Decision Tree Learning: Part 2

Yingyu Liang
Computer Sciences 760
Fall 2017

http://pages.cs.wisc.edu/~yliang/cs760/

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, and Pedro Domingos.

Goals for the last lecture

you should understand the following concepts

- the decision tree representation
- the standard top-down approach to learning a tree
- Occam's razor
- entropy and information gain
- types of decision-tree splits

Goals for this lecture

you should understand the following concepts

- test sets and unbiased estimates of accuracy
- overfitting
- early stopping and pruning
- validation sets
- regression trees
- probability estimation trees

Stopping criteria

We should form a leaf when

- all of the given subset of instances are of the same class
- we've exhausted all of the candidate splits

Is there a reason to stop earlier, or to prune back the tree?

How can we assess the accuracy of a tree?

- can we just calculate the fraction of training instances that are correctly classified?

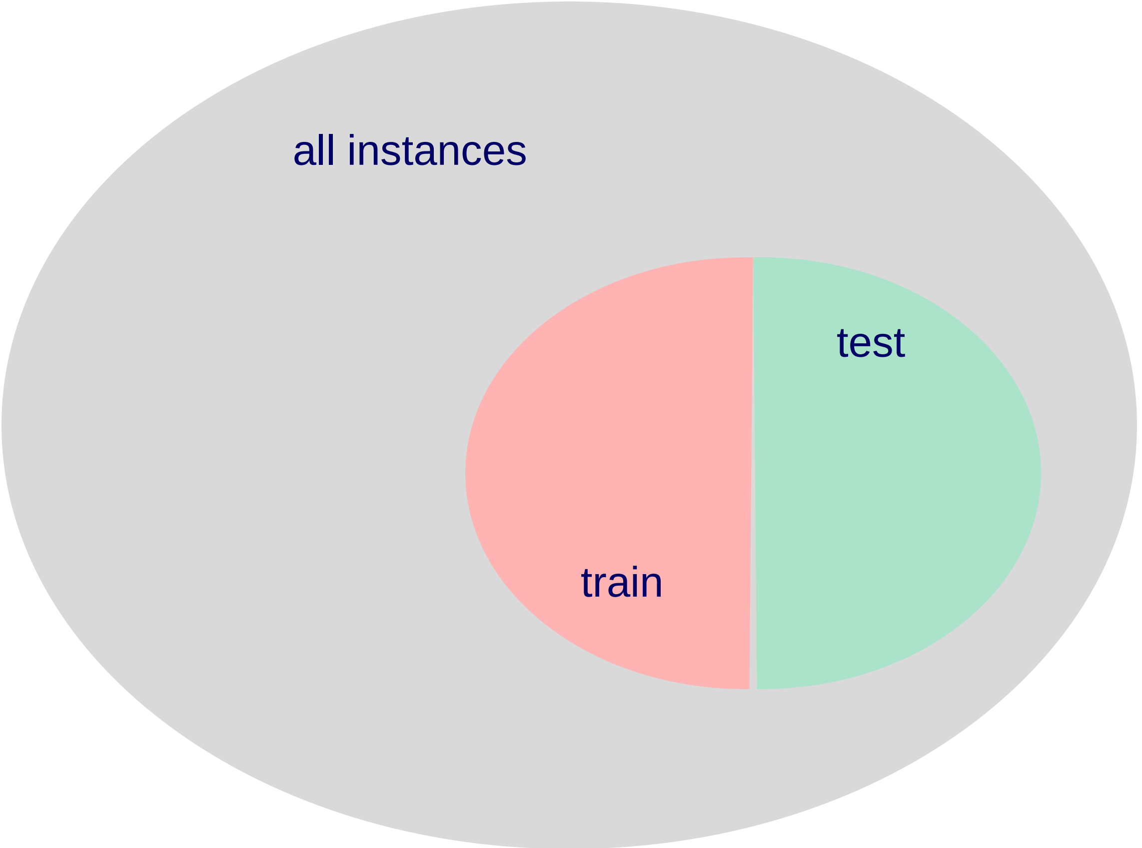
- consider a problem domain in which instances are assigned labels at random with $P(Y = \mathrm{t}) = 0.5$

  - how accurate would a learned decision tree be on previously unseen instances?

  - how accurate would it be on its training set?

How can we assess the accuracy of a tree?

- to get an unbiased estimate of a learned model's accuracy, we must use a set of instances that are held-aside during learning
- this is called a *test set*



Overfitting

- consider error of model h over
  - training data: $error_{D}(h)$
  - entire distribution of data: $error_{\mathcal{D}}(h)$

- model $h \in H$ *overfits* the training data if there is an alternative model $h' \in H$ such that

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

$$error_{D}(h) < error_{D}(h')$$

Example 1: overfitting with noisy data

suppose

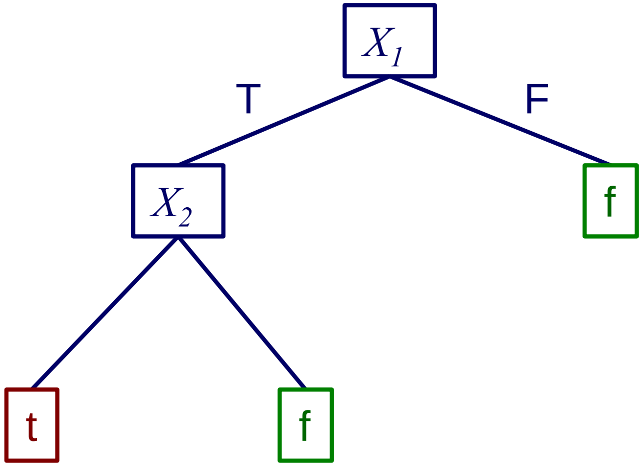
- the target concept is $Y = X_1 \wedge X_2$
- there is noise in some feature values
- we're given the following training set

X_1	X_2	X_3	X_4	X_5	…	Y
t	t	t	t	t	…	t
t	t	f	f	t	…	t
t	f	t	t	f	…	t
t	f	f	t	f	…	f
t	f	t	f	f	…	f
f	t	t	f	t	…	f

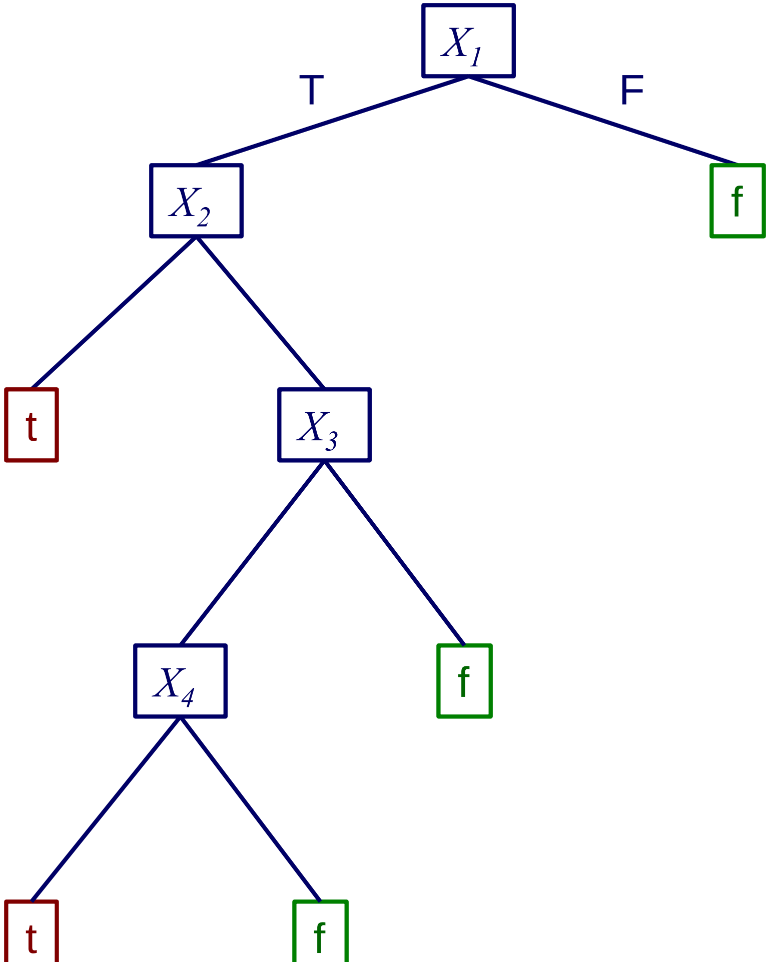
noisy value

Example 1: overfitting with noisy data

correct tree



tree that fits noisy training data



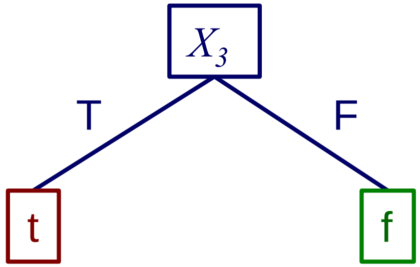
Example 2: overfitting with noise-free data

suppose

- the target concept is $Y = X_1 \wedge X_2$
- $P(X_3 = t) = 0.5$ for both classes
- $P(Y = t) = 0.67$
- we're given the following training set

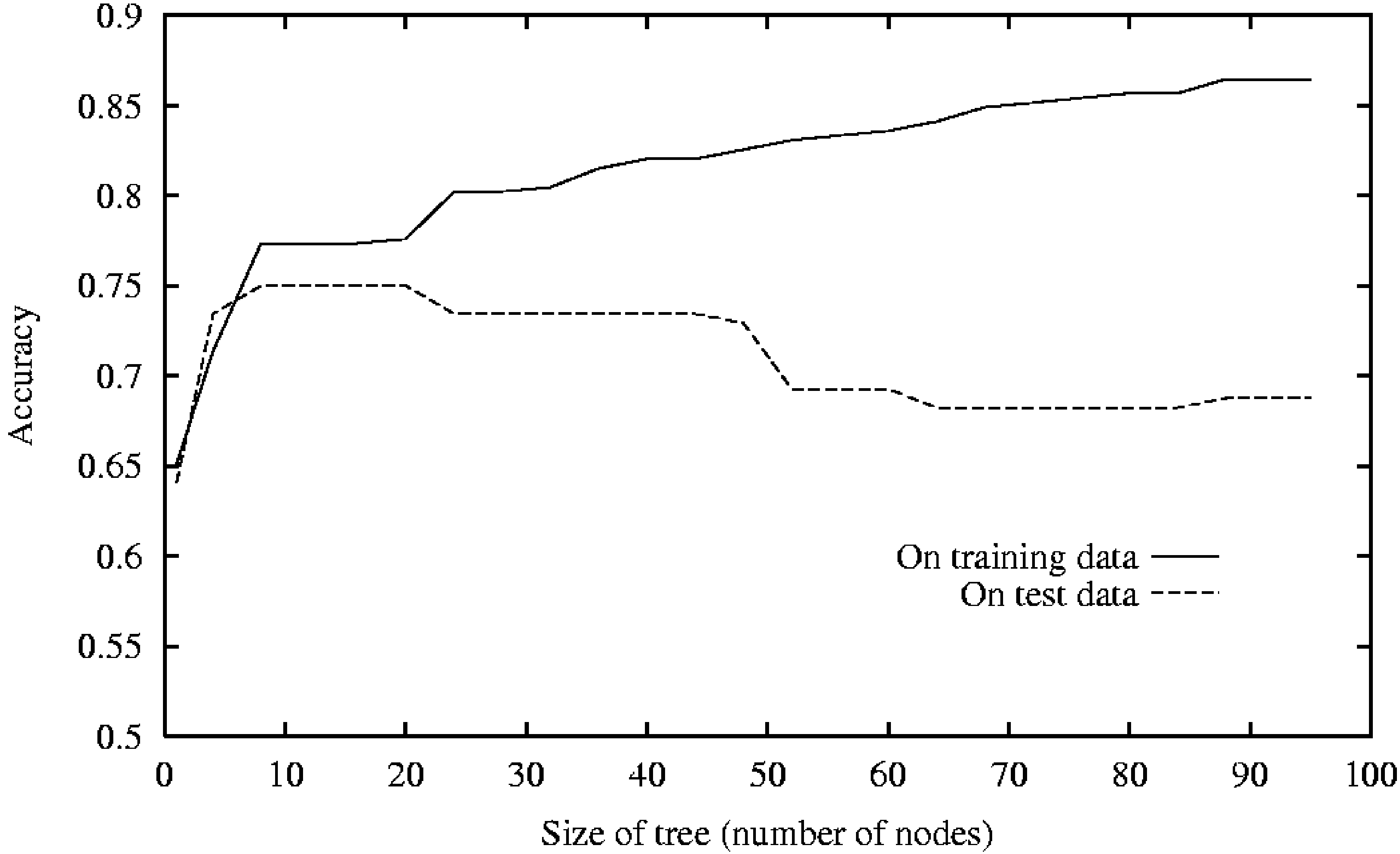
X_1	X_2	X_3	X_4	X_5	…	Y
t	t	t	t	t	…	t
t	t	t	f	t	…	t
t	t	t	t	f	…	t
t	f	f	t	f	…	f
f	t	f	f	t	…	f

Example 2: overfitting with noise-free data

	training set accuracy	test set accuracy
	100%	50%
	66%	66%

- because the training set is a limited sample, there might be (combinations of) features that are correlated with the target concept by chance

Overfitting in decision trees



Example 3: regression using polynomial

$$t = \sin(2\pi x) + \epsilon$$

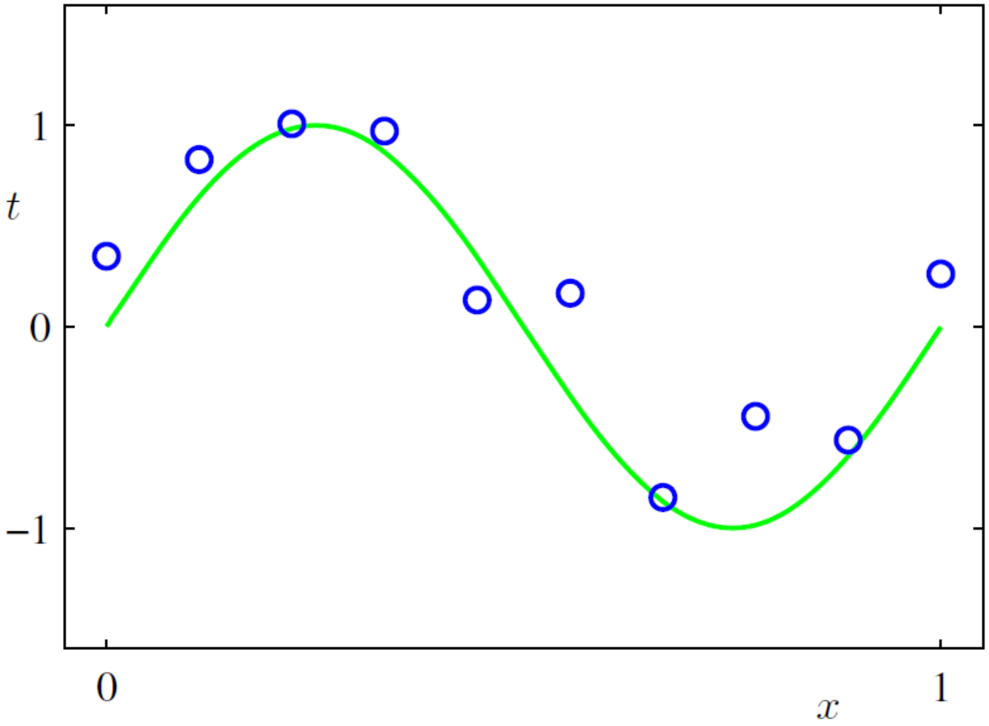
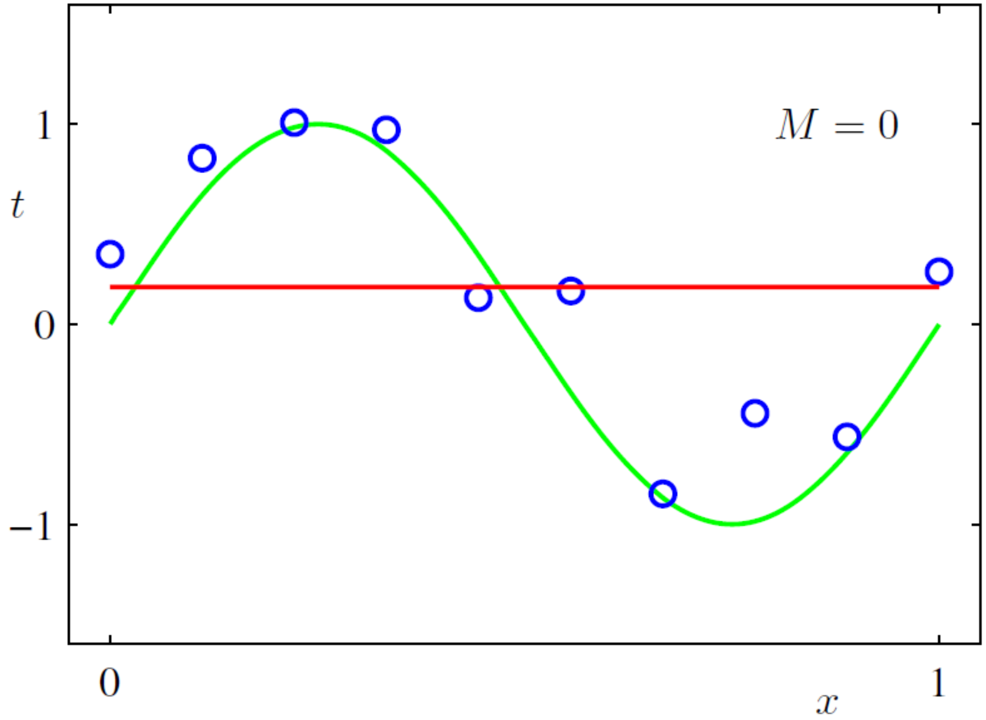


Figure from *Machine Learning and Pattern Recognition*, Bishop

Example 3: regression using polynomial

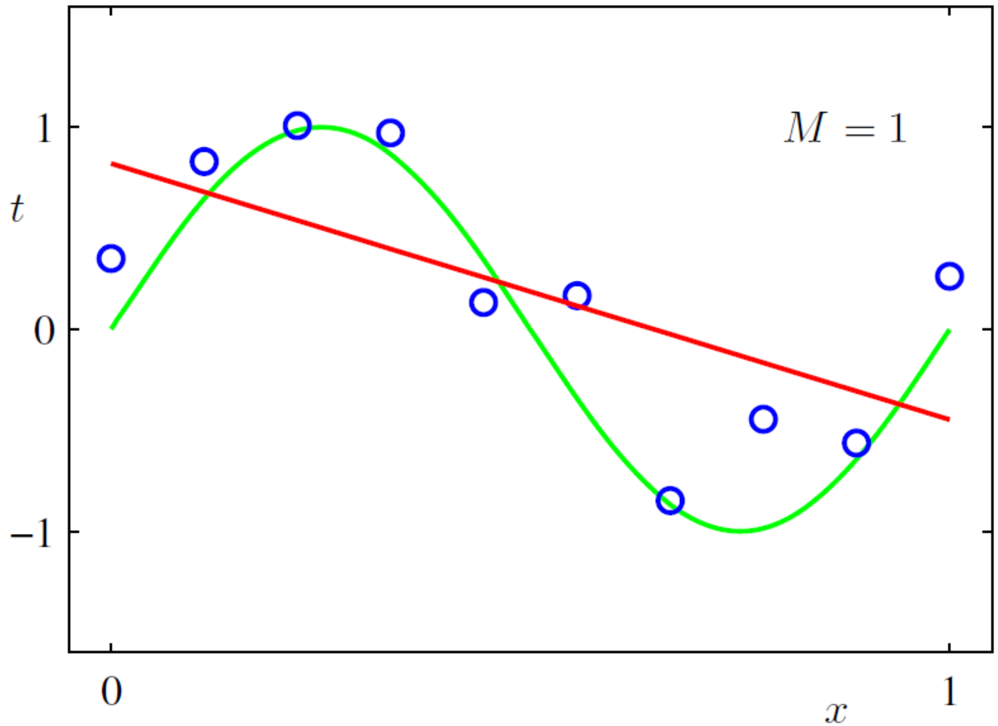
$$t = \sin(2\pi x) + \epsilon$$



Regression using polynomial of degree *M*

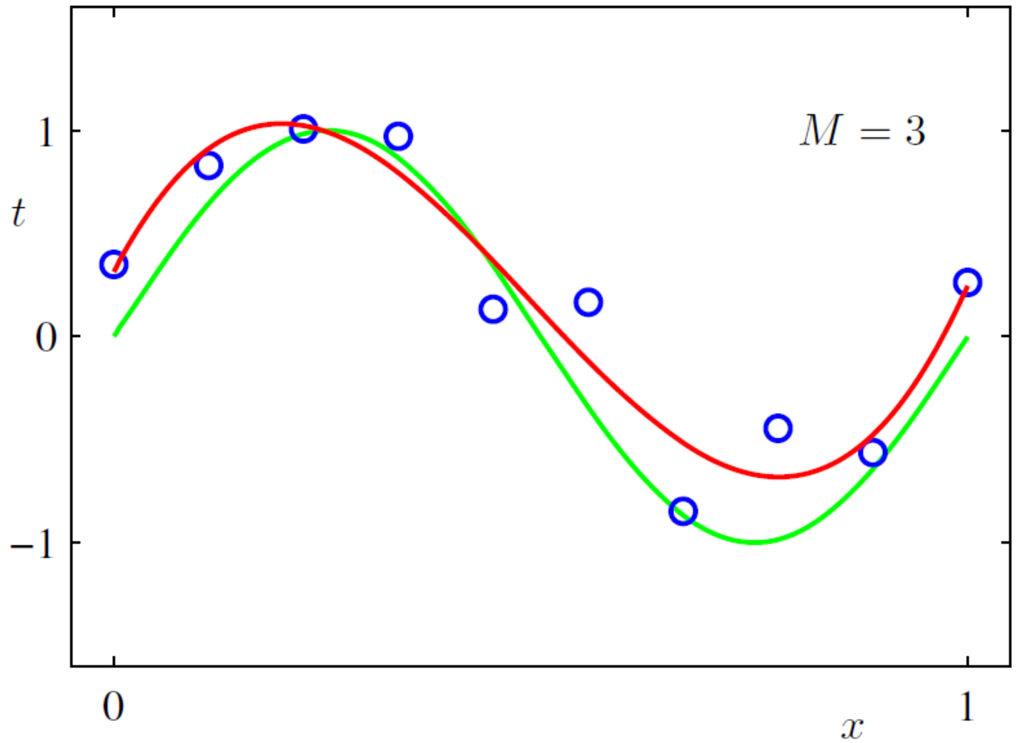
Example 3: regression using polynomial

$$t = \sin(2\pi x) + \epsilon$$



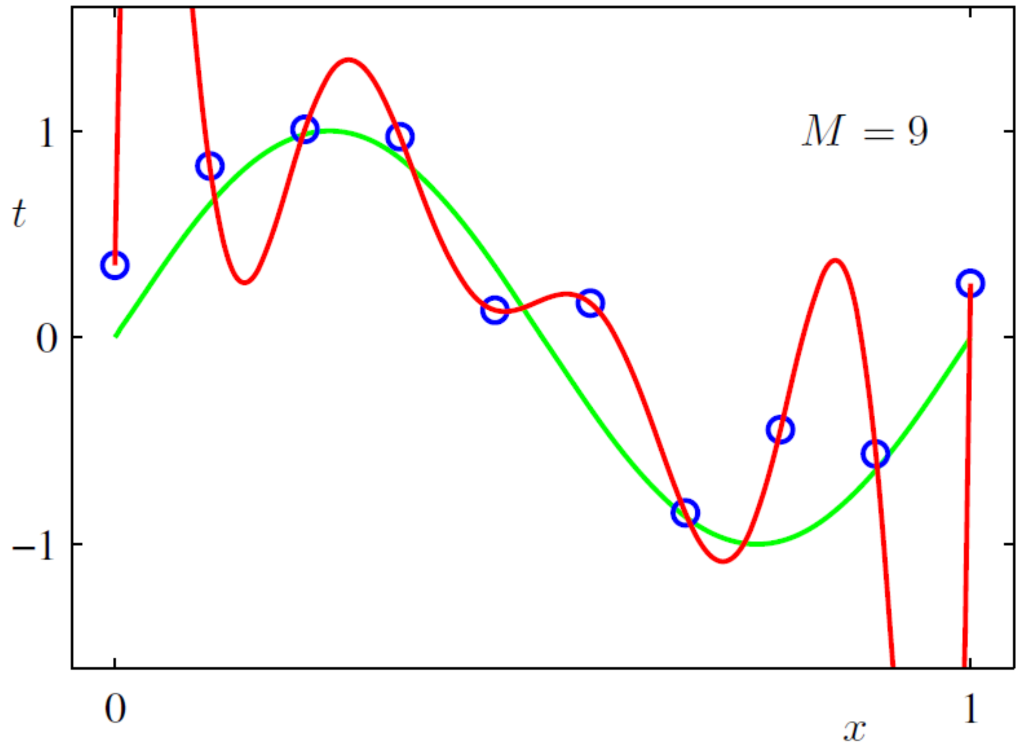
Example 3: regression using polynomial

$t = \sin(2\pi x) + \epsilon$

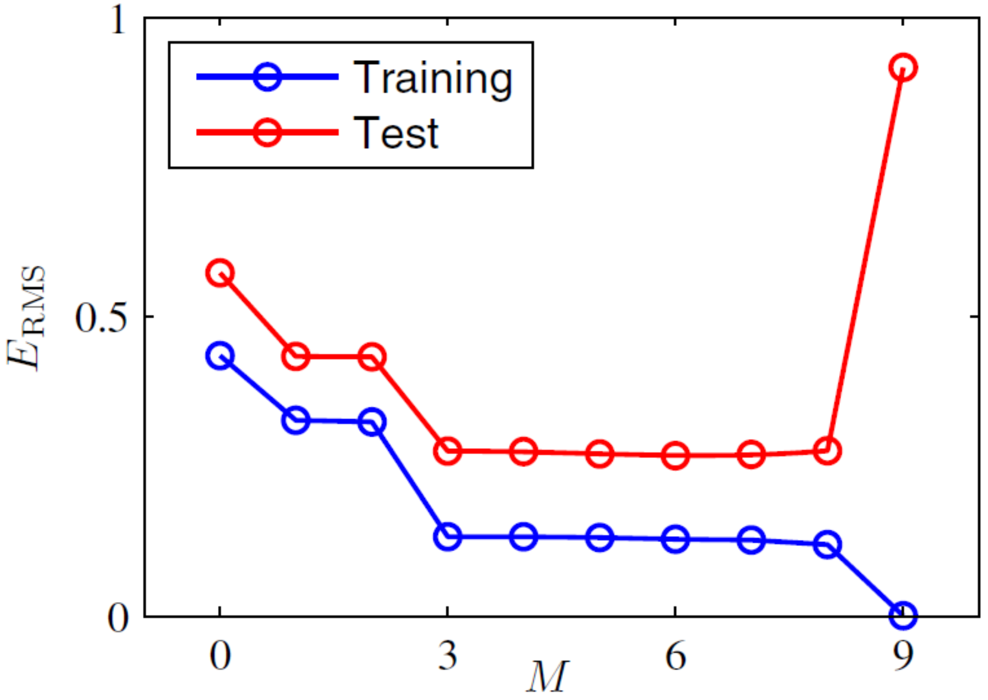


Example 3: regression using polynomial

$$t = \sin(2\pi x) + \epsilon$$



Example 3: regression using polynomial



General phenomenon

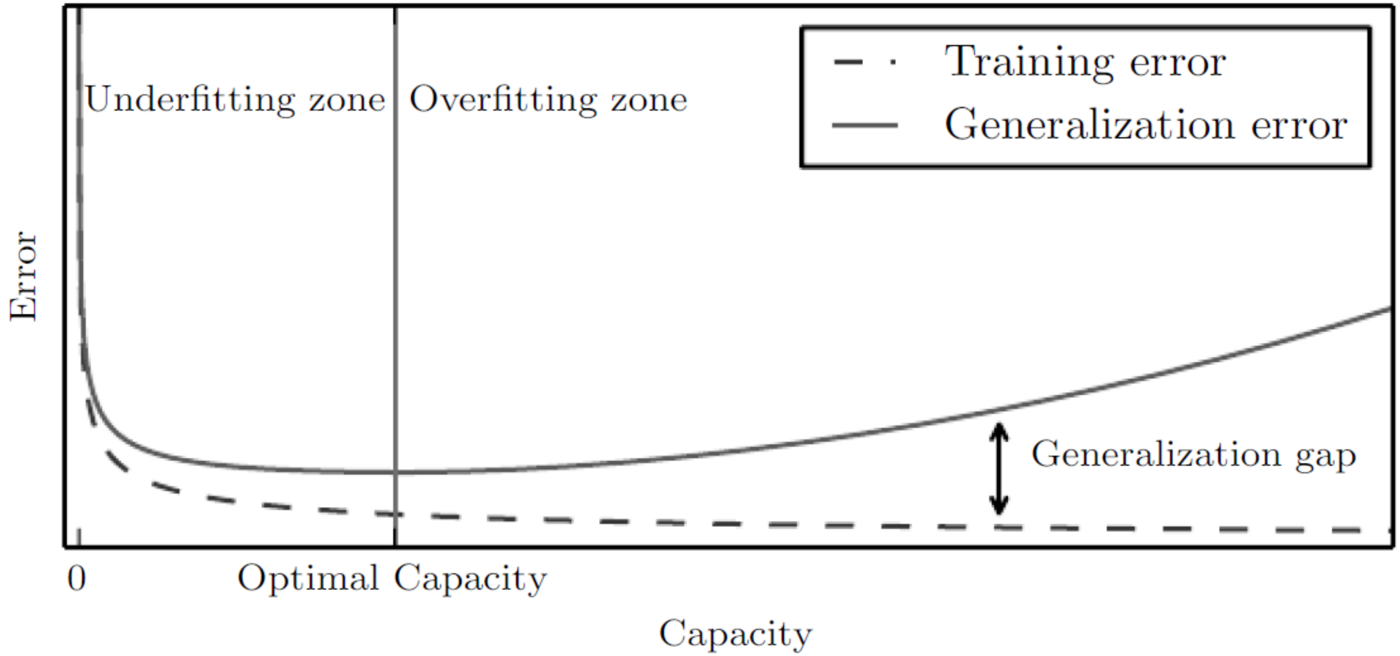


Figure from *Deep Learning*, Goodfellow, Bengio and Courville

Prevent overfitting

- cause: training error and expected error are different
    1. there may be noise in the training data
    2. training data is of limited size, resulting in difference from the true distribution
    3. larger the hypothesis class, easier to find a hypothesis that fits the difference between the training data and the true distribution

- prevent overfitting:
    1. cleaner training data help!
    2. more training data help!
    3. throwing away unnecessary hypotheses helps! (Occam's Razor)

Avoiding overfitting in DT learning

two general strategies to avoid overfitting

1. *early stopping*: stop if further splitting not justified by a statistical test
   - Quinlan's original approach in ID3

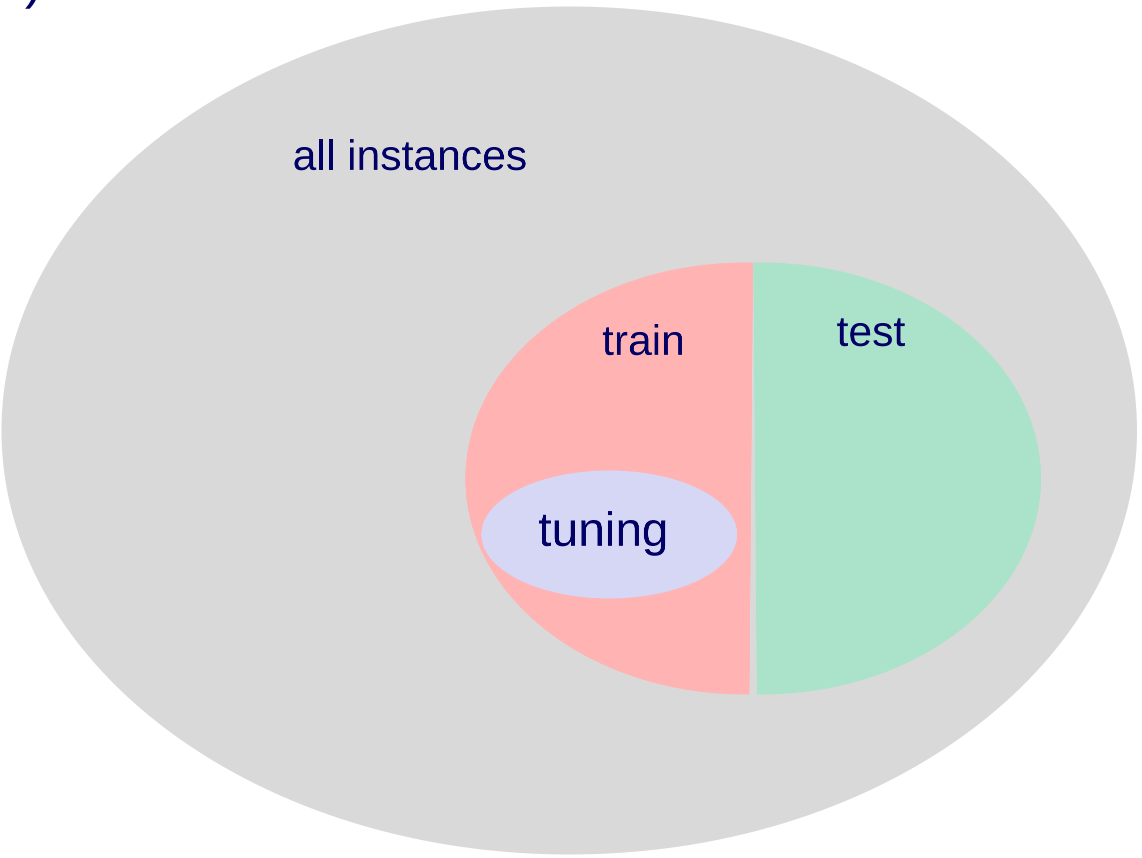
2. *post-pruning*: grow a large tree, then prune back some nodes
   - more robust to myopia of greedy tree learning

Pruning in C4.5

1. split given data into training and *validation* (*tuning*) sets
2. grow a complete tree
3. do until further pruning is harmful
    - evaluate impact on tuning-set accuracy of pruning each node
    - greedily remove the one that most improves tuning-set accuracy

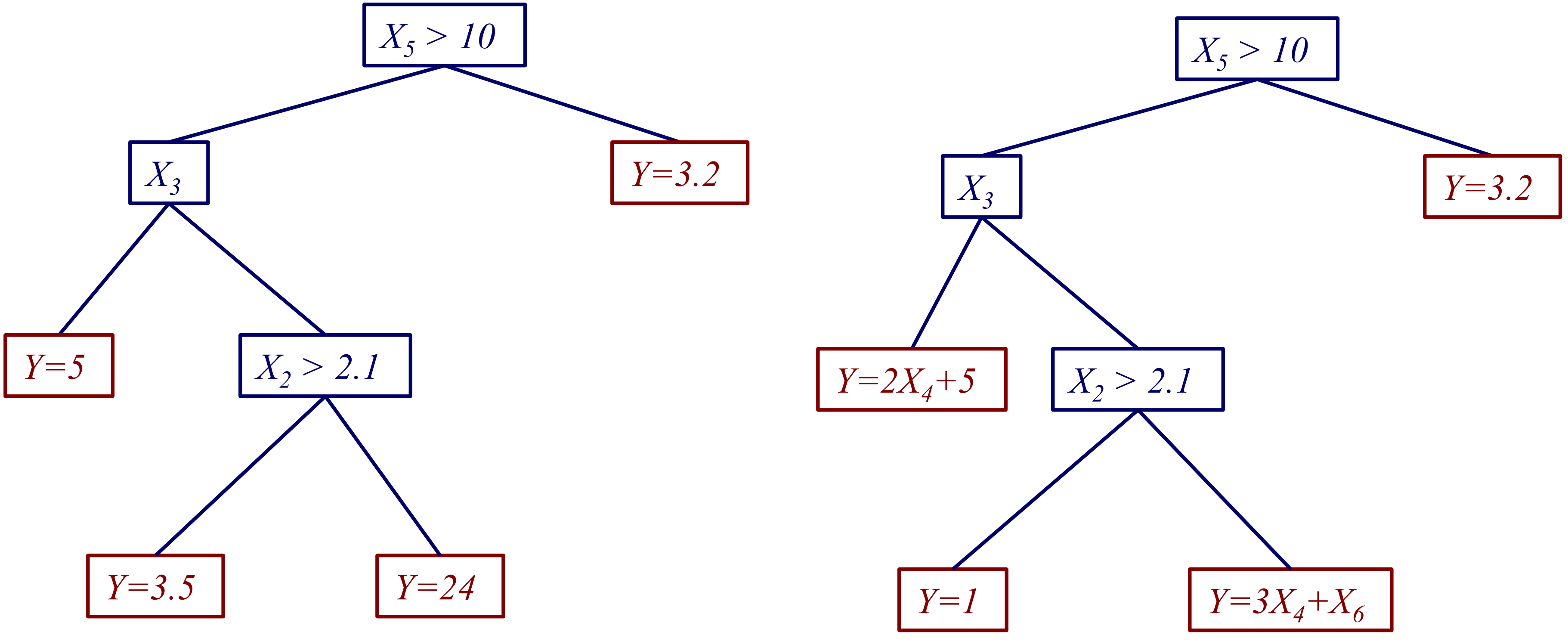
Validation sets

- a *validation set* (a.k.a. *tuning set*) is a subset of the training set that is held aside
  - not used for primary training process (e.g. tree growing)
  - but used to select among models (e.g. trees pruned to varying degrees)



Regression trees

- in a regression tree, leaves have functions that predict numeric values instead of class labels
- the form of these functions depends on the method
  - CART uses constants
  - some methods use linear functions



Regression trees in CART

- CART does *least squares regression* which tries to minimize

$$\sum_{i=1}^{|D|}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

target value for i^{th} training instance

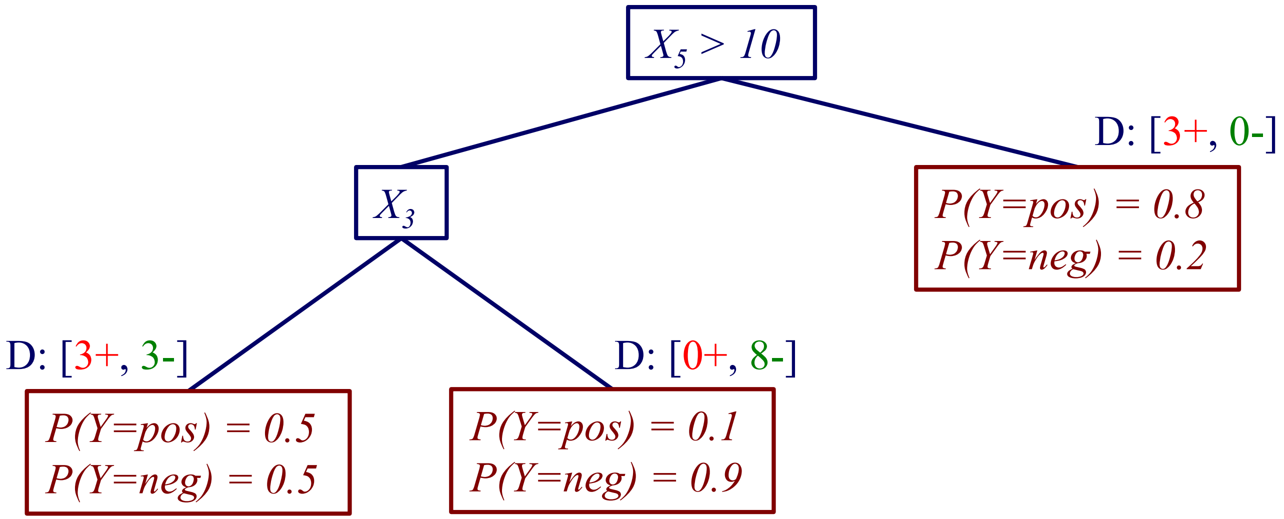
value predicted by tree for i^{th} training instance (average value of y for training instances reaching the leaf)

$$= \sum_{L \in \text{leaves}} \sum_{i \in L}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

- at each internal node, CART chooses the split that most reduces this quantity

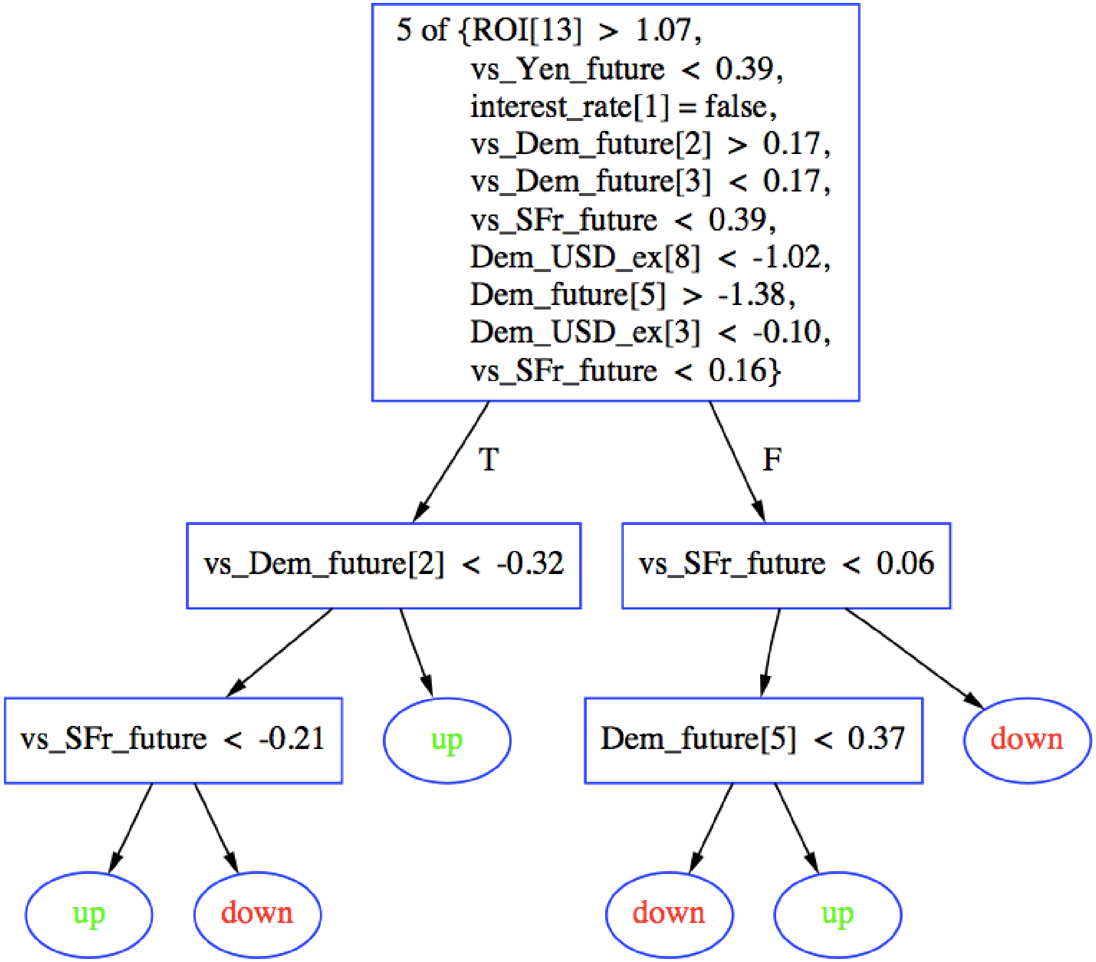
Probability estimation trees

- in a PE tree, leaves estimate the probability of each class
- could simply use training instances at a leaf to estimate probabilities, but …
- *smoothing* is used to make estimates less extreme (we'll revisit this topic when we cover Bayes nets)



m-of-*n* splits

- a few DT algorithms have used *m*-of-*n* splits [Murphy & Pazzani ‘91]
- each split is constructed using a heuristic search process
- this can result in smaller, easier to comprehend trees



test is satisfied if 5 of 10 conditions are true

tree for exchange rate prediction
[Craven & Shavlik, 1997]

Searching for m-of-n splits

m-of-n splits are found via a hill-climbing search

- initial state: best 1-of-1 (ordinary) binary split
- evaluation function: information gain
- operators:

m-of-n ➔ m-of-$(n+1)$

1 of { X_1=t, X_3=f } ➔ 1 of { X_1=t, X_3=f, X_7=t }

m-of-n ➔ $(m+1)$-of-$(n+1)$

1 of { X_1=t, X_3=f } ➔ 2 of { X_1=t, X_3=f, X_7=t }

Lookahead

- most DT learning methods use a hill-climbing search
- a limitation of this approach is myopia: an important feature may not appear to be informative until used in conjunction with other features
- can potentially alleviate this limitation by using a *lookahead* search [Norton '89; Murphy & Salzberg '95]
- empirically, often doesn't improve accuracy or tree size

Choosing best split in ordinary DT learning

OrdinaryFindBestSplit(set of training instances D, set of candidate splits C)

$maxgain = -\infty$

for each split S in C

$gain$ = InfoGain(D, S)

if $gain > maxgain$

$maxgain = gain$

$S_{best} = S$

return S_{best}

Choosing best split with lookahead (part 1)

LookaheadFindBestSplit(set of training instances D, set of candidate splits C)

$maxgain$ = -∞

for each split S in C

$gain$ = EvaluateSplit(D, C, S)

if $gain > maxgain$

$maxgain = gain$

$S_{best} = S$

return S_{best}

Choosing best split with lookahead (part 2)

EvaluateSplit(D, C, S)

if a split on S separates instances by class (i.e. $H_D(Y \mid S) = 0$)

// no need to split further

return $H_D(Y) - H_D(Y \mid S)$

else

for each outcome k of S

// see what the splits at the next level would be

D_k = subset of instances that have outcome k

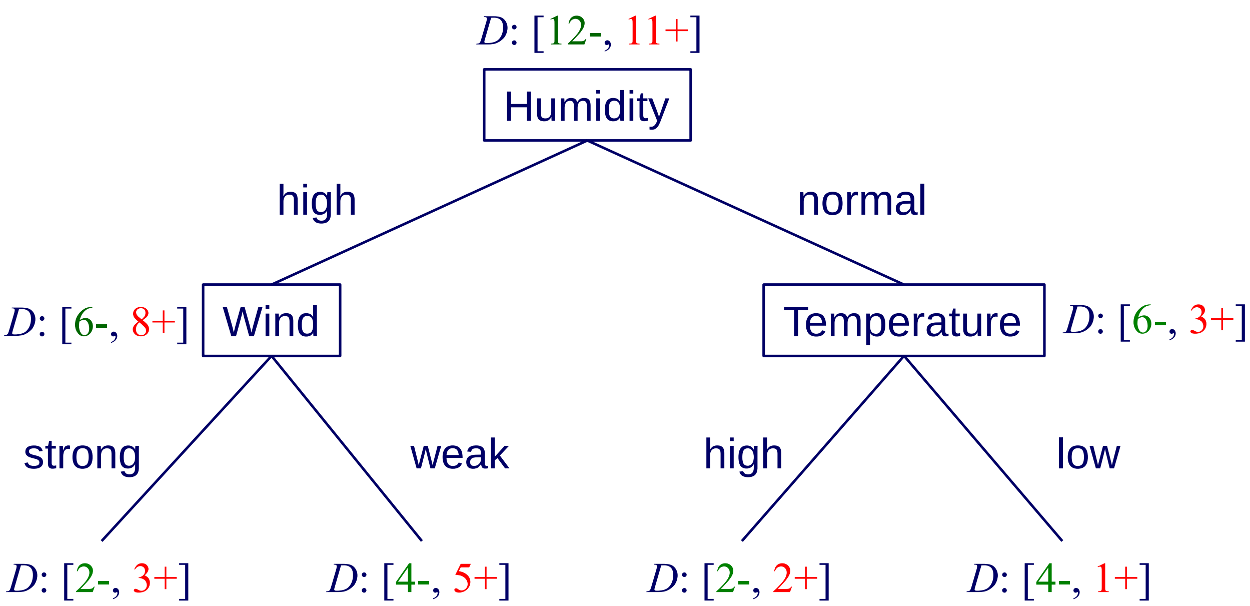
S_k = OrdinaryFindBestSplit(D_k, $C - S$)

// return information gain that would result from this 2-level subtree

return $$H_D(Y) - \left(\sum_k \frac{|D_k|}{|D|} H_{D_k}(Y \mid S = k, S_k) \right)$$

Calculating information gain with lookahead

Suppose that when considering Humidity as a split, we find that Wind and Temperature are the best features to split on at the next level



We can assess value of choosing Humidity as our split by

$$H_D(Y) - \left(\frac{14}{23} H_D(Y \mid \text{Humidity} = \text{high}, \text{Wind}) + \frac{9}{23} H_D(Y \mid \text{Humidity} = \text{low}, \text{Temperature}) \right)$$

Calculating information gain with lookahead

Using the tree from the previous slide:

$$\frac{14}{23} H_D(Y \mid \text{Humidity} = \text{high}, \text{Wind}) + \frac{9}{23} H_D(Y \mid \text{Humidity} = \text{low}, \text{Temperature})$$

$$= \frac{5}{23} H_D(Y \mid \text{Humidity} = \text{high}, \text{Wind} = \text{strong}) +$$

$$\frac{9}{23} H_D(Y \mid \text{Humidity} = \text{high}, \text{Wind} = \text{weak}) +$$

$$\frac{4}{23} H_D(Y \mid \text{Humidity} = \text{low}, \text{Temperature} = \text{high}) +$$

$$\frac{5}{23} H_D(Y \mid \text{Humidity} = \text{low}, \text{Temperature} = \text{low})$$

$$H_D(Y \mid \text{Humidity} = \text{high}, \text{Wind} = \text{strong}) = -\frac{2}{5}\log\left(\frac{2}{5}\right) - \frac{3}{5}\log\left(\frac{3}{5}\right)$$

$$\vdots$$

Comments on decision tree learning

- widely used approach
- many variations
- provides humanly comprehensible models when trees not too big
- insensitive to monotone transformations of numeric features
- standard methods learn axis-parallel hypotheses*
- standard methods not suited to on-line setting*
- usually not among most accurate learning methods

* although variants exist that are exceptions to this