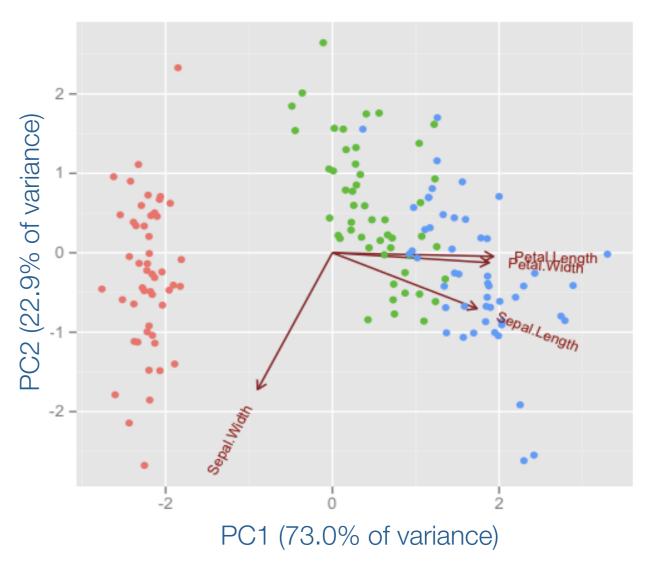
- 1. For a data matrix X with n samples, calculate mean of the columns of X.
- 2. Subtract the mean from each row of X, to give the "centered" matrix Y.
- 3. Calculate the covariance matrix $\mathbf{C} = \mathbf{Y}^\mathsf{T} \mathbf{Y} / (n-1)$
- 4. Calculate the eigenvectors of the covariance matrix C.
- 5. The PCs are given by the eigenvectors of C. The *i*-th PC is given by the eigenvector corresponding to the *i*-th largest eigenvalue of C.
- The k PCs with the highest variance provide a new reduced $n \times k$ representation of the data.

Example: PCA

Apply PCA to *Iris* data set, and examine amount of variance in each Principal Component.

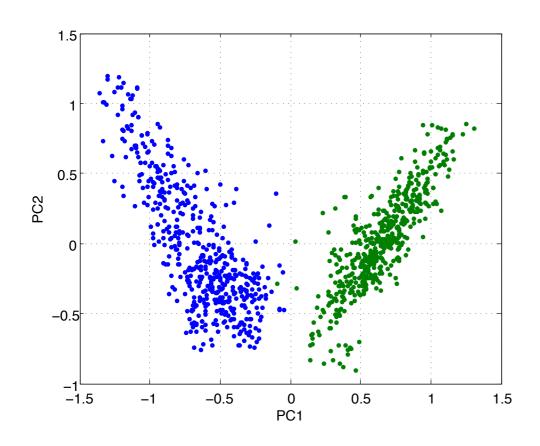
First two Principal Components account for ~96% of the variance in the data.



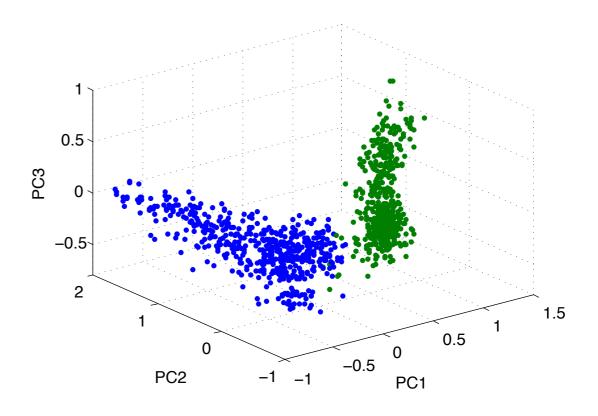


Example: PCA

- Collection of 1,021 BBC news articles on business + sport, represented by high-dimensional space with 5,570 features (words).
- Applying PCA allows us to visualise the data in a low dimensional space using a small number of PCs.



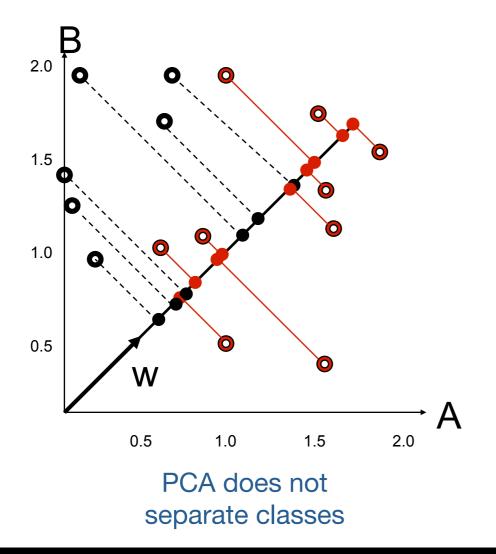
2 leading principal components (PCs)

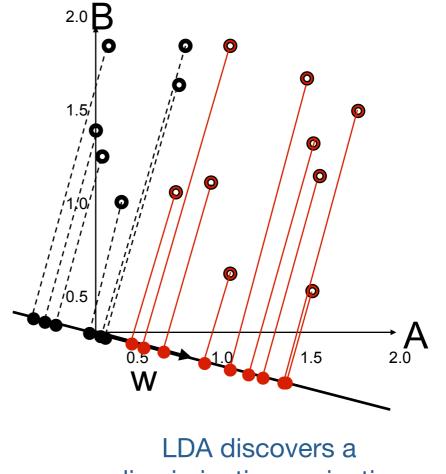


3 leading principal components (PCs)

Linear Discriminant Analysis (LDA)

- PCA is an <u>unsupervised</u> feature transformation technique. The resulting PCs are not always good for discrimination in classification.
- Linear Discriminant Analysis (LDA): Seeks to create discriminating features, by finding a linear transformation that maximises the between-class variance and minimises the within-class variance.

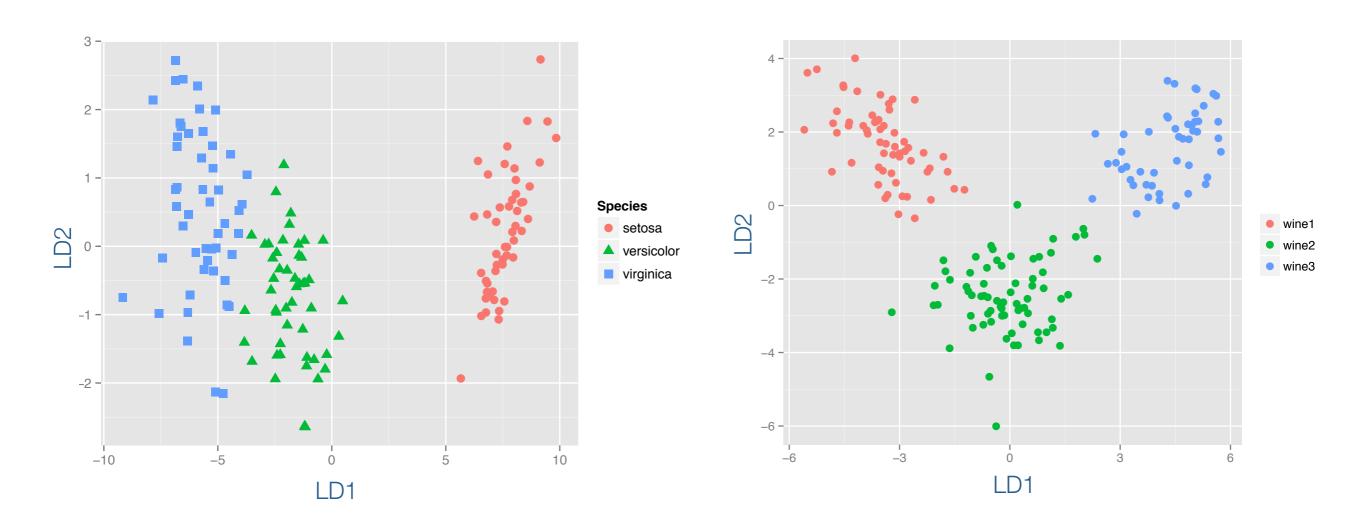




Example: LDA

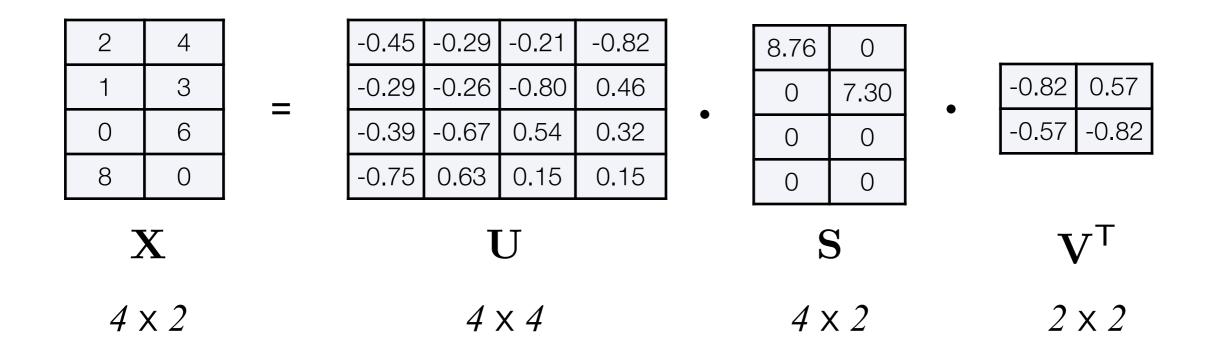
LDA applied to *Iris* data set. Attempts to maximise the variance between the three labelled classes.

LDA applied to *Wine* data set. Attempts to maximise the variance between the three labelled classes.



Singular Value Decomposition (SVD)

- Performing SVD on the data is similar to PCA.
- We can rewrite any rectangular m x n matrix as X = U · S · V^T
 Left singular vectors U: n x n matrix, eigenvectors of X · X^T
 Right singular vectors V: m x m matrix, eigenvectors of X^T · X
 Singular values S: diagonal n x m matrix



Latent Semantic Indexing (LSI)

- Latent Semantic Indexing: a method for selecting informative subspaces of feature spaces.
- Developed for information retrieval to reveal semantic information from document co-occurrences.
- Terms that do not appear in a document may still be associated with the document.
- LSI derives uncorrelated dimensions that might be considered as the latent concepts in the data.

Indexing by Latent Semantic Analysis

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ABSTRACT

A new method for automatic indexing and retrieval is described. The approach is to take advantage of implicit higher-order structure in the association of terms with documents ("semantic structure") in order to improve the detection of relevant documents on the basis of terms found in queries. The particular technique used is singular-value decomposition, in which a large term by document matrix is decomposed into a set of ca 100 orthogonal factors from which the original matrix can be approximated by linear combination. Documents are represented by ca 100 item vectors of factor weights. Queries are represented as pseudo-document vectors formed from weighted combinations of terms, and documents with supra-threshold cosine values are returned. Initial tests find this completely automatic method for retrieval to be promising.

United States Patent [19] 4,839,853 [11] Patent Number: Deerwester et al. [45] Date of Patent: Jun. 13, 1989 COMPUTER INFORMATION RETRIEVAL References Cited USING LATENT SEMANTIC STRUCTURE U.S. PATENT DOCUMENTS [75] Inventors: Scott C. Deerwester, Chicago, Ill.; 4,384,325 5/1983 Slechta Susan T. Dumais, Berkeley Heights; 4,433,392 2/1984 Beaven 1/1985 Dickinson et al. George W. Furnas, Madison, both of N.J.; Richard A. Harshman, London, 3/1985 Shaw et al. 4,575,798 3/1986 Lindstrom et al. Canada; Thomas K. Landauer, Summit, N.J.; Karen E. Lochbaum, Primary Examiner-Jerry Smith Chatham, N.J.; Lynn A. Streeter, Assistant Examiner-Steven G. Kibby Summit, N.J. Attorney, Agent, or Firm-James W. Falk; John T. [73] Assignee: Bell Communications Research, Inc., Livingston, N.J. A methodology for retrieving textual data objects is [21] Appl. No.: 244,349 disclosed. The information is treated in the statistical domain by presuming that there is an underlying, latent [22] Filed: semantic structure in the usage of words in the data objects. Estimates to this latent structure are utilized to 364/900; 364/200; represent and retrieve objects. A user query is recouched in the new statistical domain and then pro 364/225.4; 364/963.1; 364/942.71 ... 364/419, 224.1, 225.4, cessed in the computer system to extract the underlying Field of Search ... 364/253.1, 253.2, 253.3, 282.1, 282.3, 942.71, meaning to respond to the query. 942.76, 942.77, 956.1, 963.1, 200 MS File, 900 11 Claims, 2 Drawing Sheets

Latent Semantic Indexing (LSI)

• Typically represent documents as high-dimensional vectors, and a complete collection as a $m \times n$ term-document matrix.

	doc1	doc2	doc3	doc4	doc5	goop
	0	0	0	0	0	0
business	1	1	1		1	
finance						1
news		1	1		1	
apple		1	1	1		
food				1		
recipe				1		
car					1	
automobile						1

Problems

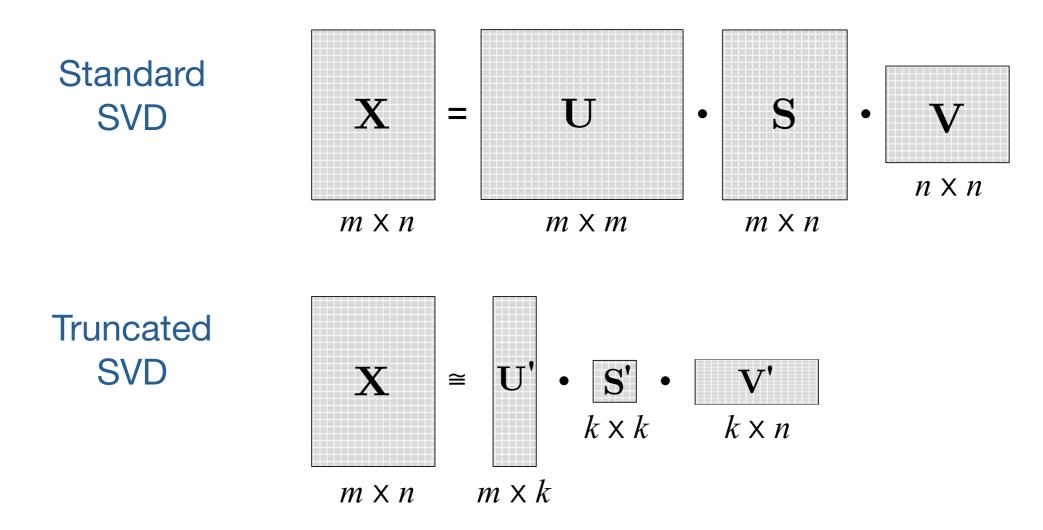
- Synonymy: different words with the same meaning (e.g "car" v "automobile").
- Polysemy: the same word having multiple meanings (e.g. "apple").
- → Semantically related documents can appear to have low similarity.

LSI Solution:

- Assume there is some underlying latent structure that is hidden by the high-dimensional representation.
- Transform the data to a reduced-dimensional space whose axes are "concepts" that effectively group similar words together.

Latent Semantic Indexing (LSI)

 Compute a k-dimensional truncated SVD of the original termdocument matrix.



• LSI only uses leading k singular vectors, discards the others, where k << m and k << n

Collection of CS paper titles (index terms in italics)...

c1	Human machine interface for Lab ABS computer applications
c2	A survey of user opinion of computer system response time
сЗ	The EPS user interface management system
с4	System and human system engineering testing of EPS
c5	Relation of <i>user</i> -perceived <i>response time</i> to error measurement
m1	The generation of random binary unordered trees
m2	The intersection <i>graph</i> of paths in <i>trees</i>
m3	Graph minors IV: Widths of trees and well quasi ordering
m4	Graph minors: A survey

Collection of CS paper titles (index terms in italics)...

c1	Human machine interface for Lab ABS computer applications										
c2	A survey of user opinic		c1	c2	с3	с4	с5	m1	m2	m3	m4
сЗ	The EPS user interface	human	1	0	0	1	0	0	0	0	0
c4	System and human sy:	interface	1	0	1	0	0	0	0	0	0
c5	Relation of <i>user</i> -percei	computer	1	1	0	0	0	0	0	0	0
		user	0	1	1	0	1	0	0	0	0
m1	The generation of rand	system	0	1	1	2	0	0	0	0	0
m2	The intersection graph	response	0	1	0	0	1	0	0	0	0
m3	Graph minors IV: Width	time	0	1	0	0	1	0	0	0	0
m4	Graph minors: A surve	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

Build 12 x 9 term-document matrix from index terms in titles.

 Apply truncated SVD to term-document matrix and extract vectors corresponding to 2 leading singular vectors.

-0.22	-0.11
-0.2	-0.07
-0.24	0.04
-0.4	0.06
-0.64	-0.17
-0.27	0.11
-0.27	0.11
-0.3	-0.14
-0.21	0.27
-0.01	0.49
-0.04	0.62
-0.03	0.45

TJ

12 x 2

3.34	0					
0	2.54					
$\overline{\mathbf{S}}$						

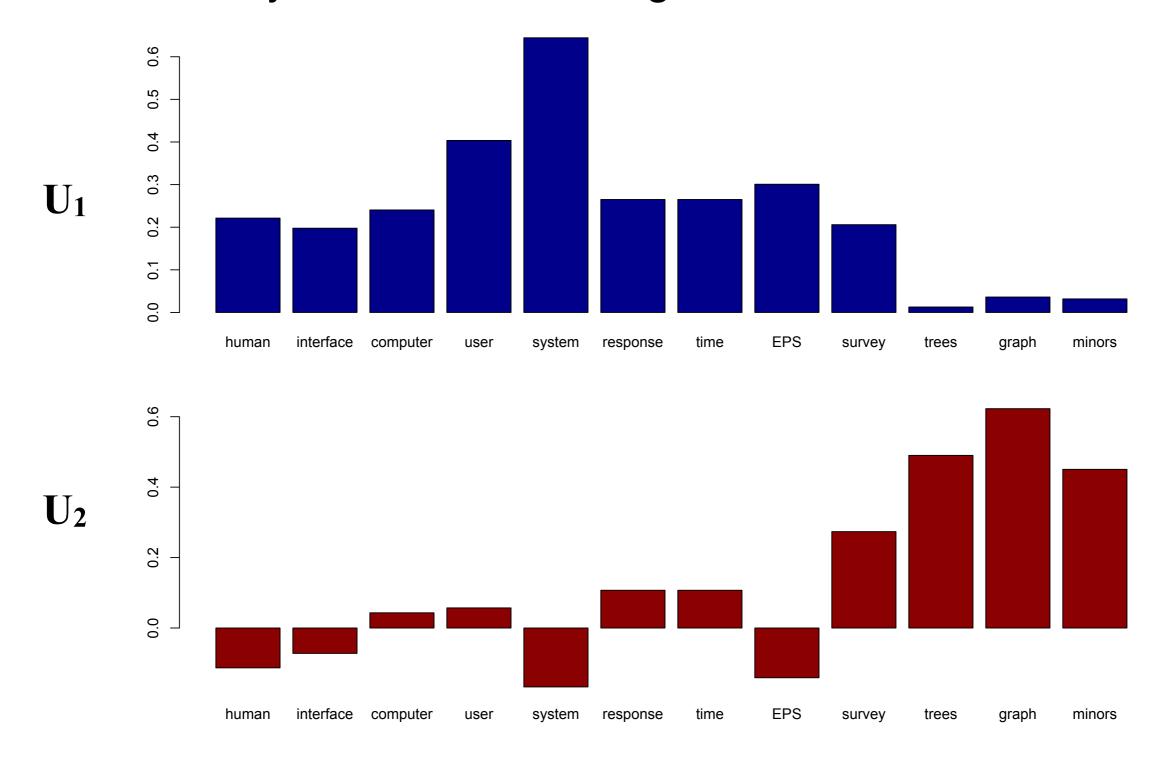
-0.20	-0.61	-0.46	-0.54	-0.28	0.00	-0.01	-0.02	-0.08
-0.06	0.17	-0.13	-0.23	0.11	0.19	0.44	0.62	0.53
\mathbf{V}^T								

Values in V define coordinates for the original 9 documents in a new latent space.

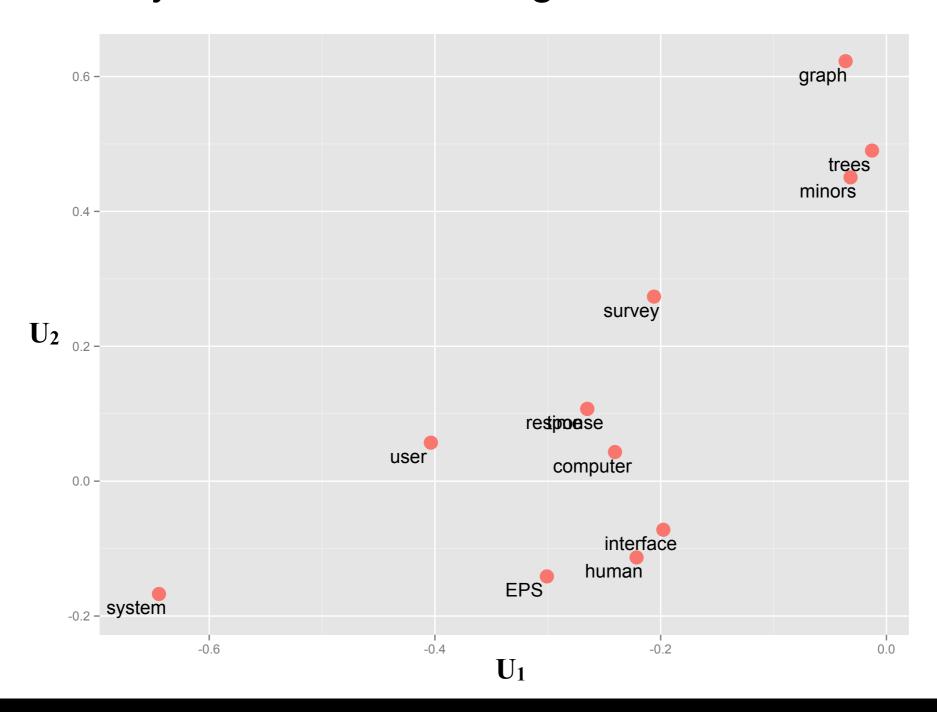
2 x 9

Values in U describe the "concepts" in the latent space, and how they relate to the 12 original index terms.

 Values in U describe the "concepts" in the 2D latent space, and how they relate to the 12 original index terms.

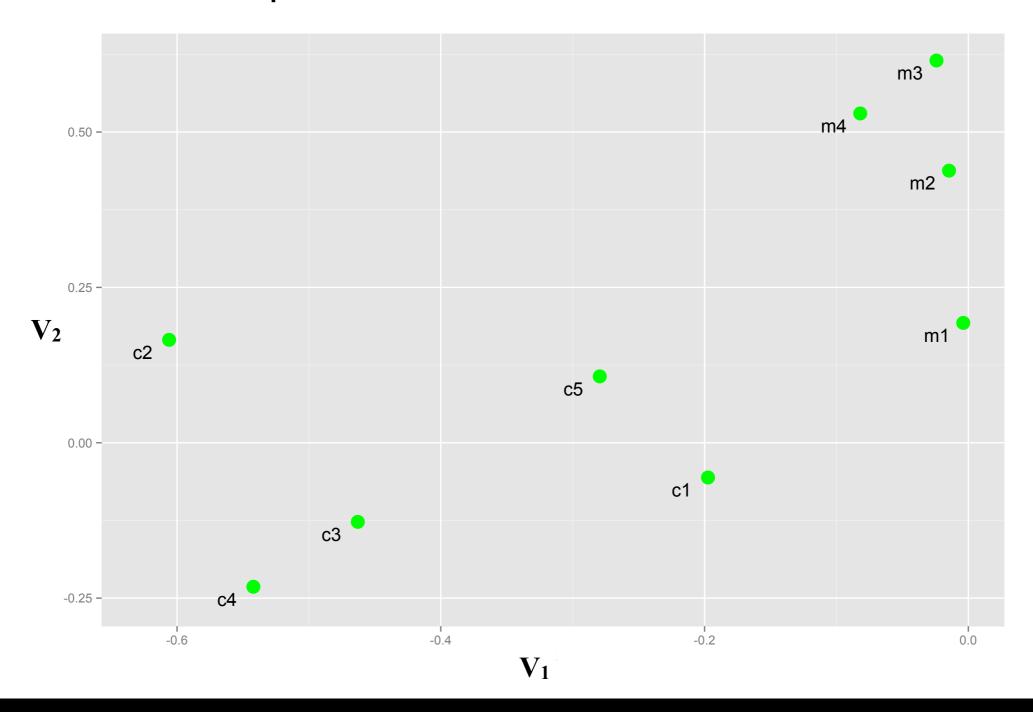


 Values in U describe the "concepts" in the 2D latent space, and how they relate to the 12 original index terms.



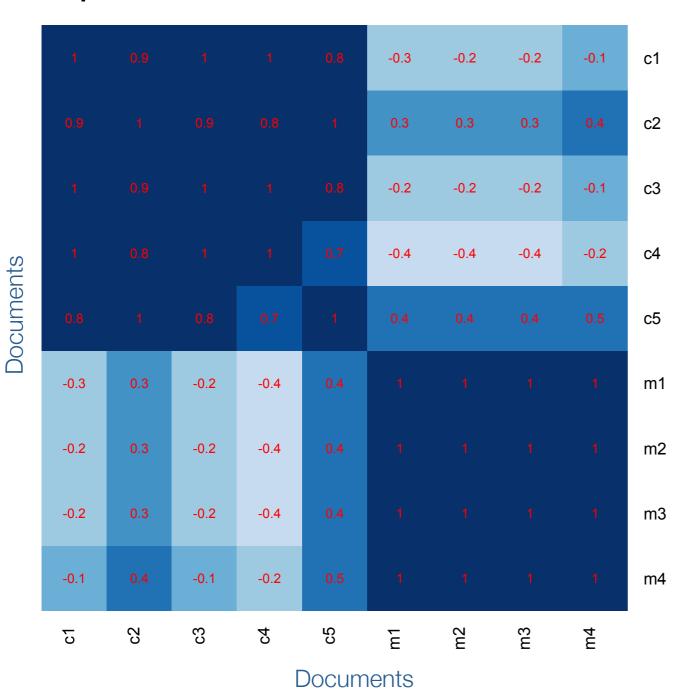
COMP30120 Machine Learning

 Values in V define coordinates for the original 9 documents in a new 2D latent space.



COMP30120 Machine Learning

 We can calculate a Cosine similarity matrix on the 2D latent space vectors in V to cluster documents.



c1	Human machine interface for Lab ABS computer applications
c2	A survey of user opinion of computer system response time
сЗ	The EPS user interface management system
с4	System and human system engineering testing of EPS
c5	Relation of user-perceived response time to error measurement
m1	The generation of random binary unordered trees
m2	The intersection graph of paths in trees
m3	Graph minors IV: Widths of trees and well quasi ordering
m4	Graph minors: A survey

We can find latent similarities between documents containing different terms (e.g. m1 & m4).

Summary

- Feature Transformation v Selection
- Feature Transformation Methods
 - Principal Component Analysis (PCA)
 - Linear Discriminant Analysis (LDA)
 - Latent Semantic Indexing (LSI)

Dimension Reduction

Pádraig Cunningham University College Dublin

Technical Report UCD-CSI-2007-7 August 8th, 2007 Technical Report on Moodle page

https://csiweb.ucd.ie/files/UCD-CSI-2007-7.pdf

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