Lecture 1: Introduction

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MSA220/MVE441 Statistical Learning for Big Data

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CHALMERS UNIVERSITY OF TECHNOLOGY | UNIVERSITY OF GOTHENBURG

The Data Deluge

- Data is getting cheap! (sometimes)
- Massive data collections across all fields! Molecular biology, health care, banking, streaming, marketing, citizen science, climate modeling, imaging, data feeds like twitter, ...
- What do we do with all this data?

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- many methods perform poorly if we overwhelm them with high-dimensional data
- is there a selection bias when we collect high-dimensional data? - which features of objects are easy to obtain?

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- Big n statistics: with a big enough n everything becomes significant - think carefully about what the analysis goals are

BIG DATA

The Parable of Google Flu: Traps in Big Data Analysis

David Lazer,[1,2*] Ryan Kennedy,[1,3,4] Gary King,[3] Alessandro Vespignani[5,6,3]

Scientific discussion article[1]

[1] Lazer et al. (2014) The Parable of Google Flu: Traps in Big Data Analysis. *Science* 343 (6176):1203–1205. DOI 10.1126/science.1248506

Big Data - Big Problems?

Big data: are we making a big mistake?

Big data is a vague term for a massive phenomenon that has rapidly become an ob
with entrepreneurs, scientists, governments and the media

Tim Harford MARCH 28, 2014

The New York Times

Opinion

THE STONE

How Democracy Can Survive Big Data

By Colin Koopman

March 22, 2018

Financial Times[1]

New York Times[2]

[1] *https://www.ft.com/content/21a6e7d8-b479-11e3-a09a-00144feabdc0#axzz2yQ2QQfQX*

[2] *https://www.nytimes.com/2018/03/22/opinion/democracy-survive-data.html*

It’s a huge topic in science!

Lot’s of research! Companies need the competence!

- Logistics, transport, banking, risk analysis, automated detection, image and video processing, molecular and systems biology
- and more...
- Methodology research: dimension reduction and visualization, computing solutions, feature selection/interpretability, scalable algorithms, ...

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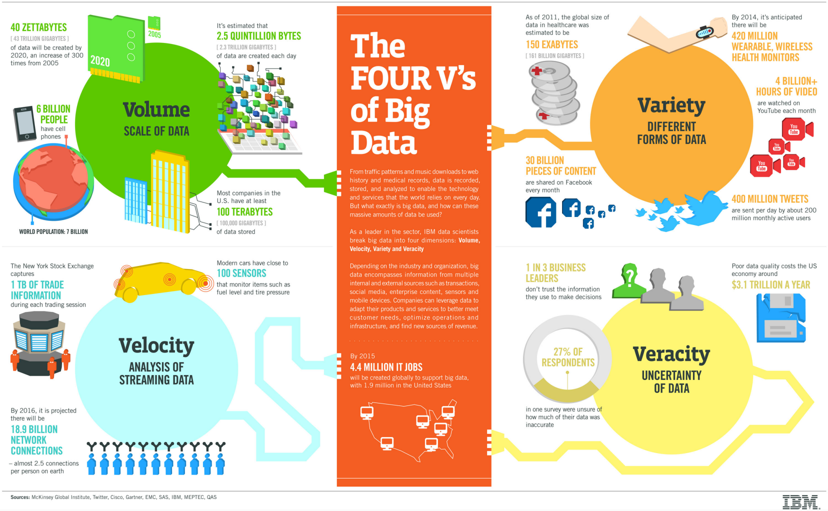
Is this all?

The Four Vs of Big Data



http://web.archive.org/web/20210506042232/https://www.ibmbigdatahub.com/infographic/four-vs-big-data

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Focus is on the last three in this course.

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- Exploration and visualisation of Big Data can already require statistics
- **Probability of extreme values:** Unlikely results become much more likely with an increase in n
- **Curse of dimensionality:** Lot's of space between data points in high-dimensional space

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- Problem: exploration and visualization may be difficult/expensive but you *need* to check assumptions! Cannot rely on automation!
- In fact: **with Big Data you may encounter selection bias, mislabeled observations, imbalance of data, noisy data, spurious correlations, ...**
- Before analysis, spend time with the people collecting the data to try to understand how, why, think about sources for bias, questions that were *not* asked, ... **Taking time to understand the data will save you a lot of headache later on!**

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  - Overfitting
  - Computational burden
  - but also blessing (e.g. SGD and ensembles, ”data hungry” methods like NN, rare-events detection, noise correction)

PAUSE!!!!

A bit of recap.....

If what comes next feels unfamiliar - spend a bit of time reviewing basic stat concepts

Terminology, Background and Basics

1. Statistics terminology recap
2. Basics of statistical learning
3. Setting the stage for the course

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$$p(0) = \theta, \quad p(1) = 1 - \theta$$

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- Where will we see this? **Classification**, where θ denotes the probability of class 1 and can be observation specific, θ_i, and depend on features of this observation, $\theta(x_i)$

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Basics about random variables

- We will consider **discrete** and **continuous** random quantities
- **Probability density function (pdf)** $p(\mathbf{x})$ for a continuous variables

  Example: Multivariate normal distribution with mean vector $\boldsymbol{\mu} \in \mathbb{R}^p$ and covariance matrix $\boldsymbol{\Sigma} \in \mathbb{R}^{p \times p}$

$$p(\mathbf{x}) = |2\pi\boldsymbol{\Sigma}|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

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Two important rules (and a consequence)

Marginalisation

For a joint density $p(x, y)$ it holds that

$$p(x) = \sum_y p(x, y) \quad \text{or} \quad p(x) = \int p(x, y)\,\mathrm{d}y$$

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Both rules together imply **Bayes' law**

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

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- Conditioning in classification/regression where we treat features of objects as known and focus on the random variation of the outcome (response, class) only, *given* the features
- Bayes law: the basis for building classification rules by updating marginal population frequencies once we observe observation specific features.

Expectation and variance

Expectations and variance depend on an underlying pdf/pmf.

Notation:

- $\mathbb{E}_{p(x)}[f(x)] = \int f(x)p(x)\,\mathrm{d}x$
- $\mathrm{Var}_{p(x)}[f(x)] = \mathbb{E}_{p(x)}\left[\left(f(x) - \mathbb{E}_{p(x)}[f(x)]\right)^2\right]$

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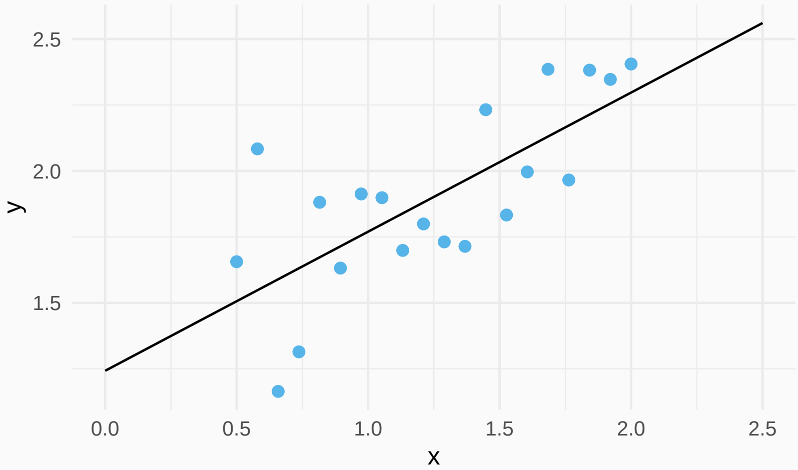
- **Data:** Data with known outcomes is needed
- **Expected prediction error:** Focus on quality of prediction (predictive modelling)
- **Loss function:** Quantifies the discrepancy between observed data and predictions

Linear regression - An old friend



- **Data:** Training data consists of independent pairs

$$(y_i, \mathbf{x}_i), \quad i = 1, \dots, n$$

Observed response $y_i \in \mathbb{R}$ for predictors $\mathbf{x}_i \in \mathbb{R}^p$

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- **Loss function: Squared error loss**

  $$L(y, \hat{y}) = (y - \hat{y})^2$$

PAUSE 2!!!!!

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- What can happen if these are violated?

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- What can happen if these are violated?
- What, if anything, can we do to handle violations?

Statistical decision theory for regression (I)

- Squared error loss between outcome y and a prediction $f(\mathbf{x})$ dependent on the variable(s) x

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- When a new pair of data $(y, \mathbf{x})$ from the same distribution (population) as the training data arrives, **expected prediction loss** for a given f is

$$J(f) = \mathbb{E}_{p(\mathbf{x},y)}\left[L(y, f(\mathbf{x}))\right] = \mathbb{E}_{p(\mathbf{x})}\left[\mathbb{E}_{p(y|\mathbf{x})}\left[L(y, f(\mathbf{x}))\right]\right]$$

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- Define 'best' by:

$$\widehat{f} = \arg\min_{f} J(f)$$

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Can we determine $\widehat{f}$?

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Can we determine $\widehat{f}$? Focus on inner expectation

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$\mathbb{E}_{p(y|\mathbf{x})}[y]$: "Average of y in vertical slice defined by x"
f(x): Our model

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Can we determine $\widehat{f}$? Focus on inner expectation

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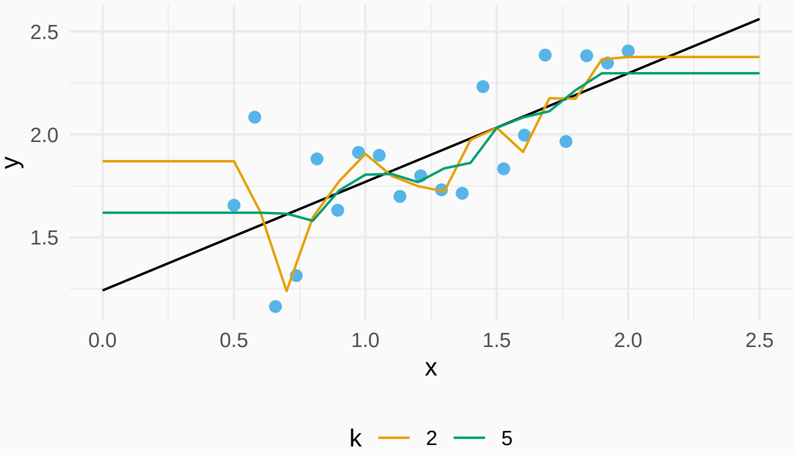
- Probably more realistic to look for the k closest neighbours of $\mathbf{x}$ in the training data $N_k(\mathbf{x}) = \{\mathbf{x}_{i_1}, \dots, \mathbf{x}_{i_k}\}$. Then

$$\mathbb{E}_{p(y|\mathbf{x})}[y] \approx \frac{1}{k} \sum_{\mathbf{x}_{i_l} \in N_k(\mathbf{x})} y_{i_l}$$

Average of k neighbours



Back to linear regression

Linear regression is a **model-based approach** and assumes that the dependence of y on $\mathbf{x}$ can be written as a weighted sum, i.e.

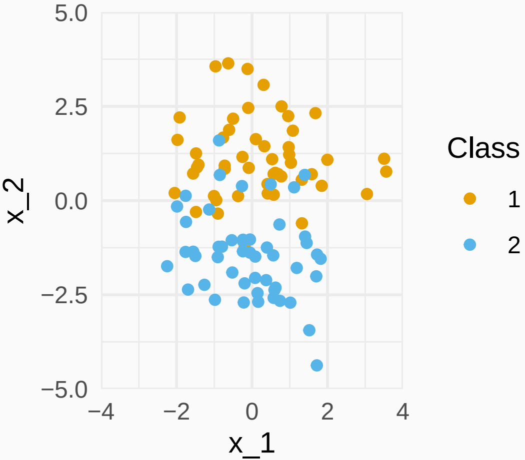
$$y = \mathbf{x}^\top \boldsymbol{\beta} + \varepsilon$$

where $\varepsilon \sim N(0, \sigma^2)$. The mean of y given $\mathbf{x}$ is therefore

$$\mathbb{E}_{p(y|x)}[y] = \mathbf{x}^\top \boldsymbol{\beta}.$$

Note that in practice this equality will only hold approximately.

A simple example of classification



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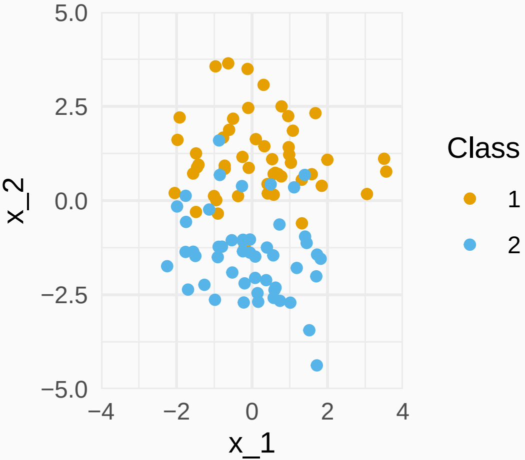

How do we classify a pair of new coordinates $\mathbf{x} = (x_1, x_2)$?

- Find the k predictors

$$N_k(\mathbf{x}) = \{\mathbf{x}_{i_1}, \dots, \mathbf{x}_{i_k}\}$$

in the training sample, that are closest to $\mathbf{x}$ in the Euclidean norm.

k-nearest neighbour classifier (kNN)

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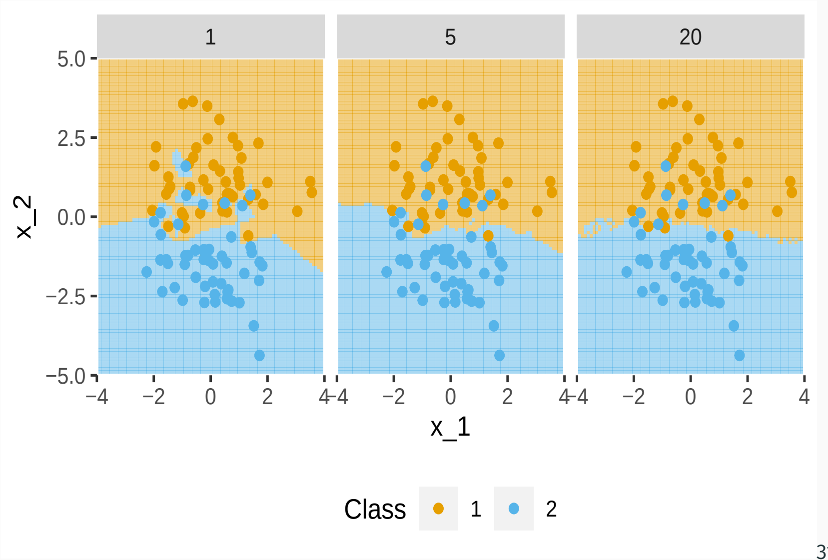
  in the training sample, that are closest to $\mathbf{x}$ in the Euclidean norm.
- **Majority vote:** Assign $\mathbf{x}$ to the class that most predictors in $N_k(\mathbf{x})$ belong to (highest frequency)

kNN and its decision boundaries



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Learn a rule $c(\mathbf{x})$ from data which maps observed features $\mathbf{x}$ to classes $\{1, \dots, K\}$.

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Statistical Learning

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What is a suitable loss?

Statistical decision theory for classification

- **0-1 misclassification loss:** Let i be the actual class of an object and $c(\mathbf{x})$ is a rule that returns the class for the variable(s) $\mathbf{x}$, then

$$L(i, c(\mathbf{x})) = \begin{cases} 0 & i = c(\mathbf{x}), \\ 1 & i \neq c(\mathbf{x}) \end{cases} = \mathbb{1}(i \neq c(\mathbf{x}))$$

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- Minimizing expected prediction error leads to the rule

$$\hat{c}(\mathbf{x}) = \arg\max_{1 \leq i \leq K} p(i|\mathbf{x})$$

This is called **Bayes' rule**.

Deriving Bayes' rule

Again, focus on inner expectation

$$\mathbb{E}_{p(i|\mathbf{x})}[\mathbb{1}(i \neq c(\mathbf{x}))] = \sum_{i=1}^{K} \mathbb{1}(i \neq c(\mathbf{x}))p(i|\mathbf{x})$$

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Back to kNN

- kNN solves the classification problem by approximating $p(i|\mathbf{x})$ with the frequency of class i among the k closest neighbours of $\mathbf{x}$.
- Given data $(i_l, \mathbf{x}_l)$ for $l = 1, \dots, n$ it holds that

$$\hat{c}(\mathbf{x}) = \underset{1 \leq i \leq K}{\arg\max} \frac{1}{k} \sum_{\mathbf{x}_l \in N_k(\mathbf{x})} \mathbb{1}(i_l = i)$$

A note on kNN

There are two choices to make when implementing a kNN method

1. The metric to determine a neighbourhood
    - e.g. Euclidean/ℓ_2 norm, Manhattan/ℓ_1 norm, max norm, …
2. The number of neighbours, i.e. k

The choice of metric changes the underlying local model of the method while k determines the size of this local model.

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Take-home message

- Big Data is complex and is multi-faceted
- Regression and classification can be formulated in the framework of Statistical Learning
- In both cases, focus is on prediction
- Next class: Dimension reduction, Logistic regression and Bias-Variance trade-off