Lecture 4: 17 January, 2023

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[Slides by Madhavan Mukund]

Data Mining and Machine Learning
January–April 2023

Decision tree algorithm

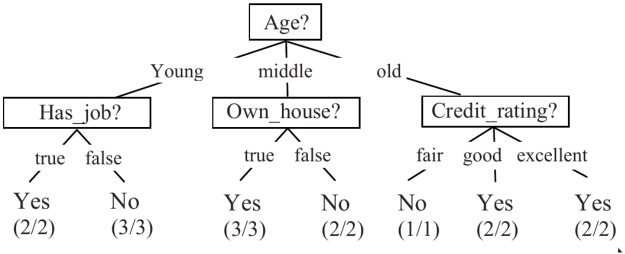
A : current set of attributes

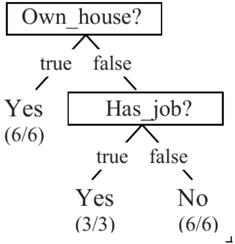
Pick $a \in A$, create children corresponding to resulting partition with attributes $A \setminus \{a\}$

Stopping criterion:

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

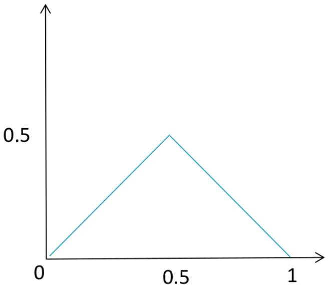
If a leaf node is not uniform, use majority class as prediction





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



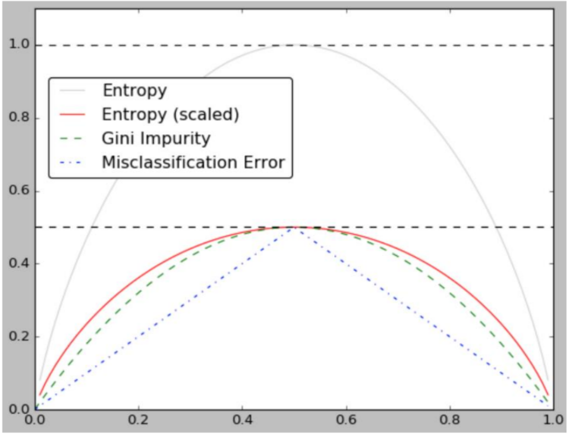
$c = 1$

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 $c = 1$, $p_1 = n_1/n$
  - $G = 1 - (p_0^2 + p_1^2)$



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Information gain

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- $Impurity(D)$ is the impurity of the dataset D.
- Suppose attribute $a \in A$ takes values $v_1, v_2, \dots, v_k$
- If we split D by using an attribute a, we get $D_1, D_2, \dots, D_k$.

$$Impurity_a(D) = \sum_{i=1}^{k} \frac{|D_i|}{|D|} \cdot Impurity(D_i)$$

- Information Gain of $a \in A$ is

$$Information - Gain(D, a) = Impurity(D) - Impurity_a(D)$$

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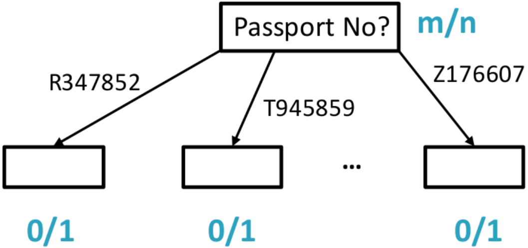
  - Roll number, passport number, Aadhaar . . .



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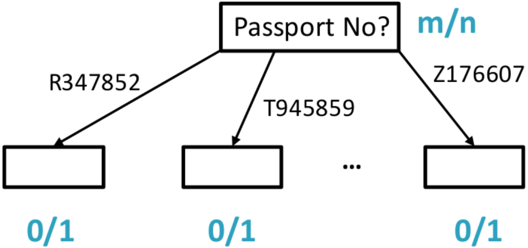

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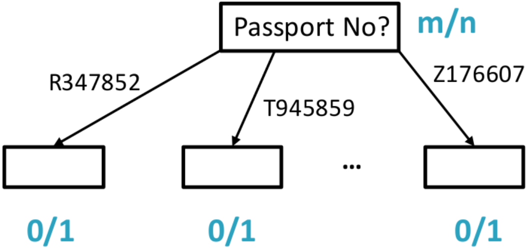
- Maximum possible impurity reduction, but useless!



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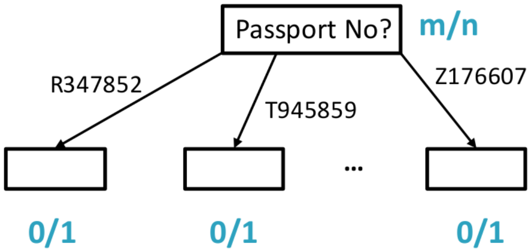

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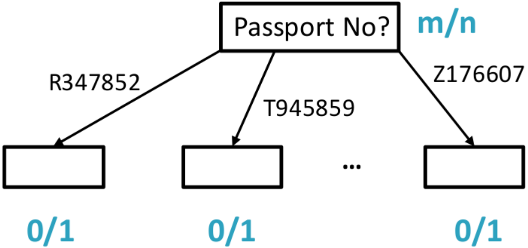

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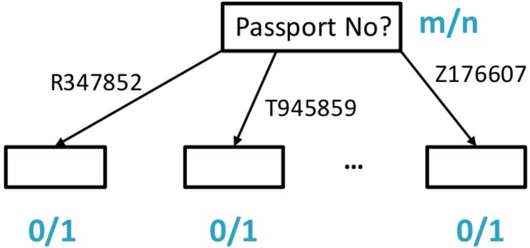
- Extend the notion of impurity to attributes



Attribute Impurity

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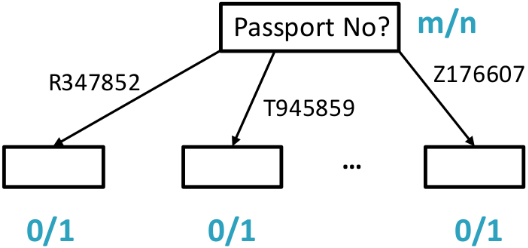

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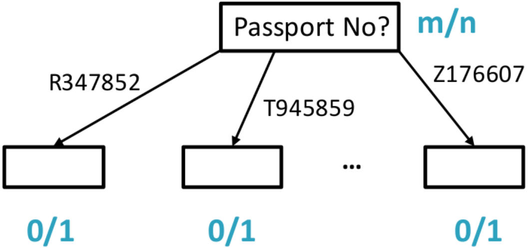

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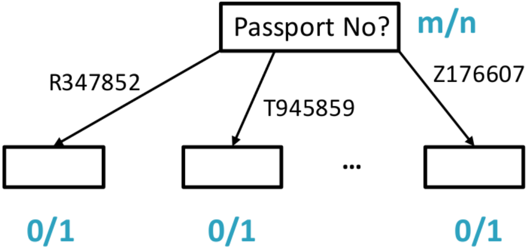

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Penalizing scattered attributes

- Divide information gain by attribute impurity
- Information gain ratio(a) for $a \in A$

$$\frac{\text{Information-Gain(D,a)}}{\text{Impurity}(a)}$$

- Scattered attributes have high denominator, counteracting high numerator

Heuristics for building decision trees

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- Can find better measures of impurity than misclassification rate
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  - 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

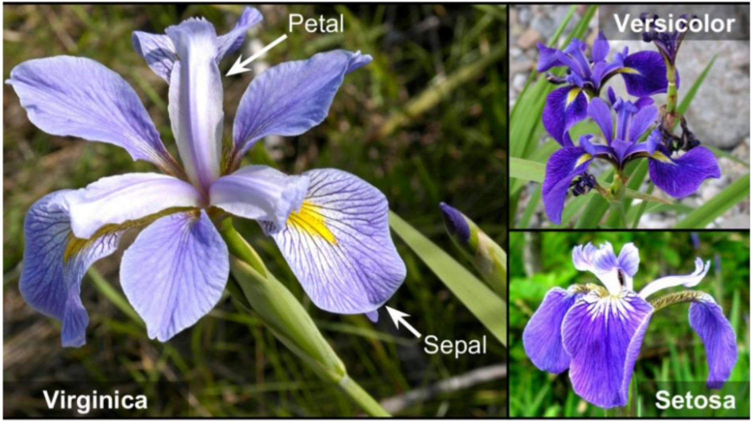
Categorical vs numeric attributes

- 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



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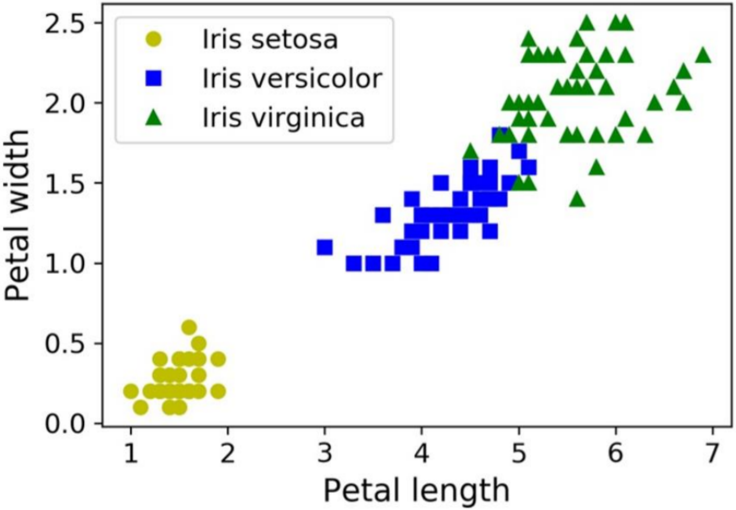

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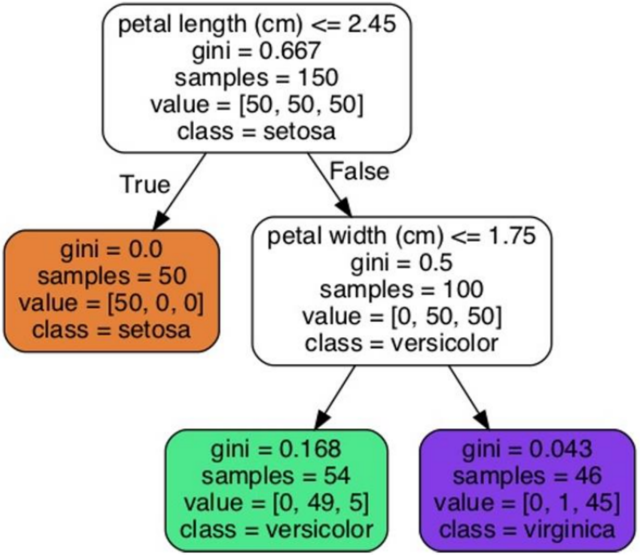
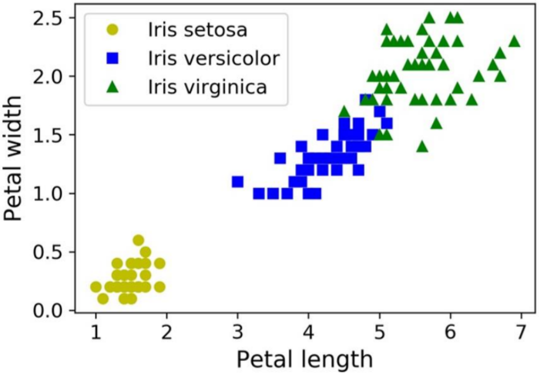
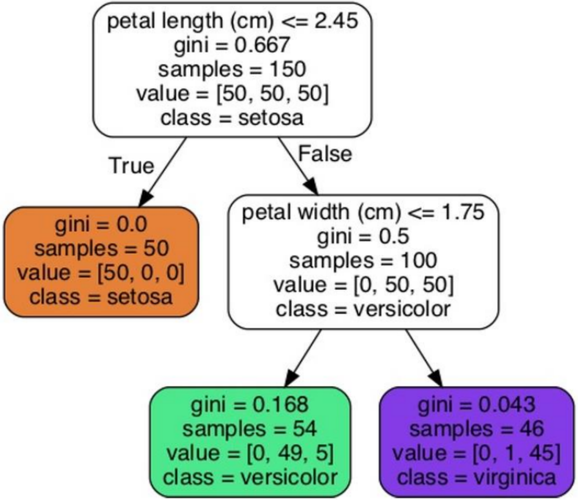


Decision tree for iris dataset

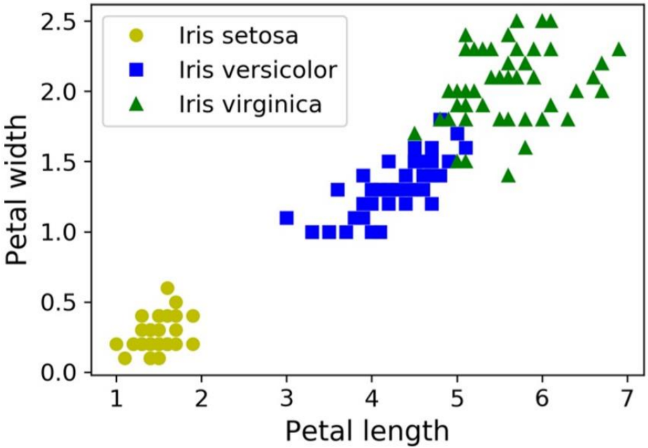
- Queries compare numerical attribute against a value
- How do we find these query values?





Querying numerical attributes

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



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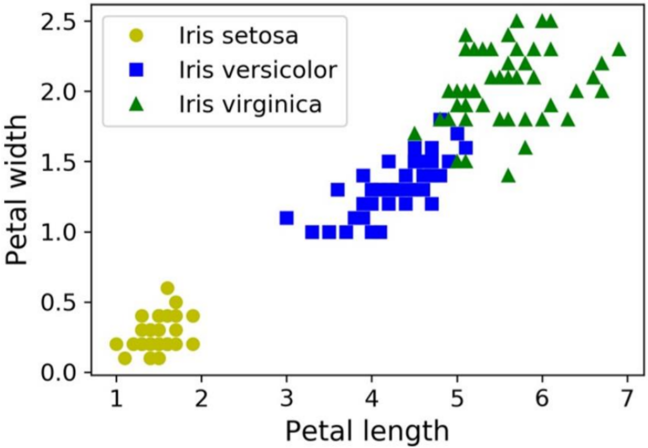

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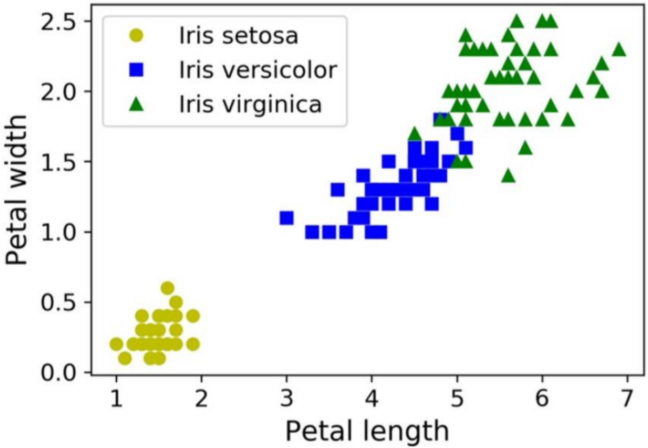
- Infinitely many choices for v
- How do we pick a sensible one?



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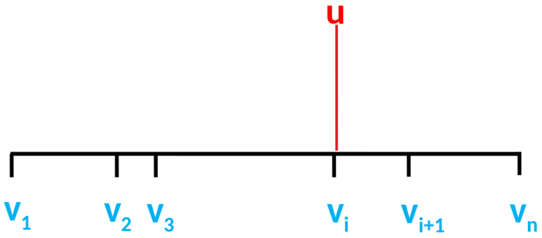

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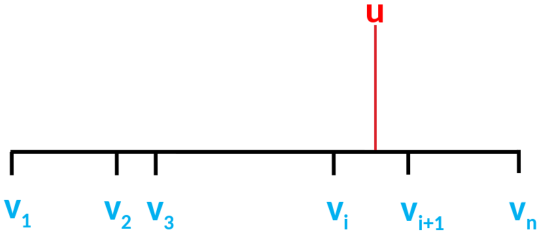

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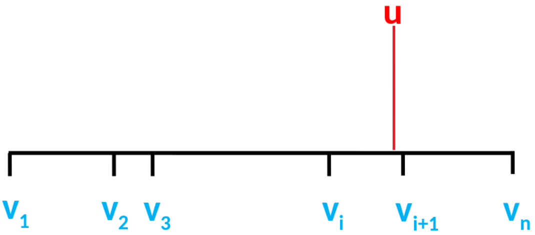

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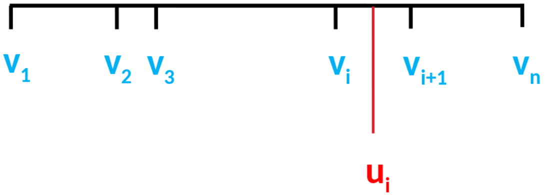

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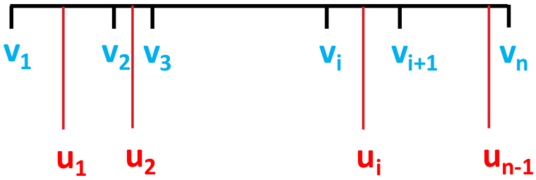

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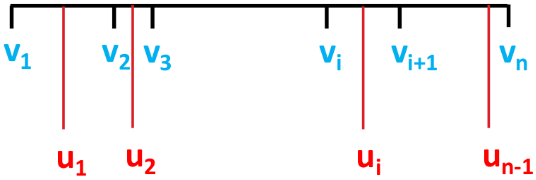

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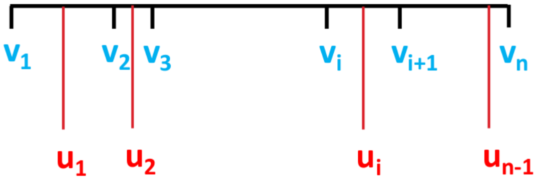

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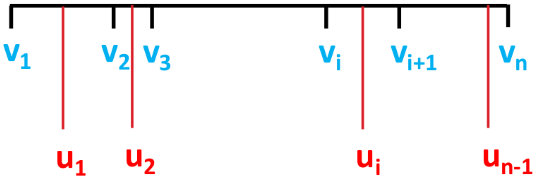

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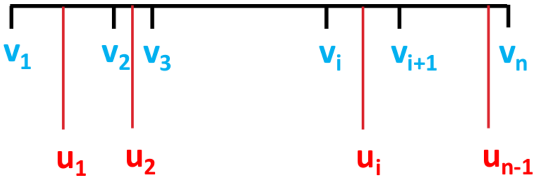

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- May prefer endpoints — midpoints may not be meaningful values

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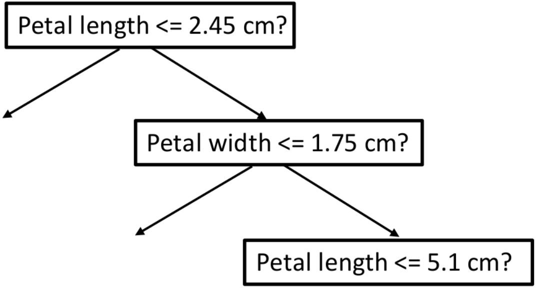
- Across all categorical and numerical attributes, choose the one with best information gain
- Categorical attrbutes can be queried only once on a path
- Numerical attributes can be queried repeatedly — interval to query keeps shrinking



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- On what basis can we evaluate a supervised learning model?

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- 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

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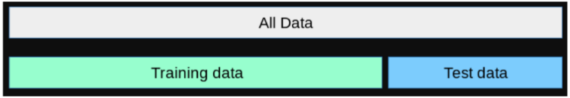
- How large should the test set be?
  - Typically 20-30% of labelled data
- Depends on labelled data available
  - Need enough training data to build the model



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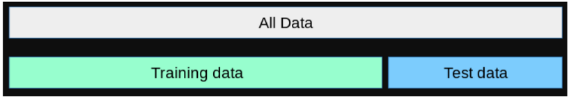
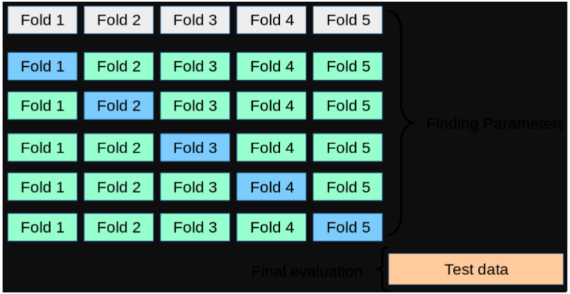


Cross validation

- 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



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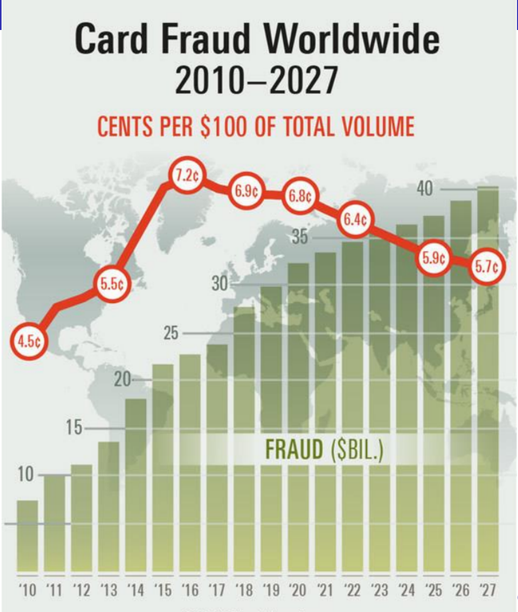

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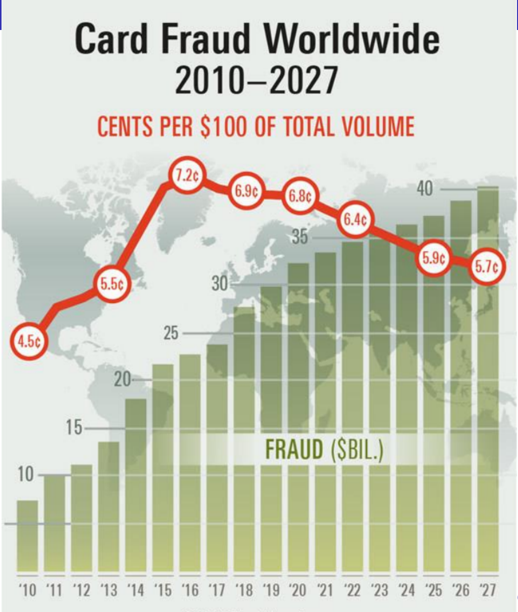
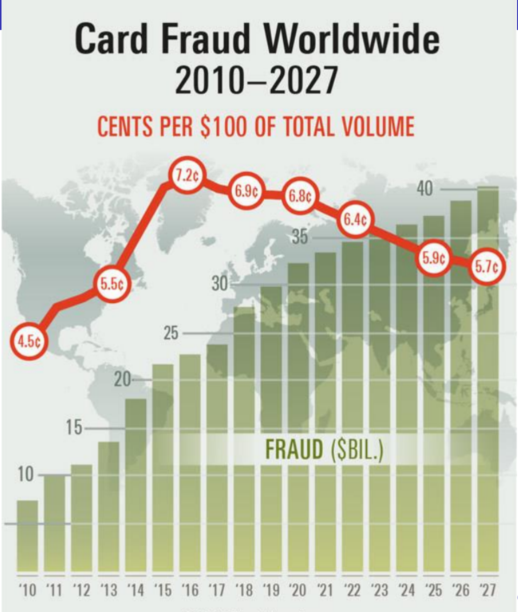
- Classifiers are often used in asymmetric situations
  - Less than 1% of credit card transactions are fraud
- "Is this transaction a fraud?"
  - Trivial classifier — always answer "No"
  - More than 99% accurate, but useless!



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



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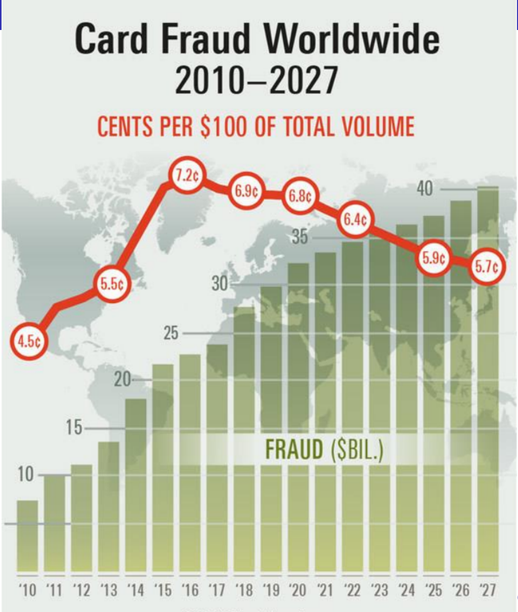

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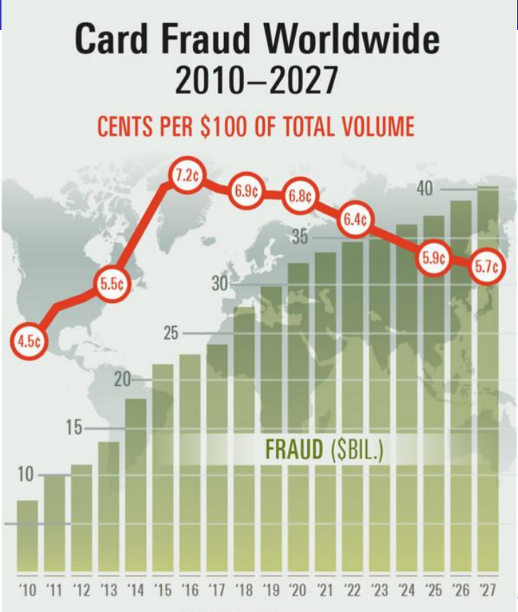
- Cautious classifier
  - Marks borderline "Yes" as "No"
  - False negatives



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
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Performance measures

- Precision 1, Recall 0.01

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

Performance measures

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

	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

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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

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F Score

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

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