Machine Learning in Real World: C4.5

Outline

- Handling Numeric Attributes
  - Finding Best Split(s)
- Dealing with Missing Values
- Pruning
  - Pre-pruning, Post-pruning, Error Estimates
- From Trees to Rules

Industrial-strength algorithms

- For an algorithm to be useful in a wide range of real-world applications it must:
  - Permit numeric attributes
  - Allow missing values
  - Be robust in the presence of noise
  - Be able to approximate arbitrary concept descriptions (at least in principle)
- Basic schemes need to be extended to fulfill these requirements

C4.5 History

- ID3, CHAID – 1960s
- C4.5 innovations (Quinlan):
  - permit numeric attributes
  - deal sensibly with missing values
  - pruning to deal with for noisy data
- C4.5 - one of best-known and most widely-used learning algorithms
  - Last research version: C4.8, implemented in Weka as J4.8 (Java)
  - Commercial successor: C5.0 (available from Rulequest)

Numeric attributes

- Standard method: binary splits
  - E.g. temp < 45
- Unlike nominal attributes, every attribute has many possible split points
- Solution is straightforward extension:
  - Evaluate info gain (or other measure) for every possible split point of attribute
  - Choose "best" split point
  - Info gain for best split point is info gain for attribute
- Computationally more demanding

Weather data – nominal values

Outlook	Temperature	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	Normal	False	Yes
…	…	…	…	…

```
If outlook = sunny and humidity = high then play = no
If outlook = rainy and windy = true then play = no
If outlook = overcast then play = yes
If humidity = normal then play = yes
If none of the above then play = yes
```

Weather data - numeric

Outlook	Temperature	Humidity	Windy	Play
Sunny	85	85	False	No
Sunny	80	90	True	No
Overcast	83	86	False	Yes
Rainy	75	80	False	Yes
…	…	…	…	…

```
If outlook = sunny and humidity > 83 then play = no
If outlook = rainy and windy = true then play = no
If outlook = overcast then play = yes
If humidity < 85 then play = yes
If none of the above then play = yes
```

Example

- Split on temperature attribute:

64	65	68	69	70	71	72	72	75	75	80	81	83	85
Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

  - E.g. temperature < 71.5: yes/4, no/2
    temperature ≥ 71.5: yes/5, no/3
  - Info([4,2],[5,3])
    = 6/14 info([4,2]) + 8/14 info([5,3])
    = 0.939 bits
- Place split points halfway between values
- Can evaluate all split points in one pass!

Avoid repeated sorting!

- Sort instances by the values of the numeric attribute
  - Time complexity for sorting: $O(n \log n)$
- ***Q. Does this have to be repeated at each node of the tree?***
- A: No! Sort order for children can be derived from sort order for parent
  - Time complexity of derivation: $O(n)$
  - Drawback: need to create and store an array of sorted indices for each numeric attribute

More speeding up

- Entropy only needs to be evaluated between points of different classes (Fayyad & Irani, 1992)

value	64	65	68	69	70	71	72	72	75	75	80	81	83	85
class	Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

X

Potential optimal breakpoints

Breakpoints between values of the same class cannot be optimal

Binary *vs.* multi-way splits

- Splitting (multi-way) on a nominal attribute exhausts all information in that attribute
  - Nominal attribute is tested (at most) once on any path in the tree
- Not so for binary splits on numeric attributes!
  - Numeric attribute may be tested several times along a path in the tree
- Disadvantage: tree is hard to read
- Remedy:
  - pre-discretize numeric attributes, *or*
  - use multi-way splits instead of binary ones

Missing as a separate value

- Missing value denoted "?" in C4.X
- Simple idea: treat missing as a separate value
- Q: When this is not appropriate?
- A: When values are missing due to different reasons
  - Example 1: gene expression could be missing when it is very high or very low
  - Example 2: field **IsPregnant**=missing for a male patient should be treated differently (no) than for a female patient of age 25 (unknown)

Missing values - advanced

Split instances with missing values into pieces

- A piece going down a branch receives a weight proportional to the popularity of the branch
- weights sum to 1

- Info gain works with fractional instances
  - use sums of weights instead of counts
- During classification, split the instance into pieces in the same way
  - Merge probability distribution using weights

Pruning

- Goal: Prevent overfitting to noise in the data
- Two strategies for "pruning" the decision tree:
  - *Postpruning* - take a fully-grown decision tree and discard unreliable parts
  - *Prepruning* - stop growing a branch when information becomes unreliable
- Postpruning preferred in practice—prepruning can "stop too early"

Prepruning

- Based on statistical significance test
  - Stop growing the tree when there is no *statistically significant* association between any attribute and the class at a particular node
- Most popular test: *chi-squared test*
- ID3 used chi-squared test in addition to information gain
  - Only statistically significant attributes were allowed to be selected by information gain procedure

Early stopping

	a	b	class
1	0	0	0
2	0	1	1
3	1	0	1
4	1	1	0

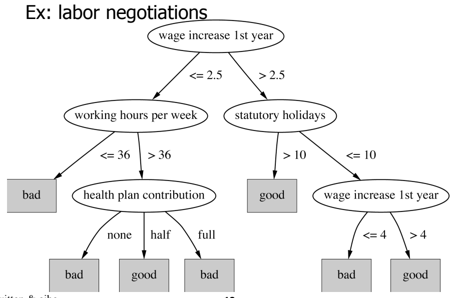
- Pre-pruning may stop the growth process prematurely: *early stopping*
- Classic example: XOR/Parity-problem
  - No *individual* attribute exhibits any significant association to the class
  - Structure is only visible in fully expanded tree
  - Pre-pruning won't expand the root node
- But: XOR-type problems rare in practice
- And: pre-pruning faster than post-pruning

Post-pruning

- First, build full tree
- Then, prune it
  - Fully-grown tree shows all attribute interactions
- Problem: some subtrees might be due to chance effects
- Two pruning operations:
  1. *Subtree replacement*
  2. *Subtree raising*
- Possible strategies:
  - error estimation
  - significance testing
  - MDL principle

Subtree replacement

- *Bottom-up*
- Consider replacing a tree only after considering all its subtrees
- Ex: labor negotiations



Subtree replacement

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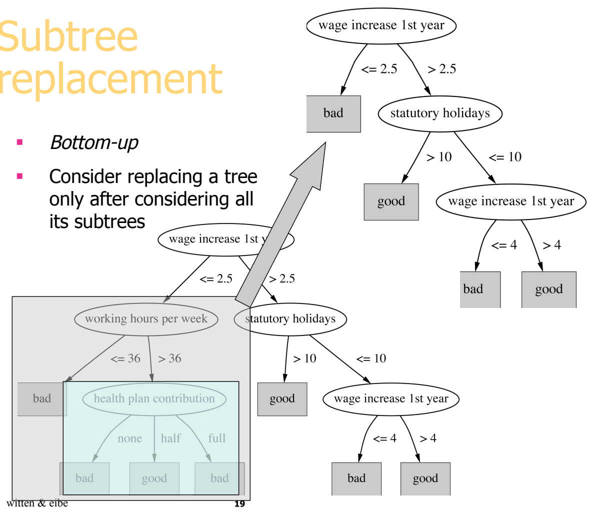
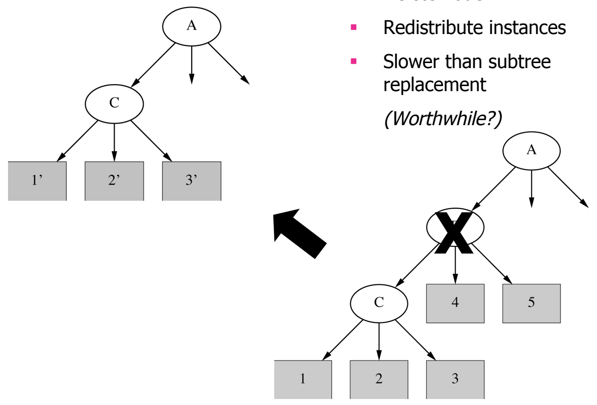


*Subtree raising

- Delete node
- Redistribute instances
- Slower than subtree replacement

  (Worthwhile?)



Estimating error rates

- Prune only if it reduces the estimated error
- Error on the training data is NOT a useful estimator
  Q: Why it would result in very little pruning?
- Use hold-out set for pruning ("reduced-error pruning")
- C4.5's method
  - Derive confidence interval from training data
  - Use a heuristic limit, derived from this, for pruning
  - Standard Bernoulli-process-based method
  - Shaky statistical assumptions (based on training data)

*Mean and variance

- Mean and variance for a Bernoulli trial: *p, p* (1–*p*)
- Expected success rate *f=S/N*
- Mean and variance for *f* : *p, p* (1–*p*)/*N*
- For large enough *N*, *f* follows a Normal distribution
- c% confidence interval [$-z \le X \le z$] for random variable with 0 mean is given by:

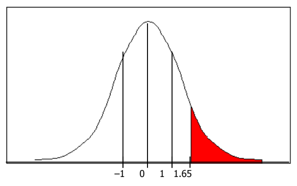
$$\Pr[-z \le X \le z] = c$$

- With a symmetric distribution:

$$\Pr[-z \le X \le z] = 1 - 2 \times \Pr[X \ge z]$$

*Confidence limits

- Confidence limits for the normal distribution with 0 mean and a variance of 1:



$\Pr[X \ge z]$	z
0.1%	3.09
0.5%	2.58
1%	2.33
5%	1.65
10%	1.28
20%	0.84
25%	0.69
40%	0.25

- Thus:

$$\Pr[-1.65 \le X \le 1.65] = 90\%$$

- To use this we have to reduce our random variable *f* to have 0 mean and unit variance

*Transforming *f*

- Transformed value for *f* : $\dfrac{f-p}{\sqrt{p(1-p)/N}}$

  (i.e. subtract the mean and divide by the *standard deviation*)

- Resulting equation:

$$\Pr\left[-z \le \frac{f-p}{\sqrt{p(1-p)/N}} \le z\right] = c$$

- Solving for *p*:

$$p = \left(f + \frac{z^2}{2N} \pm z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}}\right) \bigg/ \left(1 + \frac{z^2}{N}\right)$$

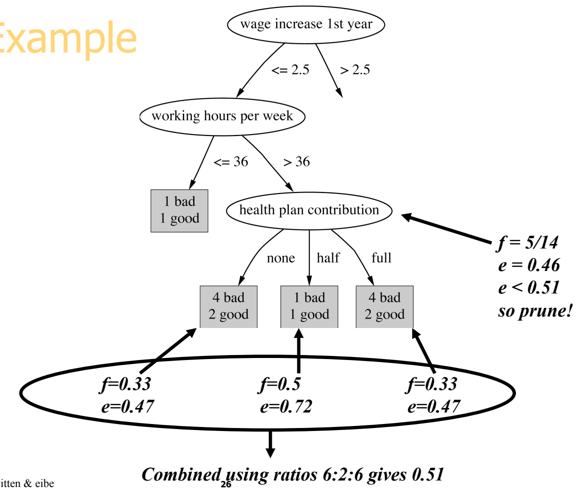
C4.5's method

- Error estimate for subtree is weighted sum of error estimates for all its leaves
- Error estimate for a node (upper bound):

$$e = \left(f + \frac{z^2}{2N} + z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}} \right) \Big/ \left(1 + \frac{z^2}{N} \right)$$

- If c = 25% then z = 0.69 (from normal distribution)
- f is the error on the training data
- N is the number of instances covered by the leaf

Example



*Complexity of tree induction

- Assume
  - m attributes
  - n training instances
  - tree depth $O(\log n)$
- Building a tree $O(m\, n \log n)$
- Subtree replacement $O(n)$
- Subtree raising $O(n (\log n)^2)$
  - Every instance may have to be redistributed at every node between its leaf and the root
  - Cost for redistribution (on average): $O(\log n)$
- Total cost: $O(m\, n \log n) + O(n (\log n)^2)$

From trees to rules

- Simple way: one rule for each leaf
- C4.5rules: greedily prune conditions from each rule if this reduces its estimated error
  - Can produce duplicate rules
  - Check for this at the end
- Then
  - look at each class in turn
  - consider the rules for that class
  - find a "good" subset (guided by MDL)
- Then rank the subsets to avoid conflicts
- Finally, remove rules (greedily) if this decreases error on the training data

C4.5rules: choices and options

- C4.5rules slow for large and noisy datasets
- Commercial version C5.0rules uses a different technique
  - Much faster and a bit more accurate
- C4.5 has two parameters
  - Confidence value (default 25%): lower values incur heavier pruning
  - Minimum number of instances in the two most popular branches (default 2)

*Classification rules

- Common procedure: *separate-and-conquer*
- Differences:
  - Search method (e.g. greedy, beam search, ...)
  - Test selection criteria (e.g. accuracy, ...)
  - Pruning method (e.g. MDL, hold-out set, ...)
  - Stopping criterion (e.g. minimum accuracy)
  - Post-processing step
- Also: Decision list
  vs. one rule set for each class

*Test selection criteria

- Basic covering algorithm:
  - keep adding conditions to a rule to improve its accuracy
  - Add the condition that improves accuracy the most
- Measure 1: *p*/*t*
  - *t* total instances covered by rule
    p number of these that are positive
  - Produce rules that don't cover *negative* instances, as quickly as possible
  - May produce rules with very small coverage —special cases or noise?
- Measure 2: Information gain *p* (log(*p*/*t*) – log(P/T))
  - *P* and *T* the positive and total numbers before the new condition was added
  - Information gain emphasizes positive rather than negative instances
- These interact with the pruning mechanism used

*Missing values, numeric attributes

- Common treatment of missing values: *for any test, they fail*
  - Algorithm must either
    - use other tests to separate out positive instances
    - leave them uncovered until later in the process
- In some cases it's better to treat "missing" as a separate value
- Numeric attributes are treated just like they are in decision trees

*Pruning rules

- Two main strategies:
  - *Incremental* pruning
  - *Global* pruning
- Other difference: pruning criterion
  - Error on hold-out set (*reduced-error pruning*)
  - Statistical significance
  - MDL principle
- Also: post-pruning vs. pre-pruning

Summary

- Decision Trees
  - splits – binary, multi-way
  - split criteria – entropy, gini, …
  - missing value treatment
  - pruning
  - rule extraction from trees
- No method is always superior – experiment!