Lecture 4: 3 February, 2022

Madhavan Mukund

https://www.cmi.ac.in/~madhavan

Data Mining and Machine Learning
January–May 2022

Decision tree algorithm

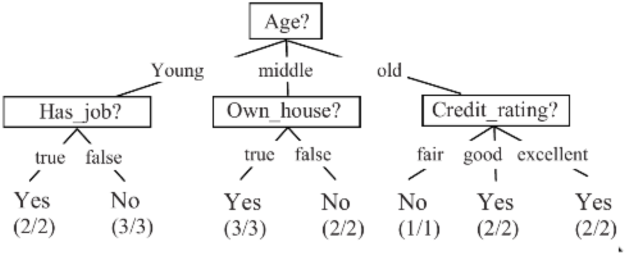
A : current set of attributes

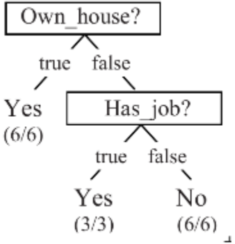
Pick $a \in A$, create children corresponding to resulting partition with attributes $A \setminus \{a\}$

Stopping criterion:

- Current node has uniform class label
- A is empty — no more attributes to query

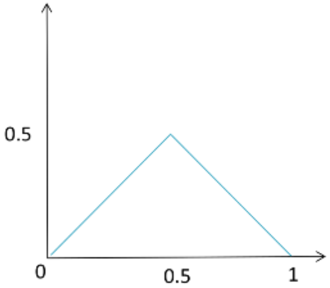
If a leaf node is not uniform, use majority class as prediction





Building small decision trees

- Prefer small trees
- Goal: partition with uniform category — pure leaf
- Impure node — best prediction is majority value
- Minority ratio is impurity
- Heuristic: reduce impurity as much as possible
- For each attribute, compute weighted average impurity of children
- Choose the minimum



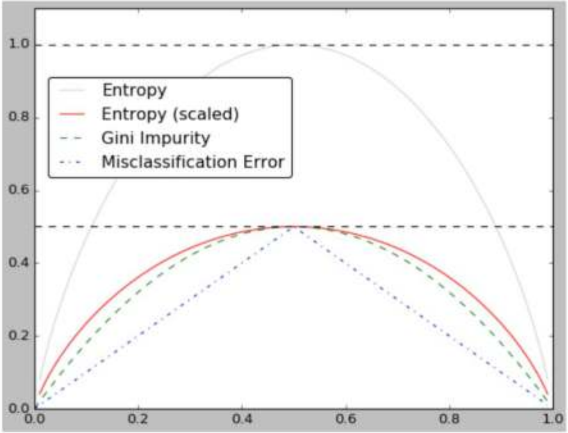
$c = 1$

Misclassification rate is linear

- $c \in \{0, 1\}$
- x-axis: fraction of inputs with $c = 1$

Better impurity functions

- Impurity measure that increases more sharply performs better, empirically
- Entropy, information theory — [Quinlan]
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
  - $E = -(p_0 \log_2 p_0 + p_1 \log_2 p_1)$
- Gini index, economics — [Breiman]
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
  - $G = 1 - (p_0^2 + p_1^2)$



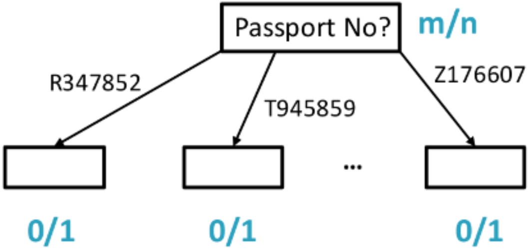
$c = 1$

Information gain

- Greedy strategy: choose attribute to maximize reduction in impurity — maximize information gain

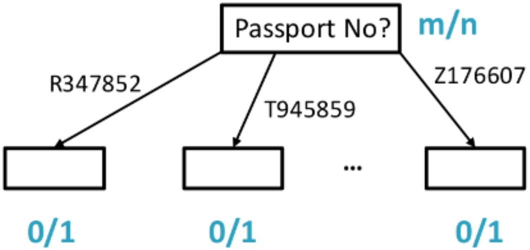
Information gain

- Greedy strategy: choose attribute to maximize reduction in impurity — maximize information gain
- Suppose an attribute is a unique identifier
  - Roll number, passport number, Aadhaar ...



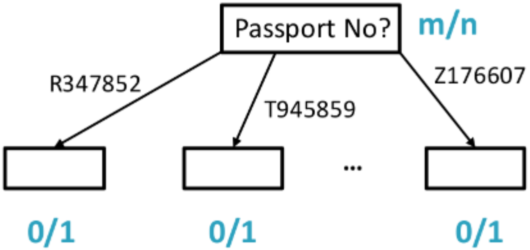
Information gain

- Greedy strategy: choose attribute to maximize reduction in impurity — maximize information gain
- Suppose an attribute is a unique identifier
  - Roll number, passport number, Aadhaar . . .
- Querying this attribute produces partitions of size 1
  - Each partition guaranteed to be pure
  - New impurity is zero



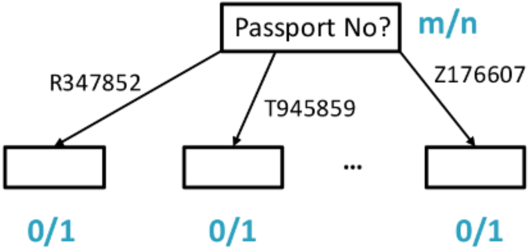
Information gain

- Greedy strategy: choose attribute to maximize reduction in impurity — maximize information gain
- Suppose an attribute is a unique identifier
  - Roll number, passport number, Aadhaar . . .
- Querying this attribute produces partitions of size 1
  - Each partition guaranteed to be pure
  - New impurity is zero
- Maximum possible impurity reduction, but useless!



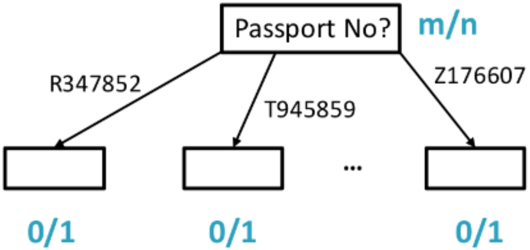
Information gain

- Tree building algorithm blindly picks attribute that maximizes information gain



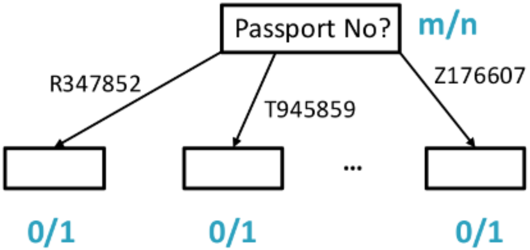
Information gain

- Tree building algorithm blindly picks attribute that maximizes information gain
- Need a correction to penalize attributes with highly scattered attributes



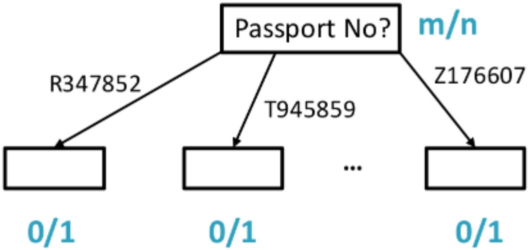
Information gain

- Tree building algorithm blindly picks attribute that maximizes information gain
- Need a correction to penalize attributes with highly scattered attributes
- Extend the notion of impurity to attributes



Attribute Impurity

- Attribute takes values $\{v_1, v_2, \ldots, v_k\}$ (n_1, n_2, n_k)
- v_i appears n_i times across n rows
- $p_i = n_i/n$

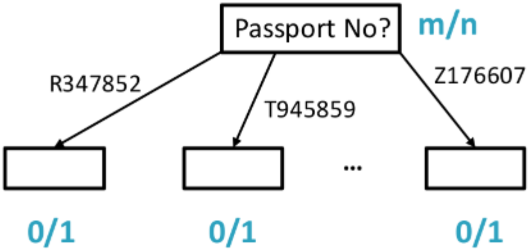


Attribute Impurity

- Attribute takes values $\{v_1, v_2, \ldots, v_k\}$
- v_i appears n_i times across n rows
- $p_i = n_i/n$
- Entropy across k values

$$-\sum_{i=1}^{k} p_i \log_2 p_i$$

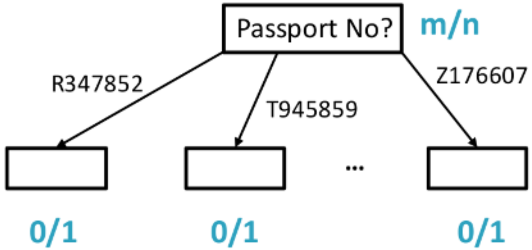
$\Sigma p_i = 1$



Attribute Impurity

- Attribute takes values $\{v_1, v_2, \ldots, v_k\}$
- v_i appears n_i times across n rows
- $p_i = n_i/n$
- Entropy across k values
  $$-\sum_{i=1}^{k} p_i \log_2 p_i$$
- Gini index across k values
  $$1 - \sum_{i=1}^{k} p_i^2$$

$1 - (p_0^2 + p_1^2)$



Attribute Impurity

- Extreme case, each $p_i = 1/n$

$p_i = n_i/n$ n_i = # times we see v_i

Attribute Impurity

- Extreme case, each $p_i = 1/n$
- Entropy

$$-\sum_{i=1}^{n} \frac{1}{n} \log_2 \frac{1}{n} = -n \cdot \frac{1}{n}(-\log_2 n) = \log_2 n$$

Attribute Impurity

- Extreme case, each $p_i = 1/n$
- Entropy

$$-\sum_{i=1}^{n} \frac{1}{n} \log_2 \frac{1}{n} = -n \cdot \frac{1}{n}(-\log_2 n) = \log_2 n$$

- Gini index

$$1 - \sum_{i=1}^{n} \left(\frac{1}{n}\right)^2 = 1 - \frac{n}{n^2} = \frac{n-1}{n}$$

$\frac{4}{5}$ $\frac{5}{6}$ $\frac{6}{7}$ - -

Attribute Impurity

- Extreme case, each $p_i = 1/n$
- Entropy

$$-\sum_{i=1}^{n} \frac{1}{n} \log_2 \frac{1}{n} = -n \cdot \frac{1}{n}(-\log_2 n) = \log_2 n$$

- Gini index

$$1 - \sum_{i=1}^{n} \left(\frac{1}{n}\right)^2 = 1 - \frac{n}{n^2} = \frac{n-1}{n}$$

- Both increase as n increases

Attribute Impurity

- Extreme case, each $p_i = 1/n$
- Entropy

$$-\sum_{i=1}^{n} \frac{1}{n} \log_2 \frac{1}{n} = -n \cdot \frac{1}{n}(-\log_2 n) = \log_2 n$$

- Gini index

$$1 - \sum_{i=1}^{n} \left(\frac{1}{n}\right)^2 = 1 - \frac{n}{n^2} = \frac{n-1}{n}$$

- Both increase as n increases

Penalizing scattered attributes

- Divide information gain by attribute impurity
- Information gain ratio(A)

$$\frac{\text{Information-Gain(A)}}{\text{Impurity}(A)}$$

- Scattered attributes have high denominator, counteracting high numerator

Heuristics for building decision trees

- Can find better measures of impurity than misclassification rate
  - Non linear impurity function works better in practice
  - Entropy, Gini index
  - Gini index is used in most decision tree libraries

Heuristics for building decision trees

- Can find better measures of impurity than misclassification rate
  - Non linear impurity function works better in practice
  - Entropy, Gini index
  - Gini index is used in most decision tree libraries
- Blindly using information gain can be problematic
  - Attributes that are unique identifiers for rows produces maximum information gain, with little utility
  - Divide information gain by impurity of attribute
  - Information gain ratio

Categorical vs numeric attributes

- So far, all attributes have been categorical
- What age groups make up young, middle, old?
- How are these boundaries defined?
- How do we query numerical attributes?
  - Height, weight, length, income,

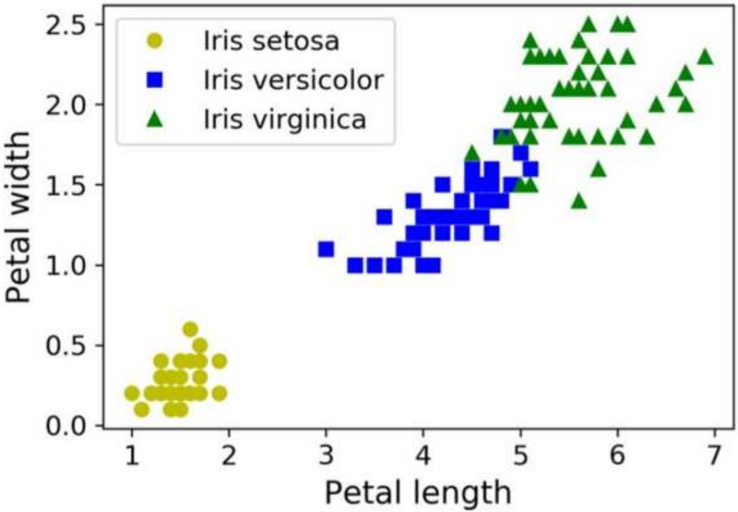
ID	Age	Has_job	Own_house	Credit_rating	Class
1	young	false	false	fair	**No**
2	young	false	false	good	**No**
3	young	true	false	good	**Yes**
4	young	true	true	fair	**Yes**
5	young	false	false	fair	**No**
6	middle	false	false	fair	**No**
7	middle	false	false	good	**No**
8	middle	true	true	good	**Yes**
9	middle	false	true	excellent	**Yes**
10	middle	false	true	excellent	**Yes**
11	old	false	true	excellent	**Yes**
12	old	false	true	good	**Yes**
13	old	true	false	good	**Yes**
14	old	true	false	excellent	**Yes**
15	old	false	false	fair	**No**

Iris dataset

- Iris is a type of flower
- Three species: *iris setosa*, *iris versicolor*, *iris virginica*
- Dataset has sepal length and width and petal length and width for 150 flowers

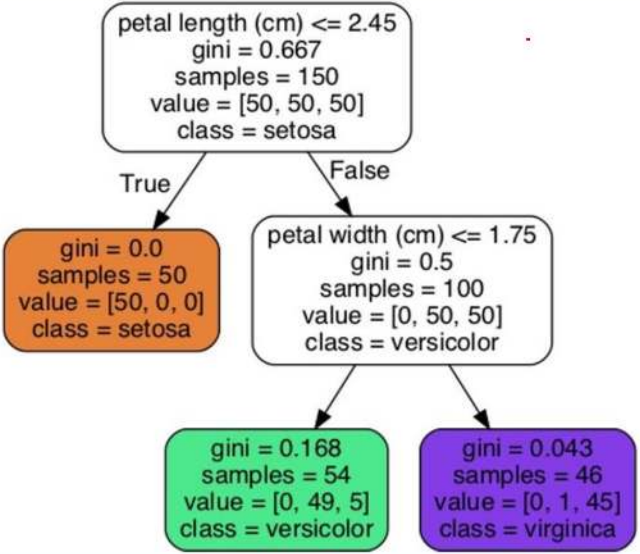
Iris dataset

- Iris is a type of flower
- Three species: *iris setosa*, *iris versicolor*, *iris virginica*
- Dataset has sepal length and width and petal length and width for 150 flowers
- Scatter plot for two attributes, petal length and petal width



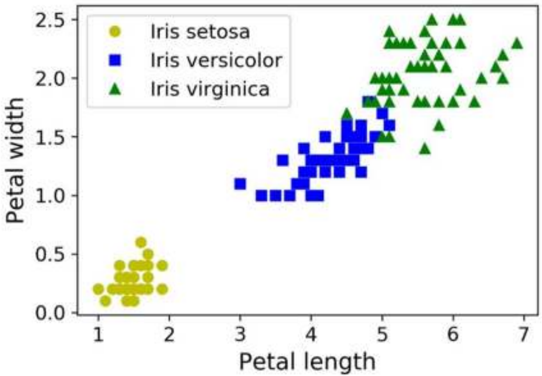
Iris dataset

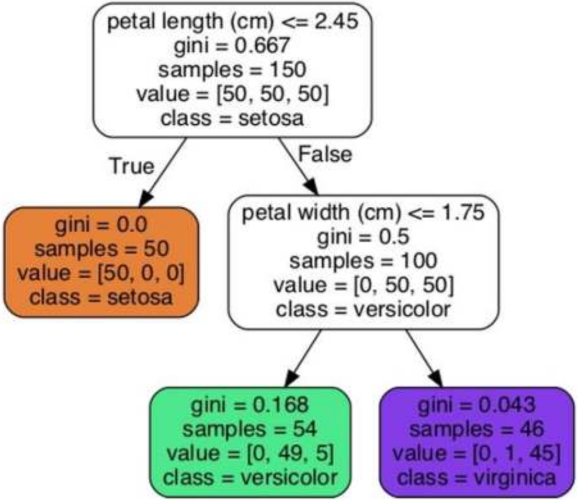
- Iris is a type of flower
- Three species: *iris setosa*, *iris versicolor*, *iris virginica*
- Dataset has sepal length and width and petal length and width for 150 flowers
- Scatter plot for two attributes, petal length and petal width
- Decision tree for this data set



Decision tree for iris dataset

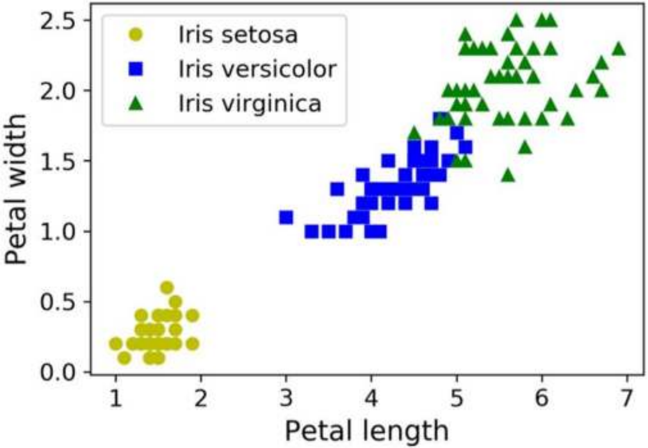
- Queries compare numerical attribute against a value
- How do we find these query values?





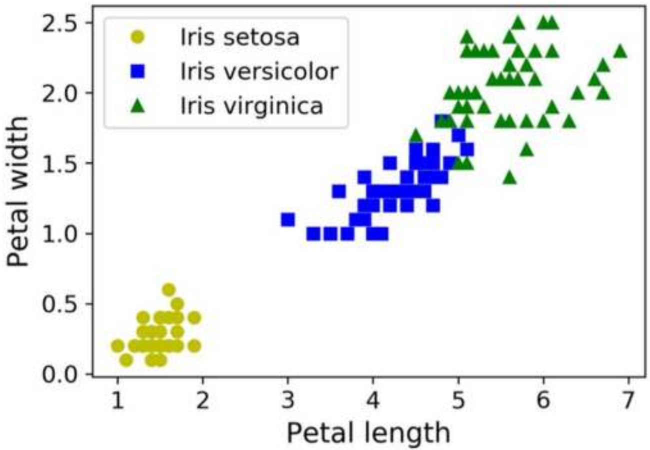
Querying numerical attributes

- Numerical attribute takes values in a range $[L, U]$
  - Petal length : $[1, 7]$
  - Petal width : $[0, 2.5]$



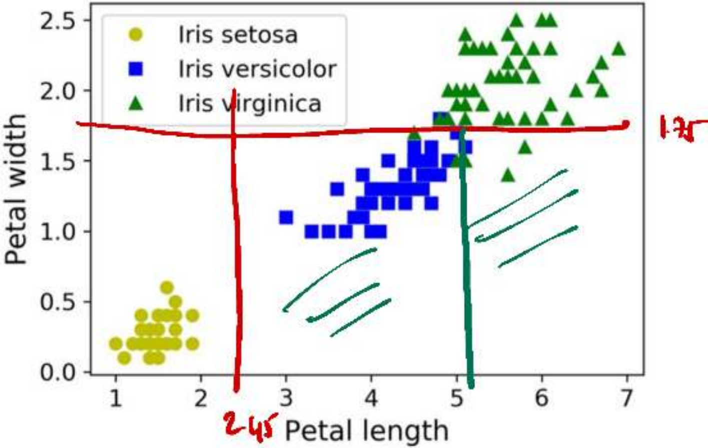
Querying numerical attributes

- Numerical attribute takes values in a range $[L, U]$
  - Petal length : $[1, 7]$
  - Petal width : $[0, 2.5]$
- Pick a value v in the range and check if $A \leq v$



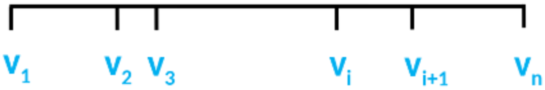
Querying numerical attributes

- Numerical attribute takes values in a range $[L, U]$
  - Petal length : $[1, 7]$
  - Petal width : $[0, 2.5]$
- Pick a value v in the range and check if $A \leq v$
- Infinitely many choices for v
- How do we pick a sensible one?



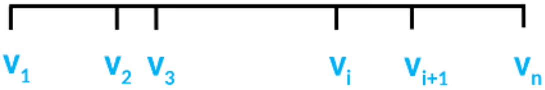
Querying numerical attributes

- Only n values for A in training data
  - Sort as $v_1 < v_2 < \cdots < v_n$



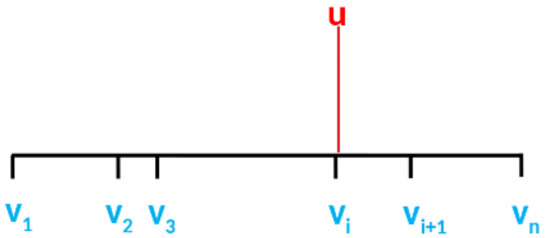
Querying numerical attributes

- Only n values for A in training data
  - Sort as $v_1 < v_2 < \cdots < v_n$
- Consider interval $[v_i, v_{i+1}]$



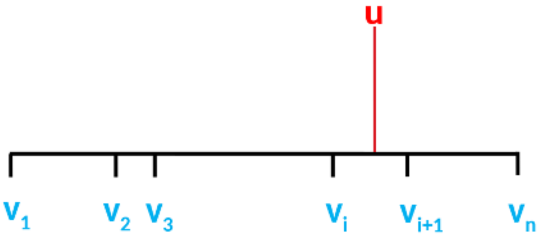
Querying numerical attributes

- Only n values for A in training data
  - Sort as $v_1 < v_2 < \cdots < v_n$
- Consider interval $[v_i, v_{i+1}]$
- For each $v_i \leq u < v_{i+1}$, query $A \leq u$ gives the same answer



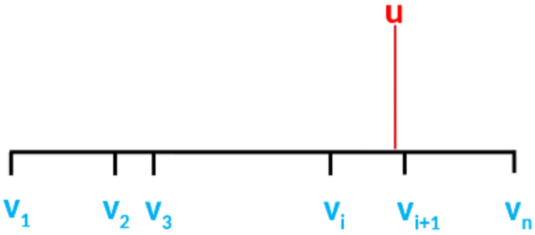
Querying numerical attributes

- Only n values for A in training data
  - Sort as $v_1 < v_2 < \cdots < v_n$
- Consider interval $[v_i, v_{i+1}]$
- For each $v_i \leq u < v_{i+1}$, query $A \leq u$ gives the same answer



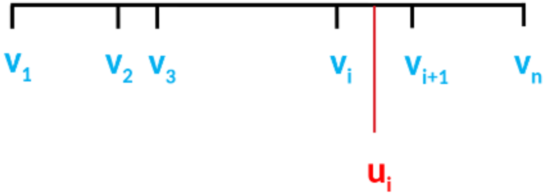
Querying numerical attributes

- Only n values for A in training data
  - Sort as $v_1 < v_2 < \cdots < v_n$
- Consider interval $[v_i, v_{i+1}]$
- For each $v_i \leq u < v_{i+1}$, query $A \leq u$ gives the same answer
- Only $n-1$ useful intervals to check

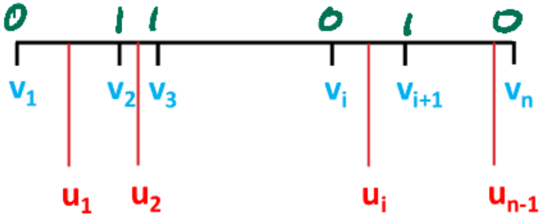


Querying numerical attributes

- Only n values for A in training data
  - Sort as $v_1 < v_2 < \cdots < v_n$
- Consider interval $[v_i, v_{i+1}]$
- For each $v_i \leq u < v_{i+1}$, query $A \leq u$ gives the same answer
- Only $n{-}1$ useful intervals to check
- Pick midpoint $u_i = (v_i + v_{i+1})/2$ as query value for each interval

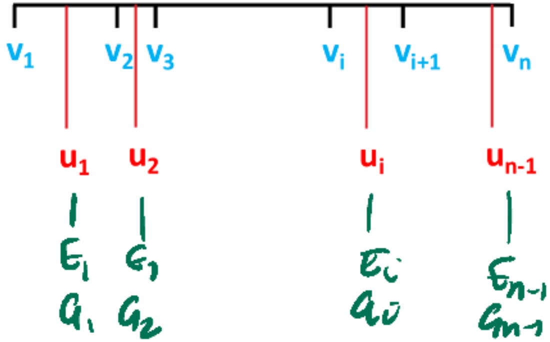


- Pick midpoint $u_i = (v_i + v_{i+1})/2$ as query value for each interval
- Each query $A \leq u_i$ partitions training data



Querying numerical attributes

- Pick midpoint $u_i = (v_i + v_{i+1})/2$ as query value for each interval
- Each query $A \leq u_i$ partitions training data
- Choose the query $A \leq u_i$ with maximum information gain
- Assign this as the information gain for this attribute

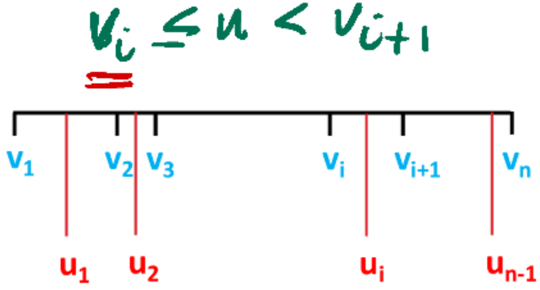


Querying numerical attributes

- Pick midpoint $u_i = (v_i + v_{i+1})/2$ as query value for each interval
- Each query $A \leq u_i$ partitions training data
- Choose the query $A \leq u_i$ with maximum information gain
- Assign this as the information gain for this attribute
- Compare across all attributes and choose best one

Querying numerical attributes

- Pick midpoint $u_i = (v_i + v_{i+1})/2$ as query value for each interval
- Each query $A \leq u_i$ partitions training data
- Choose the query $A \leq u_i$ with maximum information gain
- Assign this as the information gain for this attribute
- Compare across all attributes and choose best one



- Any point within an interval can be used

Querying numerical attributes

- Pick midpoint $u_i = (v_i + v_{i+1})/2$ as query value for each interval
- Each query $A \leq u_i$ partitions training data
- Choose the query $A \leq u_i$ with maximum information gain
- Assign this as the information gain for this attribute
- Compare across all attributes and choose best one

- Any point within an interval can be used
- May prefer endpoints — midpoints may not be meaningful values

Building a decision tree

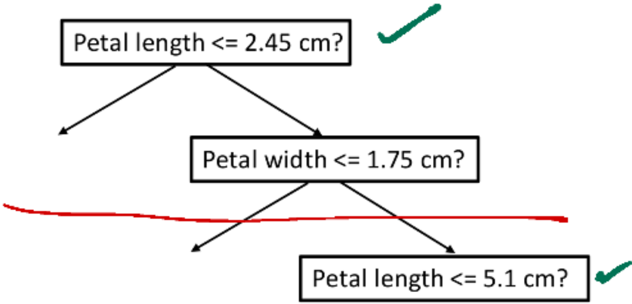
- For each numerical attribute, choose query $A \leq v$ with maximum information gain

Building a decision tree

- For each numerical attribute, choose query $A \leq v$ with maximum information gain
- Across all categorical and numerical attributes, choose the one with best information gain

Building a decision tree

- For each numerical attribute, choose query $A \leq v$ with maximum information gain
- Across all categorical and numerical attributes, choose the one with best information gain
- Categorical attrbutes can be queried only once on a path
- Numerical attributes can be queried repeatedly — interval to query keeps shrinking



Testing a supervised learning model

- How do we validate software?
  - Test suite of carefully selected inputs
  - Compare output with expected answers

Testing a supervised learning model

- How do we validate software?
  - Test suite of carefully selected inputs
  - Compare output with expected answers
- What about classification models?
  - By definition, deploy on data where the outcome is unknown
  - If expected answer available, have a deterministic solution, model not needed!

Testing a supervised learning model

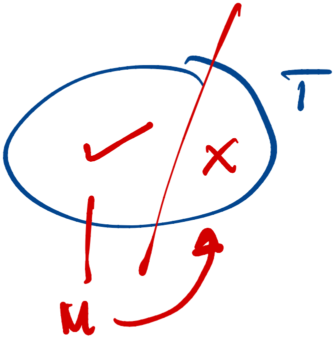
- How do we validate software?
  - Test suite of carefully selected inputs
  - Compare output with expected answers
- What about classification models?
  - By definition, deploy on data where the outcome is unknown
  - If expected answer available, have a deterministic solution, model not needed!
- On what basis can we evaluate a supervised learning model?

Creating a test set

- Training data is labelled
  - No other source of inputs with expected answers

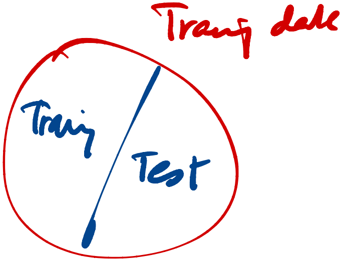
Creating a test set

- Training data is labelled
  - No other source of inputs with expected answers
- Segregate some training data for testing
  - Terminology: training set and test set
  - Build model using training set, evaluate on test set



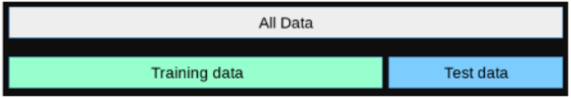
Creating a test set

- Training data is labelled
  - No other source of inputs with expected answers
- Segregate some training data for testing
  - Terminology: training set and test set
  - Build model using training set, evaluate on test set
- Creating the test set
  - Need to choose a random sample
  - Can further use stratified sampling, preserve relative ratios (e.g., age wise distribution)
  - ML libraries can do this automatically



Creating a test set

- How large should the test set be?
  - Typically 20-30% of labelled data
- Depends on labelled data available
  - Need enough training data to build the model



Creating a test set

- How large should the test set be?
  - Typically 20-30% of labelled data
- Depends on labelled data available
  - Need enough training data to build the model

Cross validation

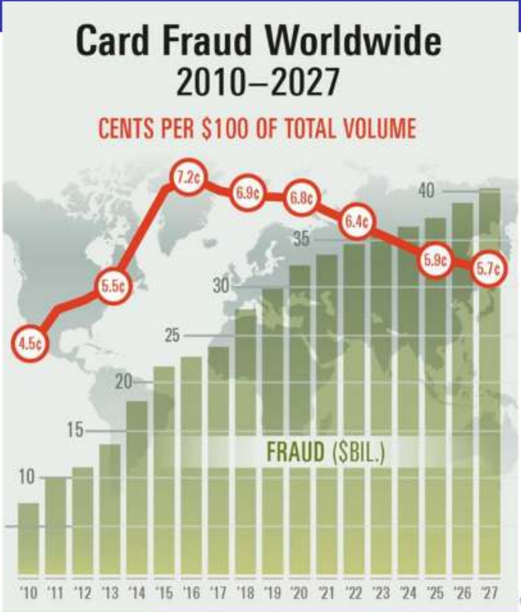
- Partition labelled data into k chunks
- Hold out one chunk at a time
- Build k models, using $k-1$ chunks for training, 1 for testing
- Useful if labelled data is scarce

What are we measuring?

- Accuracy is an obvious measure
  - Fraction of inputs where classification is correct

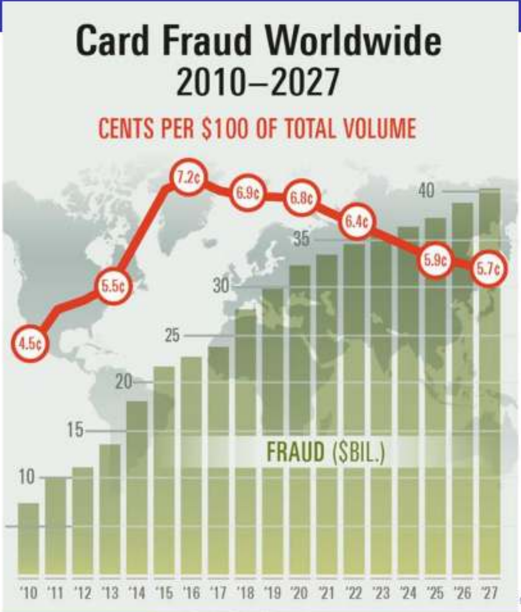
What are we measuring?

- Accuracy is an obvious measure
  - Fraction of inputs where classification is correct
- Classifiers are often used in asymmetric situations
  - Less than 1% of credit card transactions are fraud



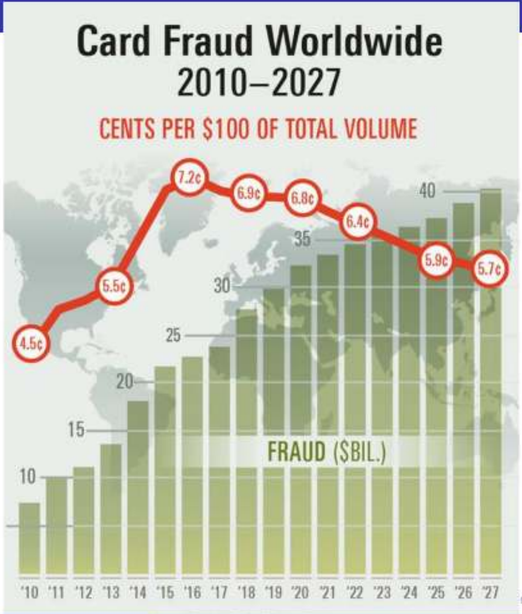
What are we measuring?

- Accuracy is an obvious measure
  - Fraction of inputs where classification is correct
- Classifiers are often used in asymmetric situations
  - Less than 1% of credit card transactions are fraud
- "Is this transaction a fraud?"
  - Trivial classifier — always answer "No"
  - More than 99% accurate, but useless!



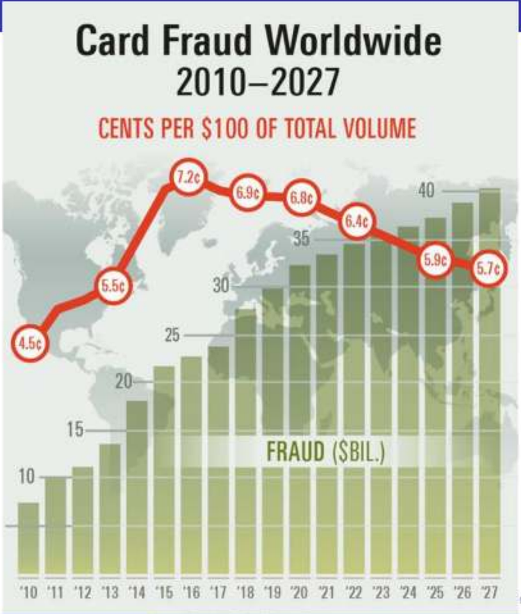
Catching the minority case

- The minority case is the useful case
  - Assume question is phrased so that minority answer is "Yes"
  - Want to flag as many "Yes" cases as possible



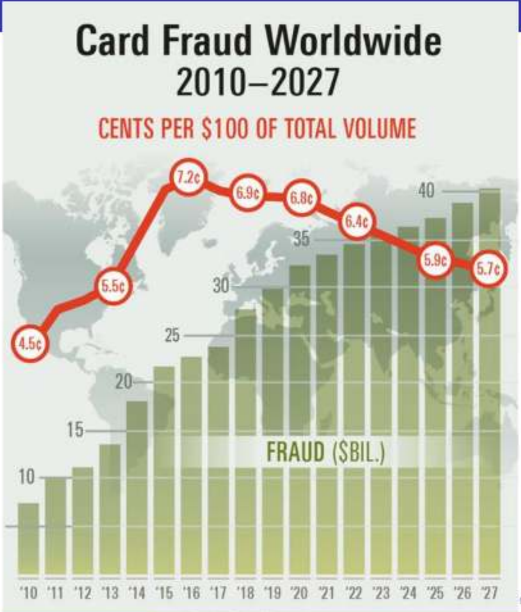
Catching the minority case

- The minority case is the useful case
  - Assume question is phrased so that minority answer is "Yes"
  - Want to flag as many "Yes" cases as possible
- Aggressive classifier
  - Marks borderline "No" as "Yes"
  - False positives



Catching the minority case

- The minority case is the useful case
  - Assume question is phrased so that minority answer is "Yes"
  - Want to flag as many "Yes" cases as possible
- Aggressive classifier
  - Marks borderline "No" as "Yes"
  - False positives
- Cautious classifier
  - Marks borderline "Yes" as "No"
  - False negatives



Confusion matrix

- Four possible combinations
  - Actual answer: Yes / No
  - Prediction: Yes / No

Confusion matrix

- Four possible combinations
  - Actual answer: Yes / No
  - Prediction: Yes / No
- Record all four possibilities in confusion matrix
  - Correct answers
    - True positives, true negatives
  - Wrong answers
    - False positives, false negatives

	Classified positive	Classified negative
Actual positive	True Positive (TP)	False Negative (FN)
Actual negative	False Positive (FP)	True Negative (TN)

Performance measures

Precision

- What percentage of positive predictions are correct?

$$\frac{\text{TP}}{\text{TP} + \text{FP}}$$

Recall

- What percentage of actual positive cases are discovered?

$$\frac{\text{TP}}{\text{TP} + \text{FN}}$$

	Classified positive	Classified negative
Actual positive	True Positive (TP)	False Negative (FN)
Actual negative	False Positive (FP)	True Negative (TN)

Performance measures

- Precision 1, Recall 0.01

	Classified positive	Classified negative
Actual positive	1	99
Actual negative	0	900

100

900

Performance measures

- Precision 1, Recall 0.01 $\frac{1}{100}$
- Recall up to 0.4, but precision down to 0.29 40/140

	Classified positive	Classified negative
Actual positive	40	60
Actual negative	100	800

Performance measures

- Precision 1, Recall 0.01
- Recall up to 0.4, but precision down to 0.29
- Recall up to 0.99, but precision down to 0.165

	Classified positive	Classified negative
Actual positive	99	1
Actual negative	500	400

Performance measures

- Precision 1, Recall 0.01
- Recall up to 0.4, but precision down to 0.29
- Recall up to 0.99, but precision down to 0.165
- Precision-recall tradeoff
  - Strict classifiers : fewer false positives (high precision), miss more actual positives (low recall)
  - Permissive classifiers : catch more actual positives (high recall) but more false positives (low precision)

	Classified positive	Classified negative
Actual positive	99	1
Actual negative	500	400

Performance measures

- Which measure is more useful?
  - Depends on situation
- Hiring
  - Screening test: high recall
  - Interview: high precision
- Medical diagnosis
  - Immunization: high recall
  - Critical illness diagnosis: high precision

	Classified positive	Classified negative
Actual positive	True Positive (TP)	False Negative (FN)
Actual negative	False Positive (FP)	True Negative (TN)

Performance measures

Other measures, terminology

- Recall is also called sensitivity
- Accuracy: (TP+TN)/(TP+TN+FP+FN)
- Specificity: TN/(TN+FP)
- Threat score: TP/(TP+FP+FN)
  - TN usually majority, ignore, not useful

	Classified positive	Classified negative
Actual positive	True Positive (TP)	False Negative (FN)
Actual negative	False Positive (FP)	True Negative (TN)

Performance measures

Other measures, terminology

- Recall is also called sensitivity
- Accuracy: (TP+TN)/(TP+TN+FP+FN)
- Specificity: TN/(TN+FP)
- Threat score: TP/(TP+FP+FN)
  - TN usually majority, ignore, not useful

	Classified positive	Classified negative
Actual positive	True Positive (TP)	False Negative (FN)
Actual negative	False Positive (FP)	True Negative (TN)

$$\frac{1}{\frac{\frac{1}{p}+\frac{1}{r}}{2}}$$

F Score

- A single combined score
- Harmonic mean of precision, recall

$$\frac{2pr}{p+r}$$

Body Mass Index

Ht, Wt

"Feature Engineering"

Performance measures

Other measures, terminology

- Recall is also called sensitivity
- Accuracy: (TP+TN)/(TP+TN+FP+FN)
- Specificity: TN/(TN+FP)
- Threat score: TP/(TP+FP+FN)
  - TN usually majority, ignore, not useful

	Classified positive	Classified negative
Actual positive	True Positive (TP)	False Negative (FN)
Actual negative	False Positive (FP)	True Negative (TN)

F Score

- A single combined score
- Harmonic mean of precision, recall

$$\frac{2pr}{p+r}$$