## Non Parametric Methods

COMP9417, 23T2

- Non Parametric Methods
- 2 Decision Trees
- **③** k-NN
- 4 Linear Smoothing

Non Parametric Methods ●○

## Section 1

## Non Parametric Methods

### Non Parametric Methods

### Parametric modelling

We make assumptions on the type of function which our data takes.

- Linear regression
- Perceptron
- Logistic regression

## Non parametric modelling

We make no assumptions on the underlying function and purely use our datapoints as guides for inference.

- k-Nearest neighbours
- Local regression
- Decision Trees

## Section 2

# **Decision Trees**

A tree-like model used for both regression and classification.

A tree-like model used for both regression and classification.

Advantages:

A tree-like model used for both regression and classification.

#### Advantages:

- Interpretable
- Useful when used in ensemble learning (we'll come back to this notion)

A tree-like model used for both regression and classification.

#### Advantages:

- Interpretable
- Useful when used in ensemble learning (we'll come back to this notion)

## Disadvantages:

A tree-like model used for both regression and classification.

#### Advantages:

- Interpretable
- Useful when used in ensemble learning (we'll come back to this notion)

### Disadvantages:

- Tend to overfit data
- Often innacurate in their most basic form

## Entropy

Entropy essentially measures the *uncertainty* or *surprise* of a random variable.

We define the entropy for a set S,

$$H(S) = \sum_{x \in X} -p(x) \log p(x)$$

where p(x) represents the *proportion* of x in S.

Entropy essentially measures the uncertainty or surprise of a random variable.

We define the entropy for a set S,

$$H(S) = \sum_{x \in X} -p(x) \log p(x)$$

where p(x) represents the *proportion* of x in S.

Say we have a random variable  $X \sim \text{Bernoulli}(p)$ . We can define the entropy of X:

## Entropy

Entropy essentially measures the uncertainty or surprise of a random variable.

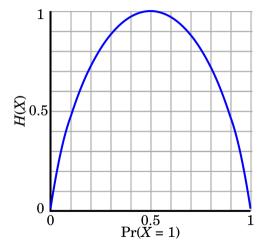
We define the entropy for a set S.

$$H(S) = \sum_{x \in X} -p(x) \log p(x)$$

where p(x) represents the *proportion* of x in S.

Say we have a random variable  $X \sim \text{Bernoulli}(p)$ . We can define the entropy of X:

$$H(x) = -(1 - p)\log(1 - p) - p\log p$$



### Gain

To measure the *information* we gain by splitting on an attribute A for a dataset S, we define:

## Gain

To measure the *information* we gain by splitting on an attribute A for a dataset S, we define:

 $\mathsf{Gain}(S,A) = \mathsf{Current} \ \mathsf{entropy} - \mathsf{Entropy} \ \mathsf{if} \ \mathsf{we} \ \mathsf{split} \ \mathsf{on} \ \mathsf{A}$ 

## Gain

To measure the *information* we gain by splitting on an attribute A for a dataset S, we define:

$$Gain(S, A) = Current entropy - Entropy if we split on A$$

If we have a dataset S with a feature A,

$$\mathsf{Gain}(S,A) = H(S) - \sum_{v \in V_A} \frac{|S_v|}{|S|} H(S_v)$$

# Basic Example

Say we have a dataset as follows: [29+,35-]:

- A1 ~ T: [21+, 5-] F: [8+, 30-]
- A2 ~ T: [18+, 33-] F: [11+, 2-]

# Basic Example

Say we have a dataset as follows: [29+,35-]:

- A1 ~ T: [21+,5-] F: [8+,30-]
- A2 ~ T: [18+, 33-] F: [11+, 2-]

$$H(S) = \sum_{x \in X} -p(x) \log p(x)$$

$$= -\frac{29}{29+35} \log \left(\frac{29}{29+35}\right) - \frac{35}{29+35} \log \left(\frac{35}{29+35}\right)$$

$$= 0.9936$$

$$H(S) = 0.9936$$

$$H(S) = 0.9936$$

$$H(S_{A_{1,T}}) = -\frac{21}{26} \log \left(\frac{21}{26}\right) - \frac{5}{26} \log \left(\frac{5}{26}\right)$$
$$= 0.7063$$

$$H(S) = 0.9936$$

$$H(S_{A_{1,T}}) = -\frac{21}{26} \log\left(\frac{21}{26}\right) - \frac{5}{26} \log\left(\frac{5}{26}\right)$$
$$= 0.7063$$

$$H(S_{A_{1,F}}) = -\frac{8}{38} \log\left(\frac{8}{38}\right) - \frac{30}{38} \log\left(\frac{30}{38}\right)$$
$$= 0.7425$$

• A2 ~ T: [18+, 33-] F: [11+, 2-]

H(S) = 0.9936  $H(S_{A_{1,T}}) = 0.7063$  $H(S_{A_{1,F}}) = 0.7425$ 

• A2 ~ T: 
$$[18+, 33-]$$
 F:  $[11+, 2-]$ 

$$H(S) = 0.9936$$
  
 $H(S_{A_{1,T}}) = 0.7063$   
 $H(S_{A_{1,F}}) = 0.7425$ 

$$H(S_{A_{2,T}}) = -\frac{18}{51} \log\left(\frac{18}{51}\right) - \frac{33}{51} \log\left(\frac{33}{51}\right)$$
$$= 0.9366$$

H(S) = 0.9936 $H(S_{A_{1:T}}) = 0.7063$  $H(S_{A_{1,F}}) = 0.7425$ 

$$H(S_{A_{2,T}}) = -\frac{18}{51} \log\left(\frac{18}{51}\right) - \frac{33}{51} \log\left(\frac{33}{51}\right)$$
$$= 0.9366$$

$$H(S_{A_{2,F}}) = -\frac{11}{13} \log \left(\frac{11}{13}\right) - \frac{2}{13} \log \left(\frac{2}{13}\right)$$
$$= 0.4674$$

 $\bullet \ \, \mathsf{A1} \sim \mathsf{T:} \, \left[21+,5-\right] \, \mathsf{F:} \, \left[8+,30-\right]$ 

• A2 ~ T: [18+, 33-] F: [11+,2-]

H(S) = 0.9936  $H(S_{A_{1,T}}) = 0.7063$   $H(S_{A_{1,F}}) = 0.7425$  $H(S_{A_{2,T}}) = 0.9366$ 

 $H(S_{A_{2}|F}) = 0.4674$ 

• A1 ~ T: 
$$[21+,5-]$$
 F:  $[8+,30-]$ 

H(S) = 0.9936

$$H(S) = 0.3366$$
 $H(S_{A_{1,T}}) = 0.7063$ 
 $H(S_{A_{1,F}}) = 0.7425$ 
 $H(S_{A_{2,T}}) = 0.9366$ 
 $H(S_{A_{2,F}}) = 0.4674$ 

$$\mathsf{Gain}(S,A_1) = H(S) - \sum_{v \in \{T,F\}} \frac{|A_{1,v}|}{|S|} H(A_{1,v})$$

• A1 ~ T: 
$$[21+,5-]$$
 F:  $[8+,30-]$ 

$$\bullet \ \, \mathsf{A2} \sim \mathsf{T:} \ [18+,33-] \ \, \mathsf{F:} \ [11+,2-]$$

H(S) = 0.9936  $H(S_{A_{1,T}}) = 0.7063$   $H(S_{A_{1,F}}) = 0.7425$  $H(S_{A_{2,T}}) = 0.9366$ 

 $H(S_{A_{2},F}) = 0.4674$ 

$$\begin{split} \mathsf{Gain}(S,A_1) &= H(S) - \sum_{v \in \{T,F\}} \frac{|A_{1,v}|}{|S|} H(A_{1,v}) \\ &= H(S) - \frac{26}{64} H(A_{1,T}) - \frac{38}{64} H(A_{1,F}) \end{split}$$

= 0.2658

• A1 ~ T: 
$$[21+,5-]$$
 F:  $[8+,30-]$ 

• A2 ~ T: 
$$[18+,33-]$$
 F:  $[11+,2-]$ 

$$\mathsf{Gain}(S, A_1) = 0.2658$$

$$H(S) = 0.9936$$

$$H(S_{A_{1:T}}) = 0.7063$$

$$H(S_{A_{1,F}}) = 0.7425$$

$$H(S_{A_{2,T}}) = 0.9366$$

$$H(S_{A_{2,F}}) = 0.4674$$

• A2 ~ T: 
$$[18+, 33-]$$
 F:  $[11+, 2-]$ 

$$\mathsf{Gain}(S, A_1) = 0.2658$$

$$H(S) = 0.9936$$

$$H(S_{A_{1.T}}) = 0.7063$$

$$H(S_{A_{1,F}}) = 0.7425$$
  
 $H(S_{A_{2,T}}) = 0.9366$ 

$$H(S_{A_{2,F}}) = 0.4674$$

$$Gain(S, A_2) = H(S) - \frac{51}{64}H(A_{2,T}) - \frac{13}{64}H(A_{2,F})$$
$$= 0.1643$$

# ID3 Algorithm

#### Basically what we just did:

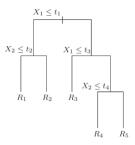
- Calculate the entropy for each attribute  $a \in A$ .
- Split on the attribute with the maximum Gain. This means creating a decision tree node using that attribute.
- Recurse on this new subset of the data.

# Regression Trees

Regression trees split the dataset up into regions and fit separate models to each region.

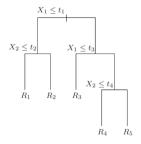
# Regression Trees

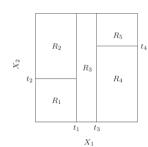
Regression trees split the dataset up into regions and fit separate models to each region.



# Regression Trees

Regression trees split the dataset up into regions and fit separate models to each region.





If we define our two regions as  $R_1(j,s) = \{X | X_j \le s\}$  and  $R_2(j,s) = \{X | X_j > s\}$ . We can find optimal regions with the formula:

If we define our two regions as  $R_1(j,s)=\{X|X_j\leq s\}$  and  $R_2(j,s)=\{X|X_j>s\}$ . We can find optimal regions with the formula:

$$\min_{j,s} \left[ \min_{c_1} \sum_{y_i \in R_1(j,s)} (y_i - c_1)^2 + \sum_{y_i \in R_2(j,s)} \min_{c_2} (y_i - c_2)^2 \right]$$

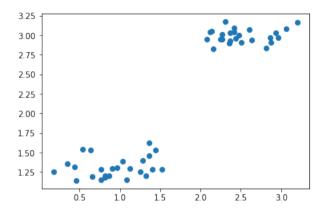
Where  $\hat{c_1} = \text{ave}(y_i | x_i \in R_1), \quad \hat{c_2} = \text{ave}(y_i | x_i \in R_2).$ 

If we define our two regions as  $R_1(j,s)=\{X|X_j\leq s\}$  and  $R_2(j,s)=\{X|X_j>s\}$ . We can find optimal regions with the formula:

$$\min_{j,s} \left[ \min_{c_1} \sum_{y_i \in R_1(j,s)} (y_i - c_1)^2 + \sum_{y_i \in R_2(j,s)} \min_{c_2} (y_i - c_2)^2 \right]$$

Where  $\hat{c_1} = \text{ave}(y_i|x_i \in R_1)$ ,  $\hat{c_2} = \text{ave}(y_i|x_i \in R_2)$ .

This essentially finds regions  $(R_1 \text{ and } R_2)$  with the minimum variance.



$$\min_{j,s} \left[ \min_{c_1} \sum_{y_i \in R_1(j,s)} (y_i - c_1)^2 + \sum_{y_i \in R_2(j,s)} \min_{c_2} (y_i - c_2)^2 \right]$$

## Section 3

*k*-NN

### k-NN

We predict  $\hat{y}_i$  for a point  $x_i$  to be the average of the k-nearest points.

### k-NN

We predict  $\hat{y}_i$  for a point  $x_i$  to be the average of the k-nearest points.

**Regression** If we define the set K as the k-nearest neighbours of a point  $X_i$ , then our k-NN estimate is:

$$\hat{y}_i = \frac{1}{k} \sum_{i=1}^n \mathbf{1} \{ X_i \in K \} y_i$$

**Classification** we assign  $X_i$  the majority

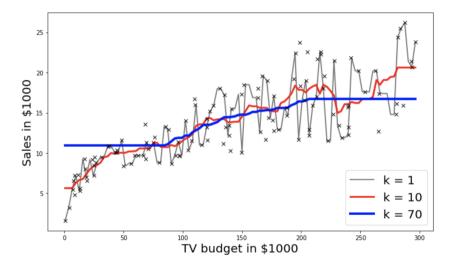
### k-NN

We predict  $\hat{y}_i$  for a point  $x_i$  to be the average of the k-nearest points.

**Regression** If we define the set K as the k-nearest neighbours of a point  $X_i$ , then our k-NN estimate is:

class in K.

$$\hat{y}_i = \frac{1}{k} \sum_{i=1}^n \mathbf{1} \{ X_i \in K \} y_i$$



We need lots of relevant data for accurate predictions.

We need lots of relevant data for accurate predictions.

#### A not-so obvious limitation:

We need lots of relevant data for accurate predictions.

#### A not-so obvious limitation:

Curse of dimensionality.

### **Curse of Dimensionality**

Certain phenomena occur when we increase the number of dimensions (i.e features) in our problem.

The most common are:

### **Curse of Dimensionality**

Certain phenomena occur when we increase the number of dimensions (i.e features) in our problem.

The most common are:

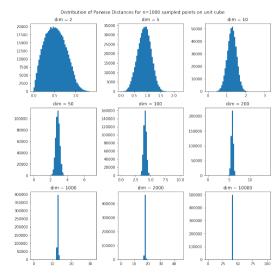
Distances between points breaking down

#### **Curse of Dimensionality**

Certain phenomena occur when we increase the number of dimensions (i.e features) in our problem.

The most common are:

- Distances between points breaking down
- The need for even more data



• 1 binary variable

• 1 binary variable - 2 unique combinations

• 1 binary variable - 2 unique combinations - 20 samples

- 1 binary variable 2 unique combinations 20 samples
- 2 binary variables 4 unique combinations 40 samples

- 1 binary variable 2 unique combinations 20 samples
- 2 binary variables 4 unique combinations 40 samples
- $\bullet$   $\it k$  binary variables  $2^{\it k}$  unique combinations  $10\times 2^{\it k}$  samples

- 1 binary variable 2 unique combinations 20 samples
- 2 binary variables 4 unique combinations 40 samples
- $\emph{k}$  binary variables  $2^\emph{k}$  unique combinations  $10 \times 2^\emph{k}$  samples

So for 20 features, we need  $10 \times 2^{20} = 10485760$  data points!

### Section 4

# Linear Smoothing

# Linear Smoothing

k-NN regression typically fits a choppy model to our data. Linear smoothing tries to smooth out the fit by incorporating a kernel to weight the influence nearest neighbours by distance.

# Linear Smoothing

k-NN regression typically fits a choppy model to our data. Linear smoothing tries to smooth out the fit by incorporating a kernel to weight the influence nearest neighbours by distance.

If we define h as the smoothing parameter and K as the kernel, the Linear Smoothing estimate is:

$$\hat{y}_i = \frac{\sum_{j=1}^n K\left(\frac{\|x_i - x_j\|}{h}\right) y_i}{\sum_{j=1}^n K\left(\frac{\|x_i - x_j\|}{h}\right)}$$

# Linear Smoothing

k-NN regression typically fits a choppy model to our data. Linear smoothing tries to smooth out the fit by incorporating a *kernel* to weight the influence nearest neighbours by distance.

If we define h as the smoothing parameter and K as the kernel, the Linear Smoothing estimate is:

$$\hat{y}_i = \frac{\sum_{j=1}^n K\left(\frac{\|x_i - x_j\|}{h}\right) y_i}{\sum_{j=1}^n K\left(\frac{\|x_i - x_j\|}{h}\right)}$$

As  $h \to 0$  our distances have a higher variance. If  $h \to \infty$  have a lower variance, and our model is in turn smoother.

