### Statistical Machine Learning

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Slide credits and other course material can be found at: http://www.stats.ox.ac.uk/~palamara/SML19\_BDI.html

### **Course Info**

#### Course material:

http://www.stats.ox.ac.uk/~palamara/SML19\_BDI.html

About me: http://www.palamaralab.org

### **Course Aims**

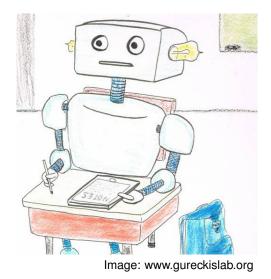
- Understand statistical fundamentals of machine learning
  - Overview of unsupervised learning.
  - Supervised learning.
- Understand difference between generative and discriminative learning frameworks.
- Learn to identify and use appropriate methods and models for given data and task.
- Learn to use the relevant R or python packages to analyse data, interpret results, and evaluate methods.

Practical

### Practical: human genomic data



- Practical discussed this afternoon: Kaggle challenge
- Link is on Canvas
- Evaluated
- Goal: try ML methods we will discuss, have fun!
- You can get 5 scores per day on a fraction of the test set



Bottom-up, data-driven approach. Incoming data "improves" a model.

#### Arthur Samuel, 1959

Field of study that gives computers the ability to **learn** without being explicitly programmed.

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Any computer program that **improves its performance** at some task **through experience**.

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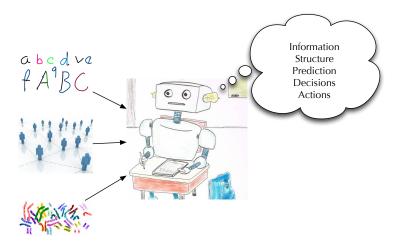
Field of study that gives computers the ability to **learn** without being explicitly programmed.

#### Tom Mitchell, 1997

Any computer program that **improves its performance** at some task **through experience**.

#### Kevin Murphy, 2012

To develop methods that can **automatically** detect **patterns in data**, and then to use the uncovered patterns to **predict** future data or other outcomes of interest.



data

### Machine Learning: Historical Perspective (Stats)

- 1763: Bayes (Prior, Likelihood, Posterior)
- 1920's: Fisher (Maximum Likelihood)
- 1937: Pitman (Exponential Family)
- 1969: Jaynes (Maximum Entropy)
- 1970: Baum (Hidden Markov Models)
- 1978: Dempster (Expectation Maximization)
- 1980's: Vapnik (VC-Dimension)
- 1990: Lauritzen, Pearl (Graphical Models)
- 1990's: ... Kalman Filtering, Hidden Markov Models, Belief Nets, Markov Random Fields, SVMs, Learning Theory, Boosting, Kernels

## Machine Learning: Historical Perspective (Bio/AI)

- 1917: Karel Capek (Robot)
- 1943: McCullogh & Pitts (Bio, Neuron)
- 1947: Norbert Weiner (Cybernetics, Multi-Disciplinary)
- 1949: Claude Shannon (Information Theory)
- 1950: Minsky, Newell, Simon, McCarthy (Symbolic AI, Logic)
- 1957: Rosenblatt (Perceptron)
- 1959: Arthur Samuel Coined "Machine Learning" (Learning Checkers)
- 1969: Minsky & Papert (Perceptron Linearity, no XOR)
- 1974: Werbos (BackProp, Nonlinearity)
- 1986: Rumelhart & McLelland (Connectionism, MLP, Verb-Conjugation)
- 1980's: NeuralNets, Genetic Algos, Fuzzy Logic, Black Boxes
- Recent years: "Big Data", Deep Learning, Machine Learning ubiquitous

## Statistics vs Machine Learning

### Traditional Problems in Applied Statistics

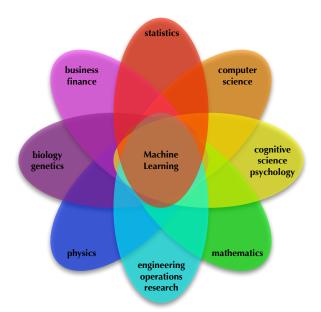
- Well formulated question that we would like to answer.
- Expensive data gathering and/or expensive computation.
- Create specially designed experiments to collect high quality data.

### Information Revolution

- Improvements in data processing and data storage.
- Powerful, cheap, easy data capturing.
- Lots of (low quality) data with **potentially valuable** information inside.
- CS and Stats forced **back together**: unified framework of data, inferences, procedures, algorithms
  - statistics taking computation seriously
  - computing taking statistical risk seriously

Michael I. Jordan: On the Computational and Statistical Interface and "Big Data" Max Welling: Are Machine Learning and Statistics Complementary?

## Machine Learning is a highly interdisciplinary field



### Machine Learning + industry



## Applications of Machine Learning



#### spam filtering



# recommendation systems



fraud detection



self-driving cars



#### image recognition



stock market analysis

ImageNet: Computer Eyesight Gets a Lot More Accurate, Krizhevsky et al, 2012

## Types of Machine Learning

#### Unsupervised learning

- Extract key features of the "unlabelled" data
- clustering, signal separation, density estimation
- Goal: representation, hypothesis generation, visualization

#### Supervised learning

- Data contains "labels": every example is an input-output pair
- classification, regression
- Goal: prediction on new examples

### Types of Machine Learning

#### Semi-supervised Learning

A database of examples, only a small subset of which are labelled.

#### Multi-task Learning

A database of examples, each of which has multiple labels corresponding to different prediction tasks.

#### **Reinforcement Learning**

An agent acting in an environment, given rewards for performing appropriate actions, learns to maximize their reward.

### Software

- Python: scikit-learn, mlpy, Theano
- R
- Matlab/Octave
- Weka, mlpack, Torch, Shogun, TensorFlow...

### Syllabus I

Part I: Introduction to unsupervised learning ( $\sim 3$  lectures)

- Dimensionality reduction
  - Principal component analysis, SVD, Biplots, Multidimensional scaling, Isomap
- Clustering
  - K-means
  - Hierarchical clustering

### Syllabus II

Part II: Supervised learning ( $\sim 7$  lectures)

- Empirical risk minimization
- Regression
  - Linear
  - Non-linear basis functions
- Overfitting, cross-validation
- Regularization
- Bias/variance tradeoff
- Classification
  - Linear discriminant analysis
  - Logistic regression
  - Naïve Bayes
  - Perceptron
  - K-nearest neighbors
- Generative vs discriminative methods
- Performance evaluation

#### Software

## Syllabus III

Part III: Useful algorithms for supervised learning ( $\sim 5$  lectures)

- Decision trees
- Ensamle methods
  - Bagging
  - Random forests
  - Boosting
- Problems / other topics TBD if time allows

# Unsupervised Learning: Visualisation and Dimensionality Reduction

### **Unsupervised Learning**

Goals:

- Find the variables that summarise the data / capture relevant information.
- Discover informative ways to visualise the data.
- Discover the subgroups among the observations.

It is often much easier to obtain unlabeled data than labeled data!

### **Exploratory Data Analysis**

#### Notation

- Data consists of *p* variables (features/attributes/dimensions) on *n* examples (items/observations).
- $\mathbf{X} = (x_{ij})$  is a  $n \times p$ -matrix with  $x_{ij} :=$  the *j*-th variable for the *i*-th example

	$x_{11}$	$x_{12}$		$x_{1j}$		$x_{1p}$
$\mathbf{X} =$	$x_{21}$	$x_{22}$	•••	$x_{2j}$	• • •	$x_{2p}$
	÷	÷	·	÷	·	:
	$x_{i1}$	$x_{i2}$		$x_{ij}$		$x_{ip}$
	÷	÷	۰.	÷	·	$\begin{array}{c} x_{1p} \\ x_{2p} \\ \vdots \\ x_{ip} \\ \vdots \end{array}$
	$x_{n1}$	$x_{n2}$		$x_{nj}$		$x_{np}$

- Denote the *i*-th data item by  $x_i \in \mathbb{R}^p$  (we will treat it as a column vector: it is the transpose of the *i*-th row of **X**).
- Assume  $x_1, \ldots, x_n$  are independently and identically distributed samples of a random vector X over  $\mathbb{R}^p$ . The *j*-th dimension of X will be denoted  $X^{(j)}$ .

#### Exploratory Data Analysis

### Crabs Data (n = 200, p = 5)

Campbell (1974) studied rock crabs of the genus **leptograpsus**. One species, **L. variegatus**, had been split into two new species according to their colour: orange and blue. Preserved specimens lose their colour, so it was hoped that morphological differences would enable museum material to be classified.

Data are available on 50 specimens of each sex of each species. Each specimen has measurements on:

- the width of the frontal lobe FL,
- the rear width RW,
- the length along the carapace midline CL,
- the maximum width CW of the carapace, and
- the body depth BD in mm.



in addition to colour/species and sex (we will later view these as labels, but will ignore for now).

### Crabs Data

```
## load package MASS containing the data
library(MASS)
```

```
## extract variables we will look at
varnames<-c("FL","RW","CL","CW","BD")
Crabs <- crabs[,varnames]</pre>
```

```
## look at raw data
Crabs
```

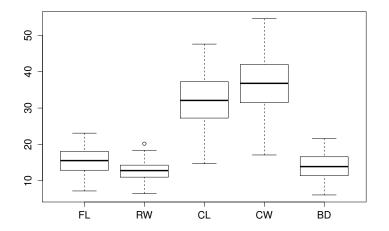
### Crabs Data

## look at raw data
Crabs

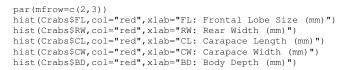
	FL	RW	CL	CW	BD
1	8.1	6.7	16.1	19.0	7.0
2	8.8	7.7	18.1	20.8	7.4
3	9.2	7.8	19.0	22.4	7.7
4	9.6	7.9	20.1	23.1	8.2
5	9.8	8.0	20.3	23.0	8.2
6	10.8	9.0	23.0	26.5	9.8
7	11.1	9.9	23.8	27.1	9.8
8	11.6	9.1	24.5	28.4	10.4
9	11.8	9.6	24.2	27.8	9.7
10	11.8	10.5	25.2	29.3	10.3
11	12.2	10.8	27.3	31.6	10.9
12	12.3	11.0	26.8	31.5	11.4
13	12.6	10.0	27.7	31.7	11.4
14	12.8	10.2	27.2	31.8	10.9
15	12.8	10.9	27.4	31.5	11.0
16	12.9	11.0	26.8	30.9	11.4
17	13.1	10.6	28.2	32.3	11.0
18	13.1	10.9	28.3	32.4	11.2
19	13.3	11.1	27.8	32.3	11.3
20	13.9	11.1	29.2	33.3	12.1

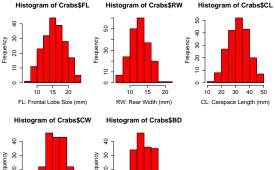
### **Univariate Boxplots**

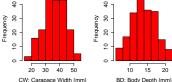
boxplot(Crabs)



### Univariate Histograms

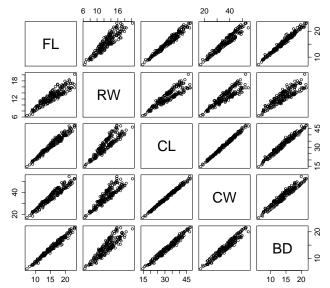






### Simple Pairwise Scatterplots

pairs(Crabs)



### Visualisation and Dimensionality Reduction

The summary plots are useful, but limited use if the dimensionality p is high (a few dozens or even thousands).

- Constrained to view data in 2 or 3 dimensions
- Approach: look for 'interesting' projections of X into lower dimensions
- Hope that even though p is large, considering only carefully selected  $k \ll p$  dimensions is just as informative.

#### **Dimensionality reduction**

- For each data item  $x_i \in \mathbb{R}^p$ , find its lower dimensional representation  $z_i \in \mathbb{R}^k$  with  $k \ll p$ .
- Map x → z should preserve the interesting statistical properties in data.