COMP9417 Machine Learning and Data Mining

May 2, 2017

#### Acknowledgements

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Material derived from slides for the book
"Elements of Statistical Learning (2nd Ed.)" by T. Hastie.
R. Tibshirani & J. Friedman. Springer (2009)
http://statweb.stanford.edu/~tibs/ElemStatLearn/
Material derived from slides for the book
"Machine Learning: A Probabilistic Perspective" by P. Murphy
MIT Press (2012)
http://www.cs.ubc.ca/~murphvk/MLbook
Material derived from slides for the book
"Machine Learning" by P. Flach
Cambridge University Press (2012)
http://cs.bris.ac.uk/~flach/mlbook
Material derived from slides for the book
"Bayesian Reasoning and Machine Learning" by D. Barber
Cambridge University Press (2012)
http://www.cs.ucl.ac.uk/staff/d.barber/brml
Material derived from figures for the book
"Python Data Science Handbook" by J. VanderPlas
O'Reilly Media (2017)
http://shop.oreillv.com/product/0636920034919.do
Material derived from slides for the course
"Machine Learning" by A. Srinivasan
```

BITS Pilani, Goa, India (2016)

### Contents

Aims

This lecture will develop your understanding of unsupervised learning methods. Following it you should be able to:

• describe the problem of dimensionality reduction

- describe the problem of dimensionality reduction
- outline the method of Principal Component Analysis

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- · describe hierarchical clustering
- outline methods of evaluation for unsupervised learning

### Contents

2 Introduction

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So: unsupervised learning methods address the problem of assigning instances to classes given only observations about the instances, i.e., without being given class "labels" for instances by a "teacher".

Why do we need unsupervised learning?

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- in principle, can use any feature as the "label"
- unfortunately, often the class is not a known feature

What is unsupervised learning good for ?

• exploratory data analysis, e.g., with visualization

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- to learn generative models for images, text, video, speech, etc.

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3 Dimensionality Reduction

### **Dimensionality Reduction**

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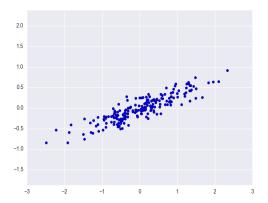
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This suggests an approach: look into using the variance-covariance matrix we recall from correlation and regression

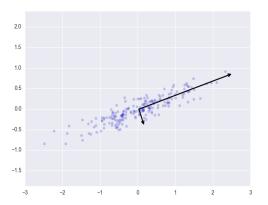
# PCA Example



PCA looks for linear combinations of the original features. This dataset of 200 points seems to show such a relationship between two feature dimensions.

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# PCA Example



PCA finds two new features on which the original data can be projected, rotated and scaled. These explain respectively 0.75 and 0.02 of the variance.

This algorithm can be presented in several ways. Here are the basic steps in terms of the variance reduction idea:

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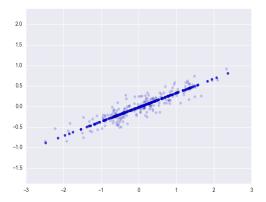
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- **5** sort columns of **S** in decreasing order (decreasing variance)
- 6 remove columns of S below some minimum threshold



# PCA Example



By rejecting the second component we reduce the dimensionality by 50% while preserving much of the original variance, seen by plotting the inverse transform of this component along with the original data.

#### PCA and friends

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- many other methods use essentially the same matrix decomposition idea, such as finding "topics" in text using Latent Semantic Analysis (next slide), finding hidden "sub-groups" for recommender systems, and so on

# Finding Topics in Text

$$\begin{bmatrix} \widetilde{\mathbf{X}} \\ \mathbf{X} \end{bmatrix} = \begin{bmatrix} \mathbf{U}_k \\ \mathbf{V}_k \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \\ s_k \end{bmatrix} \mathbf{V}_k^{\mathrm{T}}$$

$$t \times d \qquad t \times k \qquad k \times k \qquad k \times d$$

Latent Semantic Analysis (LSA) factorizes a word count matrix for t terms from d documents using the Singular Value Decomposition (SVD) to find a number k < d of topics. Here the diagonal matrix  ${\bf S}$  has the topic "strength" sorted in decreasing order.

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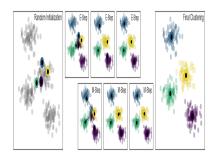
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- many alternatives, e.g., Random Projections, Independent Component Analysis, etc.

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4 Clustering

# k-Means Clustering Example



Data.

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**5** Summary

# Summary: Unsupervised Learning

Unsupervised and supervised learning are at different ends of a continuum of "degrees of supervision". Between these extremes many other approaches are possible.

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  - "reward" is a signal from the "environment"
  - learning is designed to optimize function of reward
- active learning
  - learning system acts to generate its own examples

Note: unsupervised learning an increasingly active research area, particularly in neural nets, e.g., Yann LeCun: "Unsupervised Learning: The Next Frontier in Al" https://www.youtube.com/watch?v=XTbLOjVF-y4