Lecture 4: 20 January, 2026

Madhavan Mukund

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

Data Mining and Machine Learning
January–April 2025

Decision tree algorithm

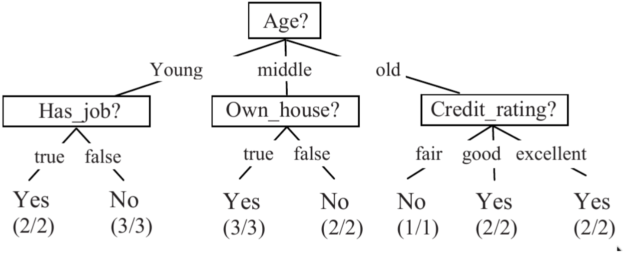
A : current set of attributes

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



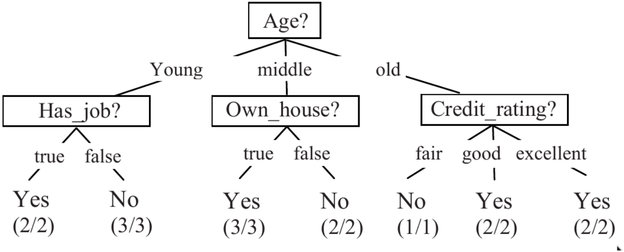
- Non-uniform leaf node — identical combination of attributes, but different classes
- Attributes do not capture all criteria used for classification

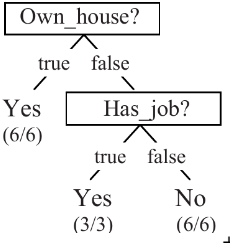
Decision trees

- Tree is not unique
- Which tree is better?
- Prefer small trees
  - Explainability
  - Generalize better (see later)

Unfortunately

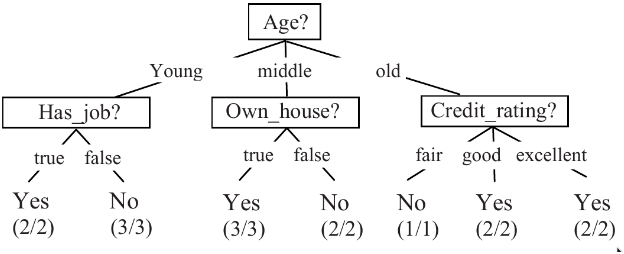
- Finding smallest tree is NP-complete — for any definition of "smallest"
- Instead, greedy heuristic

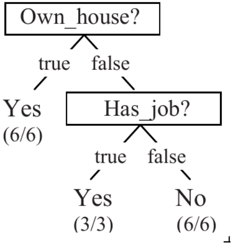




Greedy heuristic

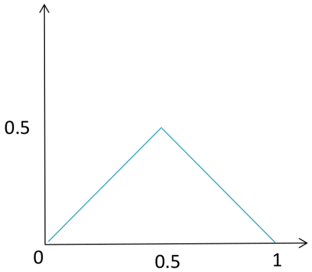
- Goal: partition with uniform category — pure leaf
- Impure node — best prediction is majority value
- Minority ratio is impurity
- Heuristic: reduce impurity as much as possible
- For each attribute, compute weighted average impurity of children
- Choose the minimum





Greedy heuristic — misclassification rate

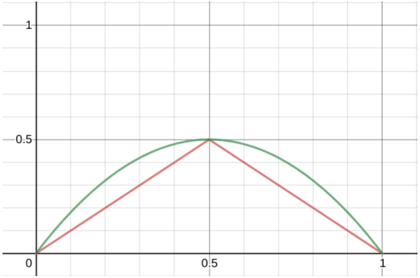
- Minority ratio is misclassification rate
- Misclassification rate is linear
  - $c \in \{0, 1\}$
  - x-axis: fraction of inputs with $c = 1$



$c = 1$

A better impurity function

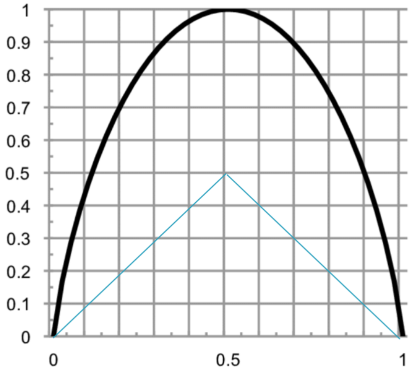
- Misclassification rate is linear
- Impurity measure that increases more sharply performs better, empirically
- Entropy — [Quinlan]
- Gini index — [Breiman]



$c = 1$

Entropy

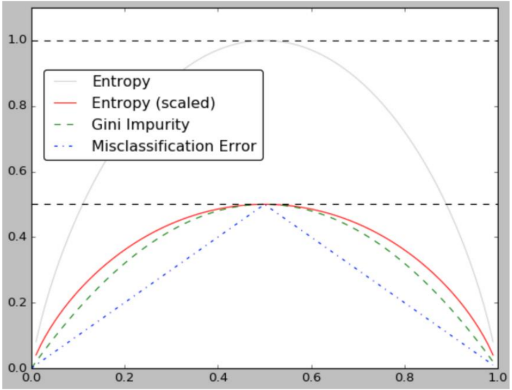
- Information theoretic measure of randomness
- Minimum number of bits to transmit a message — [Shannon]
- n data items
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
- Entropy
  $E = -(p_0 \log_2 p_0 + p_1 \log_2 p_1)$
- Minimum when $p_0 = 1, p_1 = 0$ or vice versa — note, declare $0 \log_2 0$ to be 0
- Maximum when $p_0 = p_1 = 0.5$



$c = 1$

Gini Index

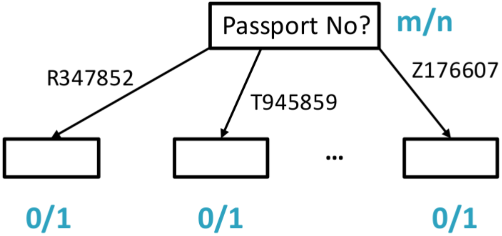
- Measure of unequal distribution of wealth
- Economics — [Corrado Gini]
- As before, n data items
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
- Gini Index $G = 1 - (p_0^2 + p_1^2)$
- $G = 0$ when $p_0 = 0$, $p_1 = 0$ or v.v.
  $G = 0.5$ when $p_0 = p_1 = 0.5$
- Entropy curve is slightly steeper, but Gini index is easier to compute
- Decision tree libraries usually use Gini index



$c = 1$

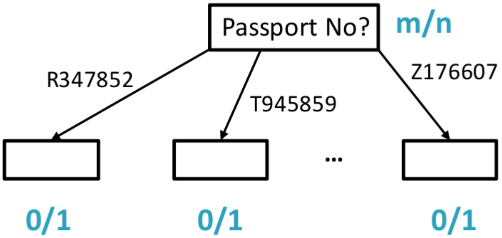
Information gain

- 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!



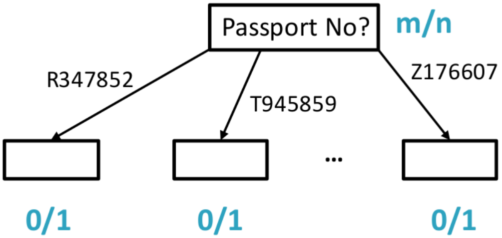
Information gain

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



Attribute Impurity

- Attribute takes values $\{v_1, v_2, \ldots, v_k\}$
- 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
  $$1 - \sum_{i=1}^{k} p_i^2$$



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

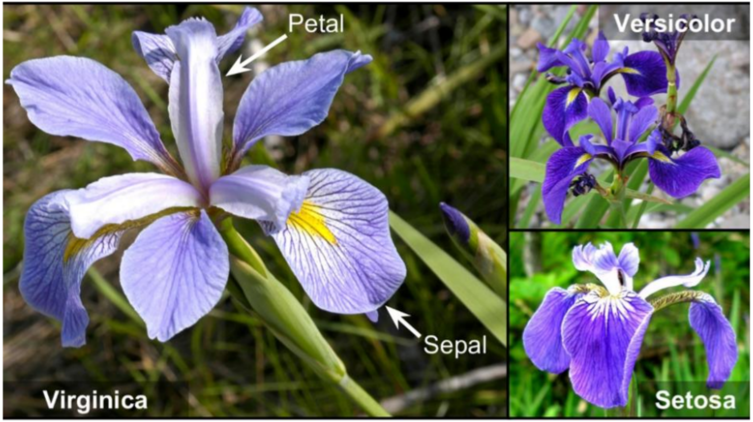
Categorical vs numeric attributes

- 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**

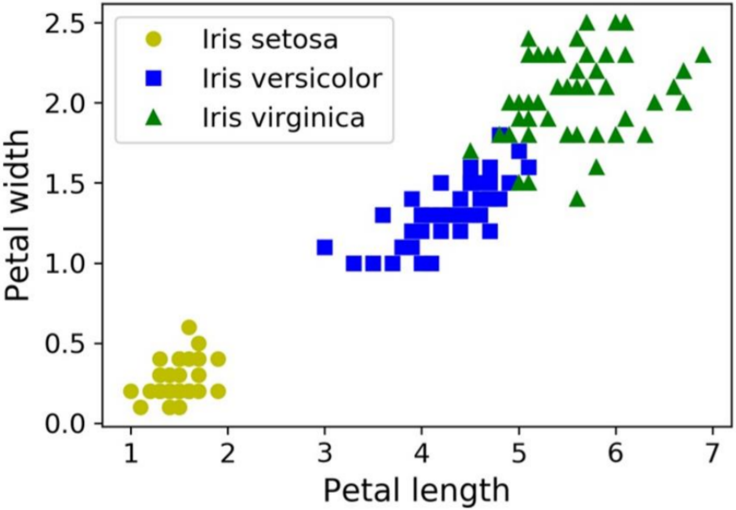
Iris dataset

- 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



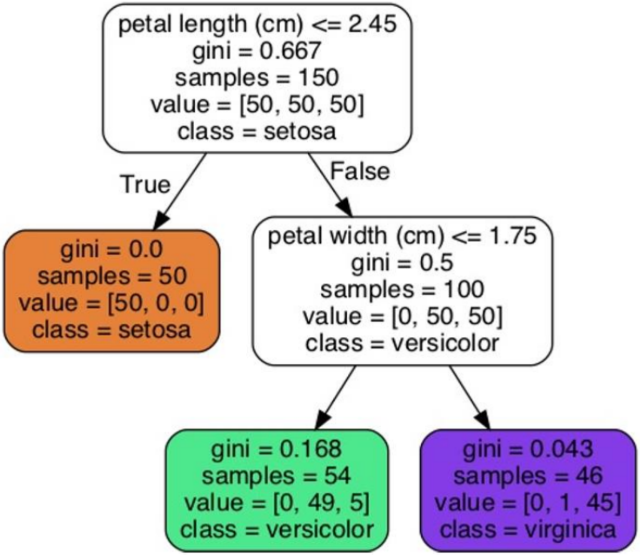
Iris dataset

- 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



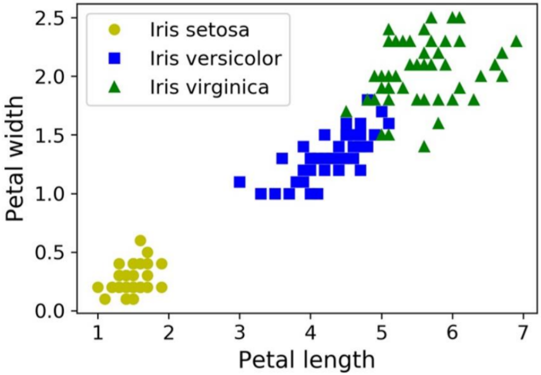
Iris dataset

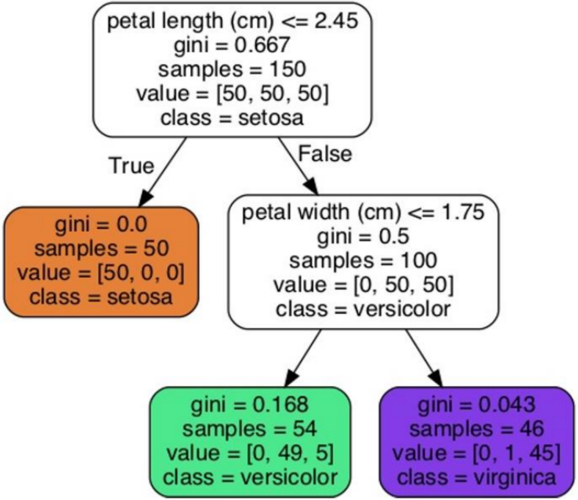
- Iris is a type of flower
- Three species: *iris setosa*, *iris versicolor*, *iris virginica*
- Dataset has sepal length and width and petal length and width for 150 flowers
- Scatter plot for two attributes, petal length and petal width
- Decision tree for this data set



Decision tree for iris dataset

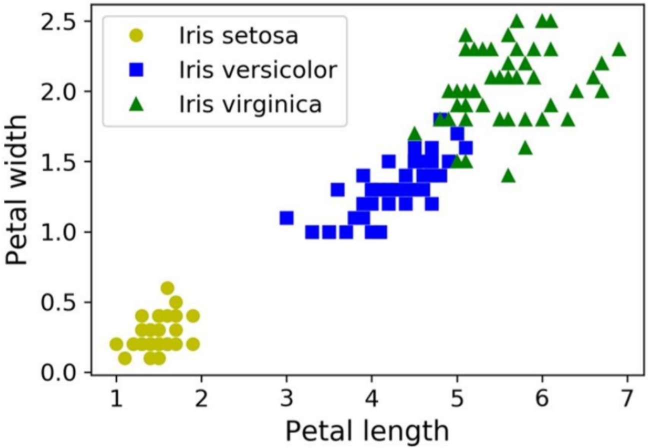
- Queries compare numerical attribute against a value
- How do we find these query values?





Querying numerical attributes

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

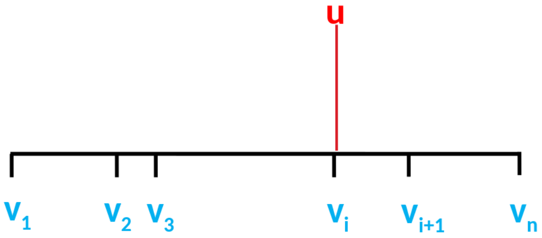


Querying numerical attributes

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

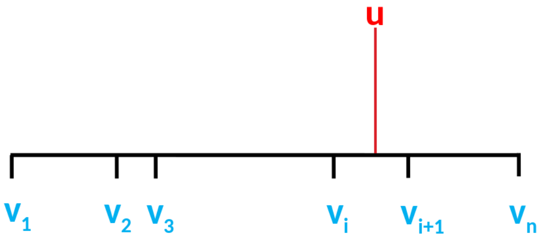
Querying numerical attributes

- 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



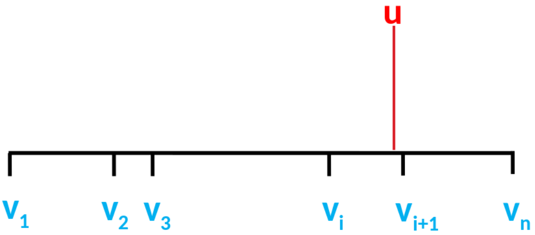
Querying numerical attributes

- 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



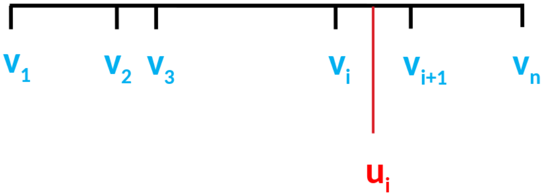
Querying numerical attributes

- 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



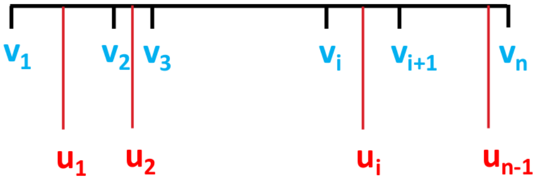
Querying numerical attributes

- 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



Querying numerical attributes

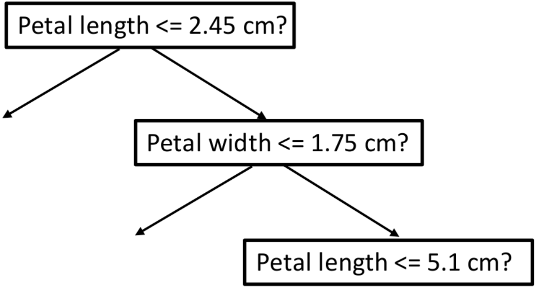
- Pick midpoint $u_i = (v_i + v_{i+1})/2$ as query value for each interval
- Each query $A \leq u_i$ partitions training data
- Choose the query $A \leq u_i$ with maximum information gain
- Assign this as the information gain for this attribute
- Compare across all attributes and choose best one



- 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
- 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

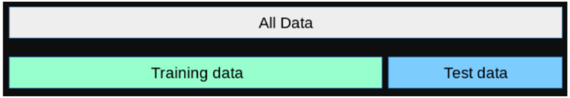
- How do we validate software?
    - Test suite of carefully selected inputs
    - Compare output with expected answers
- What about classification models?
    - By definition, deploy on data where the outcome is unknown
    - If expected answer available, have a deterministic solution, model not needed!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

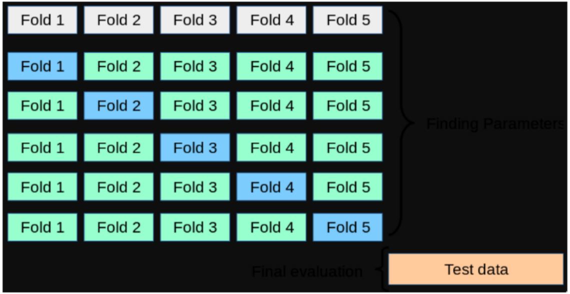
Creating a test set

- 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



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
- 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!