# Lecture 14: Classification



**COMP90049**
**Knowledge Technologies**



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THE UNIVERSITY OF MELBOURNE

# What is Classification?

Classification involves predicting a discrete class or classes. Those classes are defined in advance.



Binary (yes/no)

- Deciding whether a lone application is risky or not
- Predict whether a dwelling is an apartment or house based on its characteristics
- Predict whether a child will play or not, given weather.
- Will a student skip class on Friday?



Multi-class



- Categorise a document into newspaper sections (news, sports, entertainment, health)
- Recognise images of digits (0-9)
- Discriminating between different species of e.g. a kind of plant or an insect.
- Predicting type of cancer from gene expression data.

# What are (Supervised) Classifiers?



- Given:
  1. a fixed representation language of *attributes*
  2. a fixed set of pre-classified *training instances*
  3. a fixed set of classes $C$
  4. a “learner” algorithm which can identify patterns in the training instances
- Estimate:

  *the category of a novel input* $x : c(x) \in C$

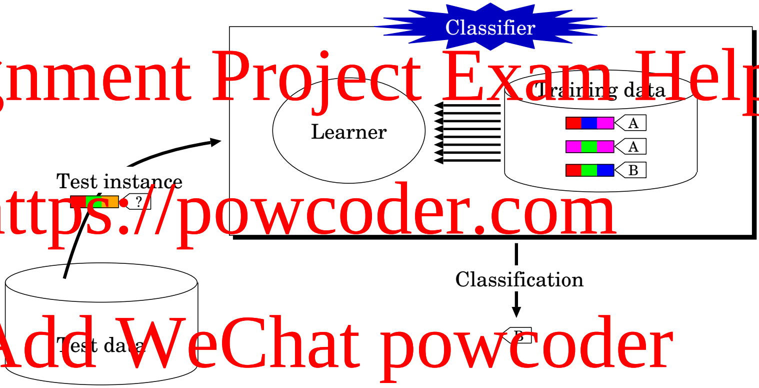
- Model:

  *discover the function that predicts the label* $c(x)$ *given a previously unseen* $x$

# Supervised classification paradigm





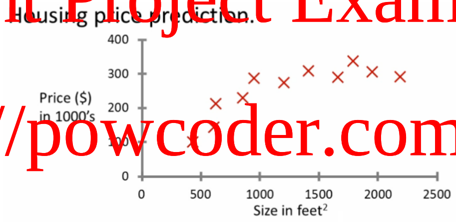



The goal of learning from examples is not to **memorise** but rather to **generalise**, e.g., predict.

# Example: Supervised Learning (Regression)



Can we predict housing prices?






A friend has a house which is 750 square feet – how much can he expect to get?

(draw a straight line vs. fit a curve)

# Linear regression, mathematically

Linear regression captures a relationship between two variables or attributes.



It makes the assumption that there is a *linear* relationship between the two variables:



1. An outcome variable (aka response variable, dependent variable, or label)
2. A predictor (aka independent variable, explanatory variable, or feature)



At its most basic, the relationship can be expressed as a *line* (a deterministic function).

$$y = f(x)$$
$$y = \beta_0 + \beta_1 * x$$
$$y = \beta \cdot x \text{ (given } x_0 = 1)$$

# A simple assumption!

Linear functions are more basic than non-linear functions (mathematically).



They capture that changes in one variable correlate linearly with changes in another variable.

For some variables, this makes sense.



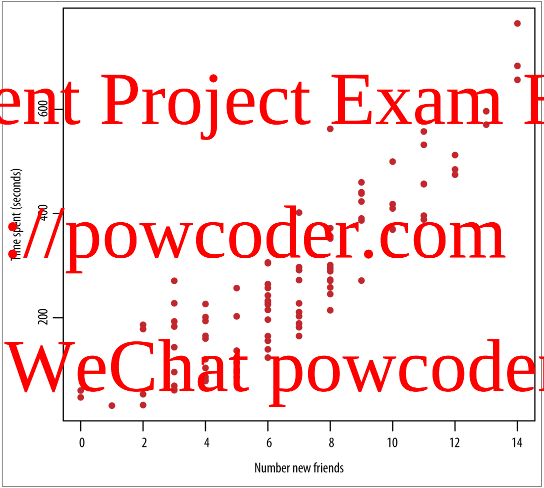
[The more umbrellas you sell, the more money you make. How much money you make is directly proportional to how many umbrellas you sell.]



**Applicability:** Regression can be applied when all variables/attributes are real numbers.

# Explore the relationship

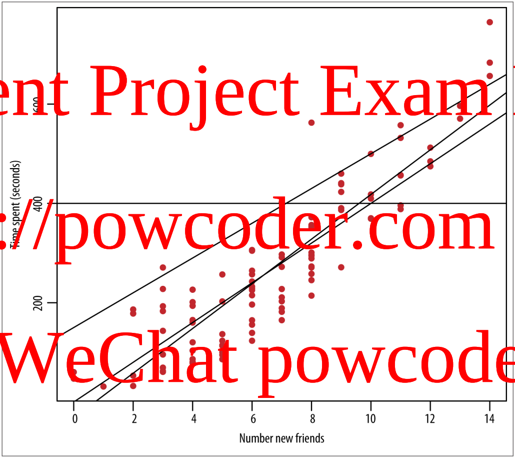





From Schutt & O'Neil, *Doing Data Science*

# Explore the relationship



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# Fitting the model

Want to choose the *best* line.

Operationally, the line that minimises the *distance* between all points and the line.



Recall Euclidean distance: $d(A, B) = \sqrt{\sum_{i=1}^{n}(a_i - b_i)^2}$



*Least squares estimation*: find the line that minimises the sum of the squares of the vertical distances between approximated/predicted $\hat{y}_i$s and observed $y_i$s. Put another way, we want to find the $\beta$ that produces $\hat{y}_i$ for each $x_i$ that is closest to the known $y_i$.



Minimise the Residual Sum of Squares (RSS) (aka Sum of Squares Due to Error (SSE)):

$$RSS(\beta) = \sum_i (y_i - \beta x_i)^2$$

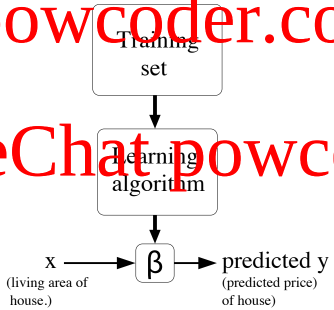
# Prediction

Armed with a linear model $y = \beta_0 + \beta_1 * x$, we can straightforwardly predict a continuous valued output for $y$ given a value of $x$.

We derive that linear model by estimating it from training examples.

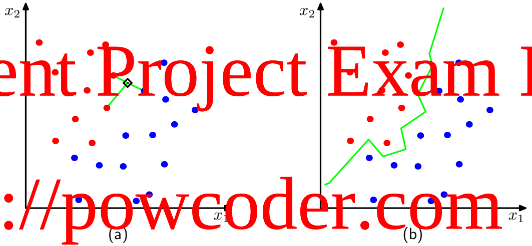
Given examples $(x_0, y_0), (x_1, y_1), ...(x_n, y_n)$ , we determine $\beta$ through least squares estimation.





# $k-$Nearest Neighbour methods in Classification






Given class assignments for existing data points, classify a new point (black).



(a) According to the class membership of the $K$ closest data points.
(b) For $k = 1$, the induced decision boundary.

See: Charles Elkan, UCSD, 2011 lecture notes (posted on LMS)

# $k-$Nearest Neighbour classification strategies



**[1-NN]:** Classify the test input according to the class of the closest training instance.

**[$k$-NN]:** Classify the test input according to the majority class of the $k$ nearest training instances.



**[weighted $k$-NN]:** Classify the test input according to the weighted accumulative class of the $k$ nearest training instances, where weights are based on similarity of the input to each of the $k$ neighbours.



**[offset-weighted $k$-NN]:** Classify the test input according to the weighted accumulative class of the $k$ nearest training instances, where weights are based on similarity of the input to each of the $k$ neighbours, factoring in an offset to indicate the prior expectation of a test input being classified as being a member of that class.

# $k-$Nearest Neighbour classification implementation

The most naive neighbour search implementation involves the brute-force computation of distances between all pairs of points in the dataset.



For N samples in D dimensions, this approach scales as $O(DN^2)$.

- Efficient brute-force neighbours searches can be very competitive for small data samples.
- However, as the number of samples N grows, the brute-force approach quickly becomes infeasible.



Alternative: tree-based data structures



- These structures attempt to reduce the required number of distance calculations by efficiently encoding aggregate distance information for the sample.
- The basic idea is that if point A is very distant from point B, and point B is very close to point C, then we know that points A and C are very distant, without having to explicitly calculate their distance.
- In this way, the computational cost of a nearest neighbours search can be reduced to $O(DN \log(N))$ or better.

# Visualisation of $k-$Nearest Neighbour classification

The nearest neighbour approach corresponds to classification by "hyper-spheres" (or "hyper-ellipsoids")



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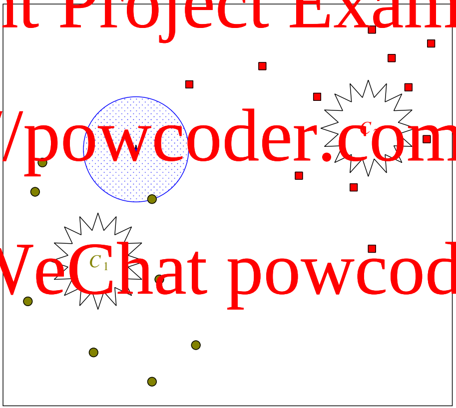
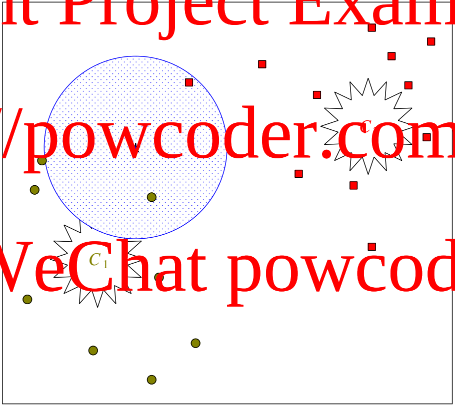


# Visualisation of $k-$Nearest Neighbour classification



The nearest neighbour approach corresponds to classification by “hyper-spheres” (or “hyper-ellipsoids”)



# Strengths and Weaknesses of Nearest Neighbour methods



Strengths

- Simple
- Can handle arbitrarily many classes (multi-class and multi-label)



Weaknesses

- We need a useful distance function, which may not be obvious to design for some sets.
- We need some sort of averaging or voting function for combining the labels of multiple training examples, which may also not be obvious to design.
- Expensive (in terms of index accesses)
- Everything is done at run time (lazy learner)
- Prone to bias
- Arbitrary k value

# Bayesian Methods



- Learning and classification methods based on probability theory
- Build a *generative model* that approximates how data is produced
- Categorisation produces a posterior probability distribution over the possible categories given a description of an instance

## Bayes' Rule



$$P(C, X) = P(C|X)P(X) = P(X|C)P(C)$$

$$P(C|X) = \frac{P(X|C)P(C)}{P(X)}$$

# Naive Bayes (NB) Classifiers



- Task: classify an instance $X = \langle x_1, x_2, ..., x_n \rangle$ according to one of the classes $c_j \in C$

$$
\begin{aligned}
c &= \operatorname{argmax}_{c_j \in C} P(c_j | x_1, x_2, ..., x_n) \\
&= \operatorname{argmax}_{c_j \in C} \frac{P(x_1, x_2, ..., x_n | c_j) P(c_j)}{P(x_1, x_2, ..., x_n)} \\
&= \operatorname{argmax}_{c_j \in C} P(x_1, x_2, ..., x_n | c_j) P(c_j)
\end{aligned}
$$

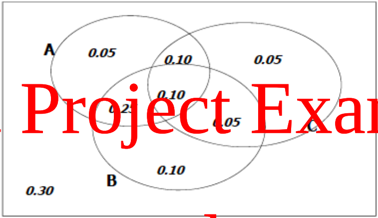


posterior $P(c_j | x_1, x_2, ..., x_n) = \frac{\textit{likelihood} * \textit{prior}}{\textit{evidence}}$



- Predicts $X$ belongs to $c_i$ iff the probability $P(c_i|X)$ is the highest among all the $P(c_k|X)$ for all the $K$ classes
- Since $P(x_1, x_2, ..., x_n)$ is constant for all classes, only $P(x_1, x_2, ..., x_n|c_j)P(c_j)$ needs to be maximised.

# Calculating the likelihood






Must determine the probability of *each combination of values* (given a class).



For large $n$,

1. Typically not enough data to estimate this accurately.
2. Common to encounter the situation where there are no training examples for a particular combination.
3. This would likely lead to over-fitting (biased to combinations for which there are examples).

# Simplifying Assumptions



- $P(c_j)$
  - can be estimated from the frequency of classes in the training examples *[maximum likelihood estimate]*



- $P(x_1, x_2, \ldots, x_n | c_j)$
  - $O(|X|^n |C|)$ parameters (cannot be estimated in practice)

- Naive Bayes Conditional Independence Assumption:
  - assume that the probability of observing the conjunction of attributes is equal to the product of the individual probabilities $P(x_i | c_j)$ *[hence "naive"]*

# The Final NB Formulation

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Classification
Definition
Methods
Linear Regression
Prediction
$k$ — Nearest Neighbour
Naive Bayes
Summary



- Applying the conditional independence assumption:

$$
\begin{aligned}
c &= \text{argmax}_{c_j \in C} P(x_1, x_2, \ldots, x_n | c_j) P(c_j) \\
&= \text{argmax}_{c_j \in C} P(c_j) \prod_i P(x_i | c_j)
\end{aligned}
$$

# Naive Bayes Example

Given a training data set, what are the probabilities we need to estimate?

| Headache | Sore | Temperature | Cough | Diagnosis |
|---|---|---|---|---|
| severe | mild | high | yes | Flu |
| no | severe | normal | yes | Cold |
| mild | mild | normal | yes | Flu |
| mild | no | normal | no | Cold |
| severe | severe | normal | yes | Flu |

Ann comes to the clinic with severe headache, no soreness, normal temperature and with cough. What does she have? Choose the case with highest probability.

$P(Flu|Headache = severe, Sore = no, Temperature = normal, Cough = yes)$
$\sim \; P(Flu) * P(Headache = severe|Flu) * P(Sore = no|Flu) * P(Temperature = normal|Flu) * P(Cough = yes|Flu)$

$P(Cold|Headache = severe, Sore = no, Temperature = normal, Cough = yes)$
$\sim \; P(Cold) * P(Headache = severe|Cold) * P(Sore = no|Cold) * P(Temperature = normal|Cold) * P(Cough = yes|Cold)$

# Estimating probabilities

$$P(Flu) = 3/5$$
$$P(Headache = severe|Flu) = 2/3$$
$$P(Headache = mild|Flu) = 1/3$$
$$P(Headache = no|Flu) = 0/3\ (= e)$$
$$P(Sore = severe|Flu) = 1/3$$
$$P(Sore = mild|Flu) = 2/3$$
$$P(Sore = no|Flu) = 0/3\ (= e)$$
$$P(Temp = high|Flu) = 1/3$$
$$P(Temp = normal|Flu) = 2/3$$
$$P(Cough = yes|Flu) = 3/3$$
$$P(Cough = no|Flu) = 0/3\ (= e)$$

$$P(Cold) = 2/5$$
$$P(Headache = severe|Cold) = 0/2\ (= e)$$
$$P(Headache = mild|Cold) = 1/2$$
$$P(Headache = no|Cold) = 1/2$$
$$P(Sore = severe|Cold) = 1/2$$
$$P(Sore = mild|Cold) = 0/2\ (= e)$$
$$P(Sore = no|Cold) = 1/2$$
$$P(Temp = high|Cold) = 0/2\ (= e)$$
$$P(Temp = normal|Cold) = 2/2$$
$$P(Cough = yes|Cold) = 1/2$$
$$P(Cough = no|Cold) = 1/2$$

Set $0/y$ to $e$, a small value like $10^{-7}$ (or less than $\frac{1}{n}$ where $n$ is the number of training instances)

$P(Flu|Headache = severe, Sore = no, Temperature = normal, Cough = yes)$
$\sim\ P(Flu) * P(Headache = severe|Flu) * P(Sore = no|Flu) * P(Temperature = normal|Flu) * P(Cough = yes|Flu) = 3/5 * 2/3 * e * 2/3 * 3/3 = 0.26e$

$P(Cold|Headache = severe, Sore = no, Temperature = normal, Cough = yes)$
$\sim\ P(Cold) * P(Headache = severe|Cold) * P(Sore = no|Cold) * P(Temperature = normal|Cold) * P(Cough = yes|Cold)$
$= 2/5 * e * 1/2 * 1 * 1/2 = 0.1e$ *Diagnosis is Flu*

# Naive Bayes, analysis





Naive Bayes (NB) Classifier is very simple to build, extremely fast to make decisions, and easy to change the probabilities when the new data becomes available.



- Works well in many application areas.
- Scales easily for large number of dimensions (100s) and data sizes.
- Easy to explain the reason for the decision made.
- One should apply NB first before launching into more sophisticated classification techniques.

# Summary





- How does the k-nearest neighbour method operate, and what are some of the variants on the original algorithm?
- How does the Naive Bayes algorithm work? What assumptions are required to make the computation tractable?

# Resources



Charles Elkan, UCSD, lecture notes
`http://cseweb.ucsd.edu/~elkan/250Bwinter2010/nearestn.pdf`



Witten, Frank, Hall (2011) Data Mining. Chapter 4. ($kD - tree$, ball tree)