Decision Trees

Decision Trees

- Decision trees have a long history in ML
  - First popular algorithms 1979
- Very popular in many real world settings
- Intuitive to understand
- Easy to build

History

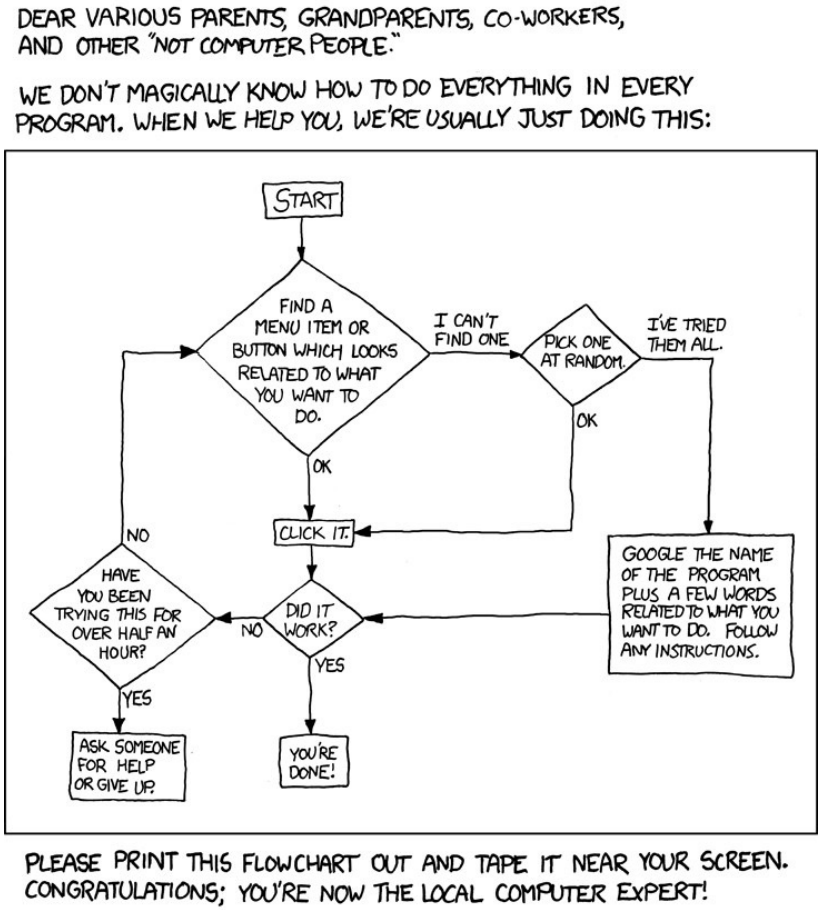
- EPAM- Elementary Perceiver and Memorizer
  - Feigenbaum 1961
  - Cognitive simulation model of human concept learning
- CLS- Early algorithm for decision tree construction
  - Hunt 1966
- ID3 based on information theory
  - Quinlan 1979
- C4.5 improved over ID3
  - Quinlan 1993

- Also has history in statistics as CART (Classification and regression tree)

Motivation

- How do people make decisions?
  - Consider a variety of factors
  - Follow a logical path of checks
- Should I eat at this restaurant?
  - If there is no wait
    - Yes
  - If there is short wait and I am hungry
    - Yes
  - Else
    - No

Decision Graph Example



Example: Should We Play Tennis?

Play Tennis	**Outlook**	**Temperature**	**Humidity**	**Windy**
No	Sunny	Hot	High	No
No	Sunny	Hot	High	Yes
Yes	Overcast	Hot	High	No
Yes	Rainy	Mild	High	No
Yes	Rainy	Cold	Normal	No

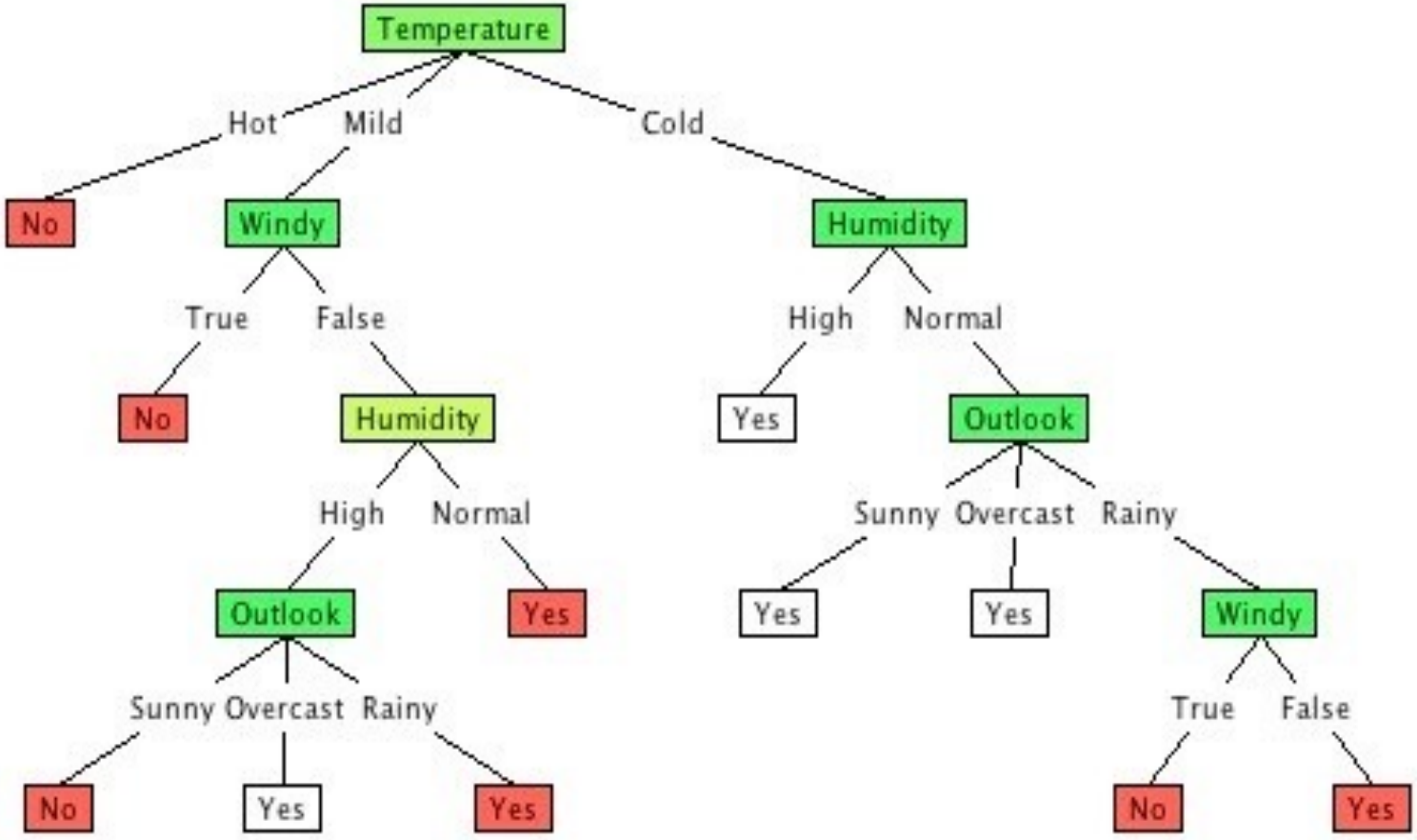
y

x

- If temperature is not hot
  - Play tennis
- If outlook is overcast
  - Play tennis
- Otherwise
  - Don’t play tennis

Decision Tree

Play Tennis	Outlook	Temperature	Humidity	Windy
Yes	Sunny	Cold	Normal	No



Decision Trees

- A decision tree is formed of
  - Nodes
    - Attribute tests
  - Branches
    - Results of attribute tests
  - Leaves
    - Classifications

Hypothesis Class

Y	X_1	X_2	X_3
1	0	0	0
0	0	0	1
1	0	1	0

- What functions can decision trees model?
  - Non-linear: very powerful hypothesis class
  - A decision tree can encode any Boolean function
  - Proof
    - Given a truth table for a function
    - Construct a path in the tree for each row of the table
    - Given a row as input, follow that path to the desired leaf (output)
- Problem: exponentially large trees!

Smaller Trees

- Can we produce smaller decision trees for functions?
  - Yes (most of the time)
  - Counter examples
    - Parity function
      - Return 1 on even inputs, 0 on odd inputs
    - Majority function
      - Return 1 if more than half of inputs are 1

- Decision trees are good for some functions but bad for others
- Recall: tradeoff between hypothesis class expressiveness and learnability

Decision Trees

- **Fitting a function to data**

- Fitting: ?
- Function: any boolean function
- Data: Batch: construct a tree using all the data

Building Decision Trees

What Makes a Good Tree?

- Small
  - Ockham's razor
    - Simpler is better
  - Avoids over-fitting
    - We'll discuss this again later
- A decision tree may be human readable, but not use human logic
  - The decision tree you would write for a problem may differ from computer

Small Trees

- How do we build small trees that accurately capture data?
- Optimal decision tree learning is NP-complete

- Constructing Optimal Binary Decision Trees is NP-complete. Laurent Hyafil, RL Rivest. Information Processing Letters, Vol. 5, No. 1. (1976), pp. 15-17.

Greedy Algorithms

- Like many NP-complete problems we can get pretty good solutions
- Most decision tree learning is by greedy algorithms
  - Adjustments are usually to fix greedy selection problems
- Top down decision tree learning
  - Recursive algorithms

ID3

- function BuildDecisionTree(data, labels):
  - if all labels are the same
    - return leaf node for that label
  - else
    - let f be the best feature for splitting
    - left = BuildDecisionTree(data with f=0, labels with f=0)
    - right= BuildDecisionTree(data with f=1, labels with f=1)
    - return Tree(f, left, right)
- Does this always terminate?

Base Cases

- All data have same label
  - Return that label
- No examples
  - Return majority label of all data
- No further splits possible
  - Return majority label of passed data

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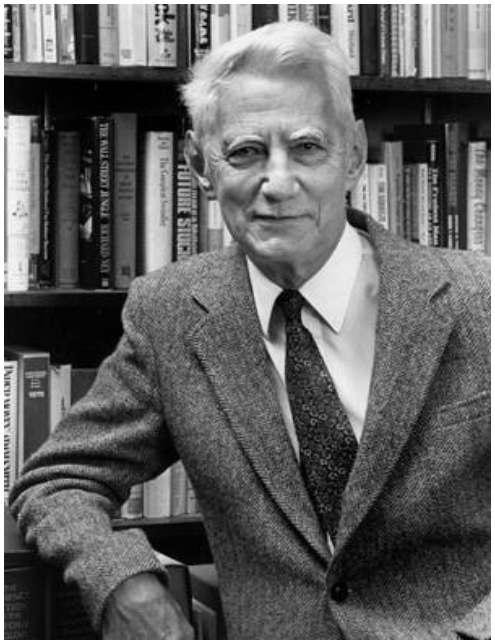
Selecting Features

- The best feature for splitting
  - The most informative feature
  - Select the feature that is most informative about the labels
- Information theory

Information Theory

- The quantification of information
- Founded by Claude Shannon
  - Landmark paper in 1948
  - Noisy channel theorem



Information Theory

- A brief introduction…

Information Theory

- Entropy

$$H(\mathrm{X}) = -\sum_{X} P(X = x)\log P(X = x)$$

- Conditional Entropy

$$H(Y|X) = \sum_{X} P(X = x)H(Y|X = x)$$

- Information Gain

$$IG(Y|X) = H(Y) - H(Y|X)$$

Selecting Features

- The best feature for splitting
  - The most informative feature
  - The feature with the highest information gain

Notes for Decision Trees

- Since we compare H(Y|X) across all features, H(Y) is a constant
  - We can omit it for comparisons
- The base of the log doesn't matter as long as it is consistent

Example: Should We Play Tennis?

Play Tennis	**Outlook**	**Temperature**	**Humidity**	**Windy**
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Yes	Rainy	Mild	High	No
Yes	Rainy	Cold	Normal	No

y

x

- H(Tennis) = -3/5 $\log_2$ 3/5 - 2/5 $\log_2$ 2/5 = 0.97

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y

x

- H(Tennis|Outlook=Sunny) = -2/2 $\log_2$ 2/2 – 0/2 $\log_2$ 0/2 = 0
- H(Tennis|Outlook=Overcast) = -0/1 $\log_2$ 0/1 – 1/1 $\log_2$ 1/1 = 0
- H(Tennis|Outlook=Rainy) = -0/2 $\log_2$ 0/2 – 2/2 $\log_2$ 2/2 = 0
- H(Tennis|Outlook) = 2/5 * 0 + 1/5 * 0 + 2/5 * 0 = 0

Example: Should We Play Tennis?

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y

x

- IG(Tennis|Outlook) = 0.97 – 0 = 0.97
- If we knew the Outlook we'd be able to perfectly predict Tennis!

- Outlook is a great feature to pick for our decision tree

ID3

- function BuildDecisionTree(data, labels):
  - if basecase
    - return appropriate leaf node
  - Else
    - f = arg max IG(label|f)
    - left = BuildDecisionTree(data with f=0, labels with f=0)
    - right= BuildDecisionTree(data with f=1, labels with f=1)
    - return Tree(f, left, right)

Basecase

- All data have same label
  - Return that label
- No examples
  - Return majority label of all data
- No further splits possible
  - Return majority label of passed data
- If max IG = 0?

IG=0 As a Base Case

- Consider the following

Y	X_1	X_2
0	0	0
1	0	1
1	1	0
0	1	1

- Both features give 0 IG
- Once we divide the data, perfect classification!

Training vs. Test Accuracy

- On the tree shown for tennis
- 100% training accuracy
- 30% testing accuracy
- Why?

Outlook	Temperature	Humidity	Windy	PlayTennis
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

An artificial example

- We'll create a training dataset

Five inputs, all bits, are generated in all 32 possible combinations

Output y = copy of e, Except a random 25% of the records have y set to the opposite of e

32 records

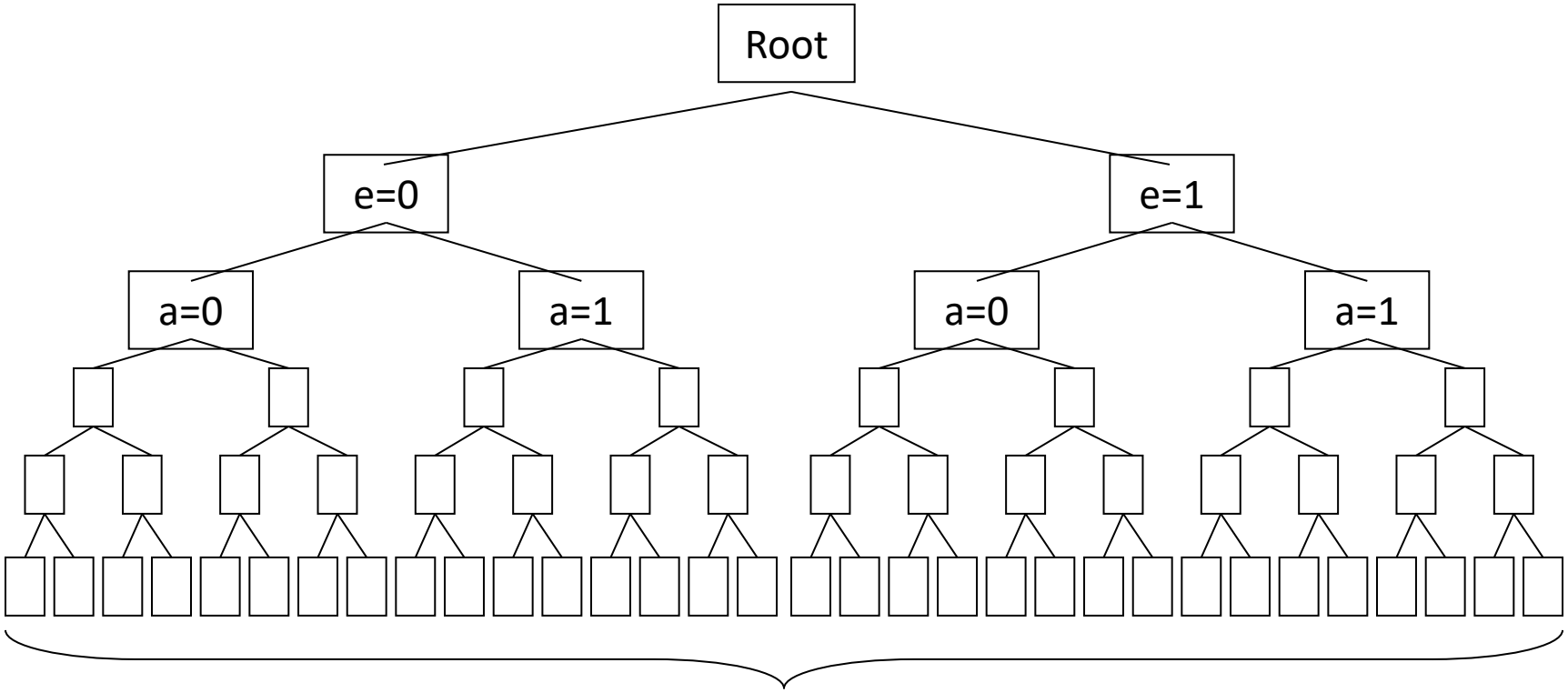
a	b	c	d	e	y
0	0	0	0	0	0
0	0	0	0	1	0
0	0	0	1	0	0
0	0	0	1	1	1
0	0	1	0	0	1
:	:	:	:	:	:
1	1	1	1	1	1

In our artificial example

- Suppose someone generates a test set according to the same method.
- The test set is identical, except that some of the y's will be different.
- Some y's that were corrupted in the training set will be uncorrupted in the testing set.
- Some y's that were uncorrupted in the training set will be corrupted in the test set.

Building a tree with the artificial training set

- Suppose we build a full tree (we always split until base case 2)



25% of these leaf node labels will be corrupted

Training set error for our artificial tree

All the leaf nodes contain exactly one record and so…

- We would have a training set error of zero

Testing the tree with the test set

	1/4 of the tree nodes are corrupted	3/4 are fine
1/4 of the test set records are corrupted	1/16 of the test set will be correctly predicted for the wrong reasons	3/16 of the test set will be wrongly predicted because the test record is corrupted
3/4 are fine	3/16 of the test predictions will be wrong because the tree node is corrupted	9/16 of the test predictions will be fine

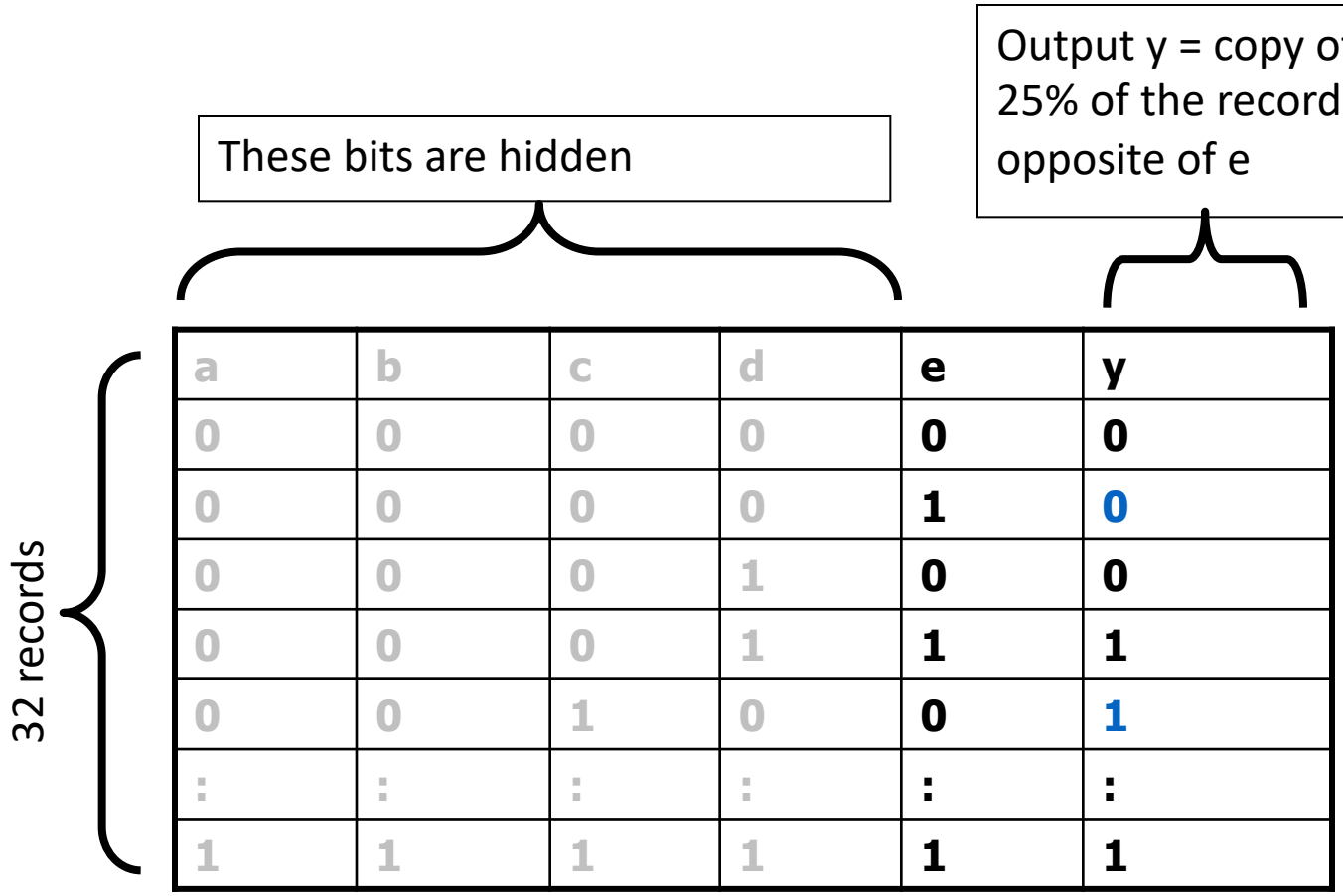
In total, we expect to be wrong on 3/8 of the test set predictions

What's this example shown us?

- This explains the discrepancy between training and test set error
- But more importantly… …it indicates there's something we should do about it if we want to predict well on future data.

Suppose we had less data

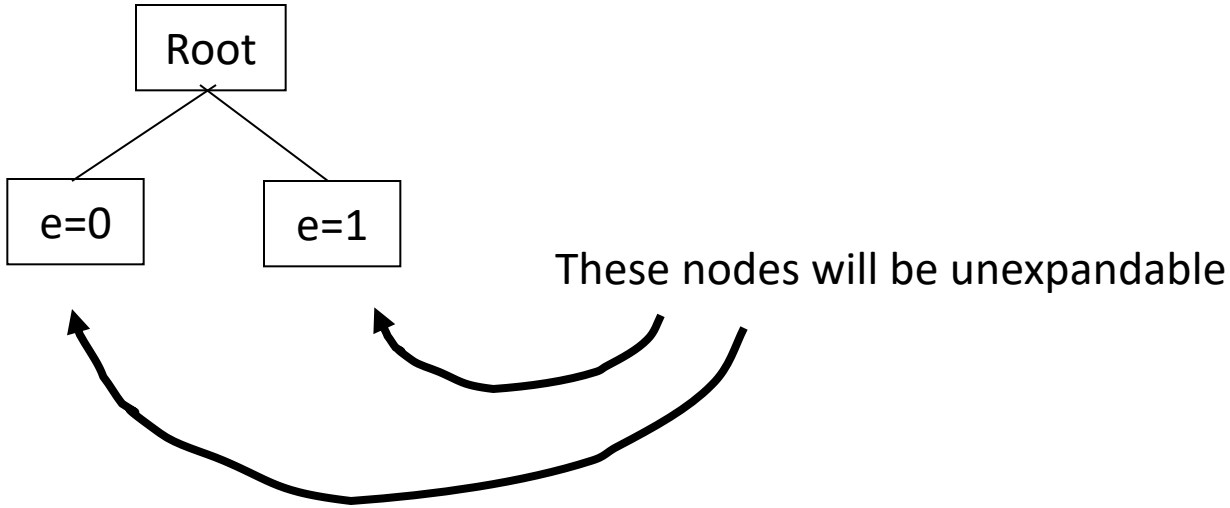
- Let's not look at the irrelevant bits



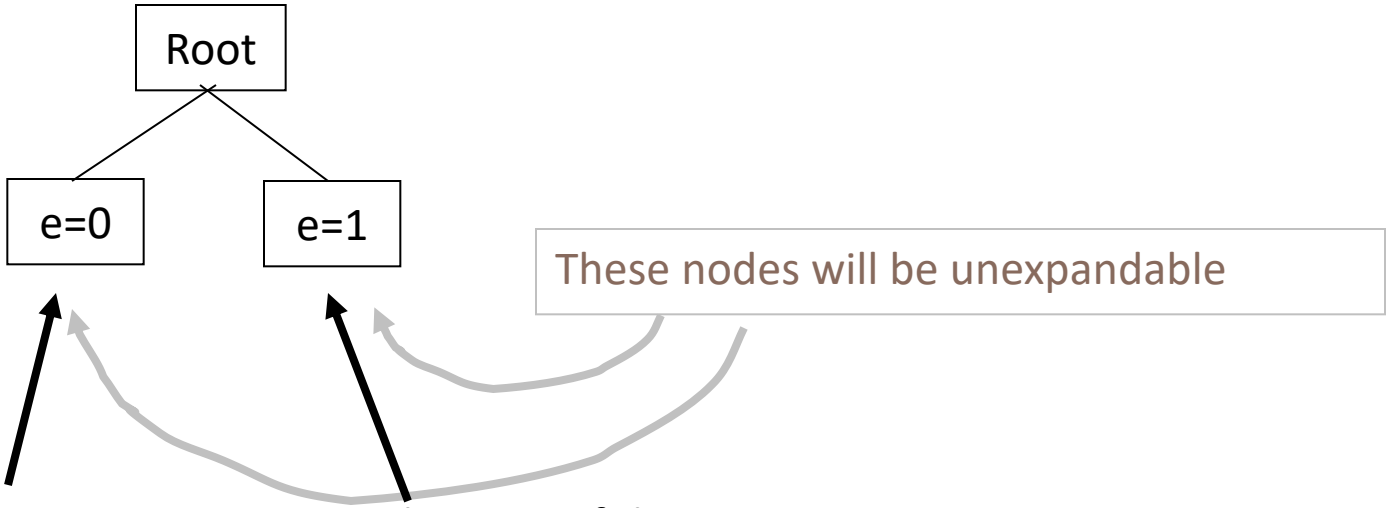
a	b	c	d	e	y
0	0	0	0	0	0
0	0	0	0	1	0
0	0	0	1	0	0
0	0	0	1	1	1
0	0	1	0	0	1
:	:	:	:	:	:
1	1	1	1	1	1

What decision tree would we learn now?

Without access to the irrelevant bits…



Without access to the irrelevant bits…



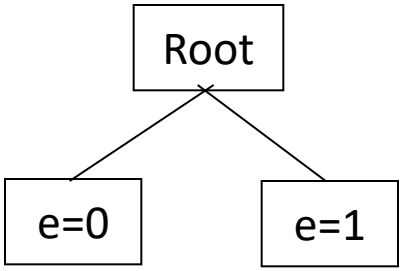
In about 12 of the 16 records in this node the output will be 0

So this will almost certainly predict 0

In about 12 of the 16 records in this node the output will be 1

So this will almost certainly predict 1

Without access to the irrelevant bits…



	almost certainly none of the tree nodes are corrupted	almost certainly all are fine
1/4 of the test set records are corrupted	n/a	1/4 of the test set will be wrongly predicted because the test record is corrupted
3/4 are fine	n/a	3/4 of the test predictions will be fine

In total, we expect to be wrong on only 1/4 of the test set predictions

Overfitting

- Definition: If your machine learning algorithm fits noise (i.e. pays attention to parts of the data that are irrelevant) it is overfitting.
- Fact (theoretical and empirical): If your machine learning algorithm is overfitting then it may perform less well on test set data.

Bias/Variance Tradeoff

- Complete trees have no bias
  - But can over-fit badly
  - Lots of variance
- 0 depth trees (return most likely label) have no variance
  - Totally biased towards majority label
- A good tree balances between these two
  - How do we learn balanced trees?

Pruning: New Base Cases

- Stop when too few examples
- Stop when max depth reached
- Stop when my classification error is not much more than average of my children
- X^2 pruning- stop when remainder is no more likely than chance

Parameters

- All of these are parameters
- How do you select parameter values?
  - Train data?
  - Test data?
  - Development data!

Extensions

- Non-binary attributes
  - Categorical
  - Continuous (real valued)
- Handle by thresholding- find the best single threshold to split the range
- Regression trees
- Missing attributes
- Alternatives to information gain: Gini index, miss-classification rate
- Non-greedy algorithms?