Trees and Rules

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Algorithms for learning trees and rules

- Decision trees
  - From ID3 to C4.5 (pruning, numeric attributes, ...)
- Classification rules
  - From PRISM to RIPPER and PART (pruning, numeric data, …)
- Association Rules
  - Faster rule mining with frequent-pattern trees

Decision Trees

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
- Basic scheme needs to be extended to fulfill these requirements

From ID3 to C4.5

- Extending ID3:
  - to permit numeric attributes: *straightforward*
  - to deal sensibly with missing values: *trickier*
  - stability for noisy data: *requires pruning mechanism*
- End result: C4.5 (Quinlan)
  - Best-known and (probably) most widely-used learning algorithm
  - Commercial successor: C5.0

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 (again!)

Outlook	Temperature	Humidity	Windy	Play
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
…	…	…	…	…

```
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 (again!)

Outlook	Temperature	Humidity	Windy	Play
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
…	…	…	…	…

Outlook	Temperature	Humidity	Windy	Play
Sunny	85	85	False	No
Sunny	80	90	True	No
Overcast	83	86	False	Yes
Rainy	70	96	False	Yes
Rainy	68	80	False	Yes
Rainy	65	70	True	No
…	…	…	…	…

```
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
```

```
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 = no
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!

Can avoid repeated sorting

- Sort instances by the values of the numeric attribute
  - Time complexity for sorting: $O\ (n \log n)$
- Does this have to be repeated at each node of the tree?
- 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

Binary vs. multiway 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

Computing multi-way splits

- Simple and efficient way of generating multi-way splits: greedy algorithm
- But: dynamic programming can find optimum multi-way split in $O\ (n^2)$ time
  - imp (k, i, j) is the impurity of the best split of values $x_i \ldots x_j$ into k sub-intervals
  - imp (k, 1, i) =
    $\min_{0<j<i}$ imp (k–1, 1, j) + imp (1, j+1, i)
  - imp (k, 1, N) gives us the best k-way split
- In practice, greedy algorithm works as well

Missing values

- C4.5 applies method of fractional instances:
  - 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

- Prevent overfitting the training data: “prune the decision tree
- Two strategies:
  - Postpruning
    take a fully-grown decision tree and discard unreliable parts
  - Prepruning
    stop growing a branch when information becomes unreliable
- Postpruning is preferred in practice—prepruning can “stop 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*
- Quinlan's classic tree learner ID3 used chi-squared test in addition to information gain
  - Only statistically significant attributes were allowed to be selected by the information gain procedure

Early stopping

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

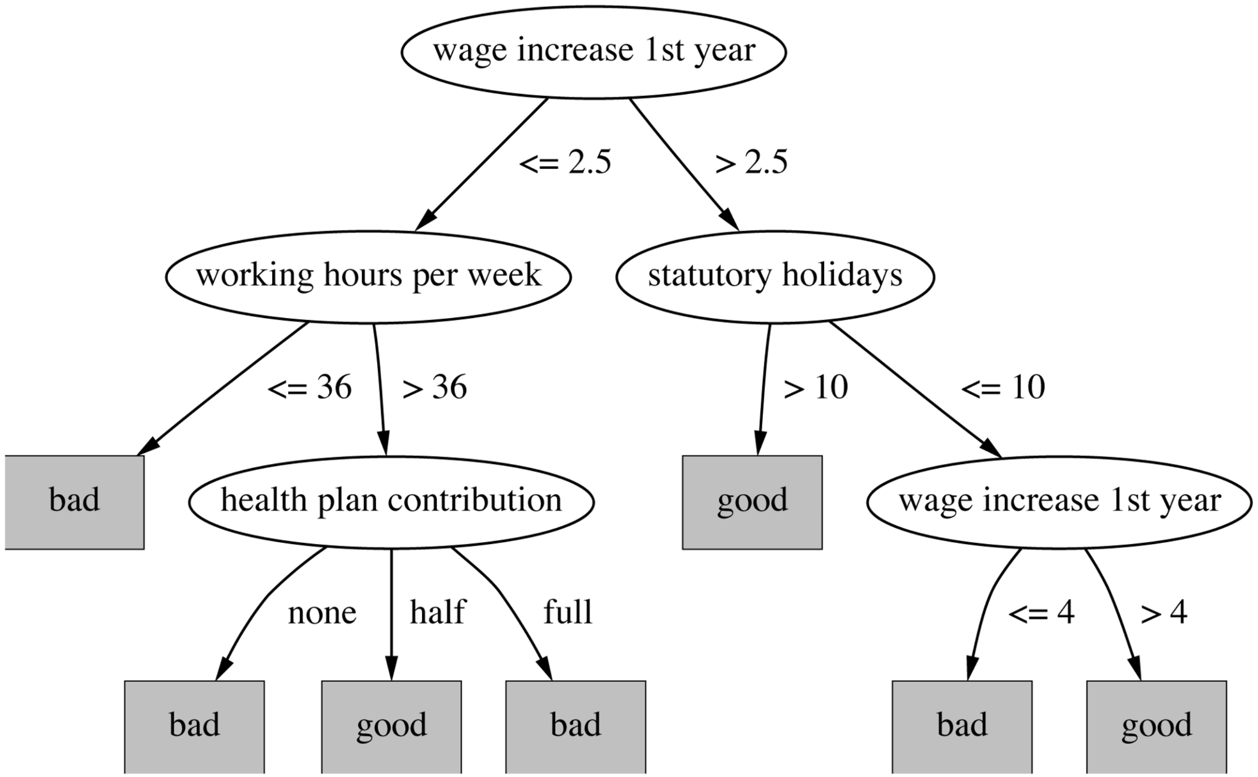
- Pre-pruning may stop the growth process prematurely: early stopping
- Classic example: XOR/Parity-problem
  - No individual attribute exhibits any significant association with the class
  - Structure is only visible in fully expanded tree
  - Prepruning won't expand the root node
- But: XOR-type problems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

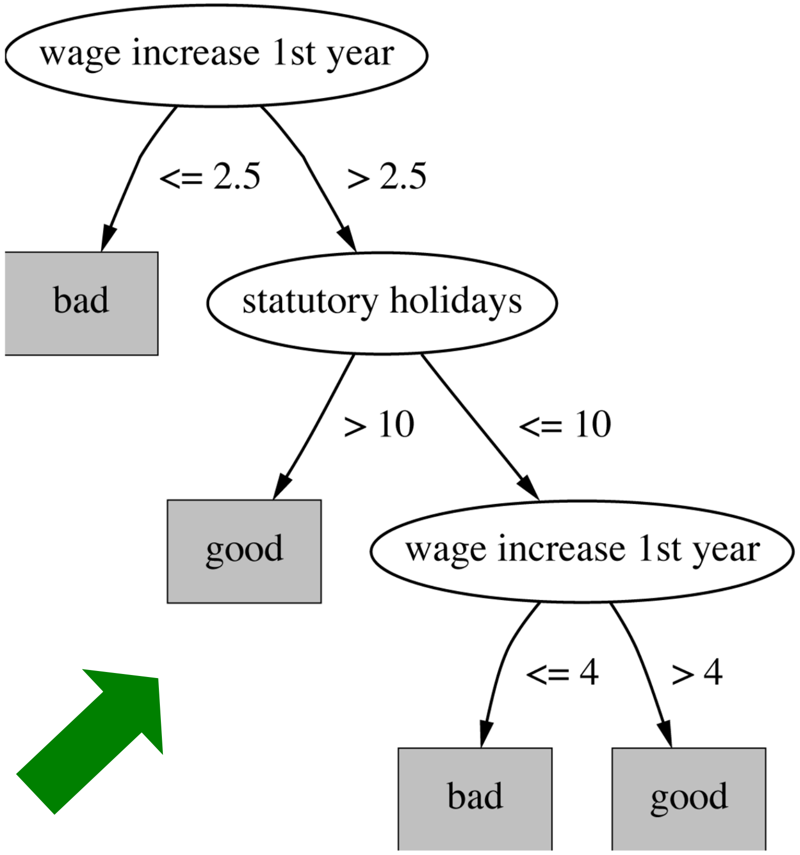
Postpruning

- 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:
  - Subtree replacement
  - Subtree raising
- Possible strategies:
  - error estimation
  - significance testing
  - MDL principle

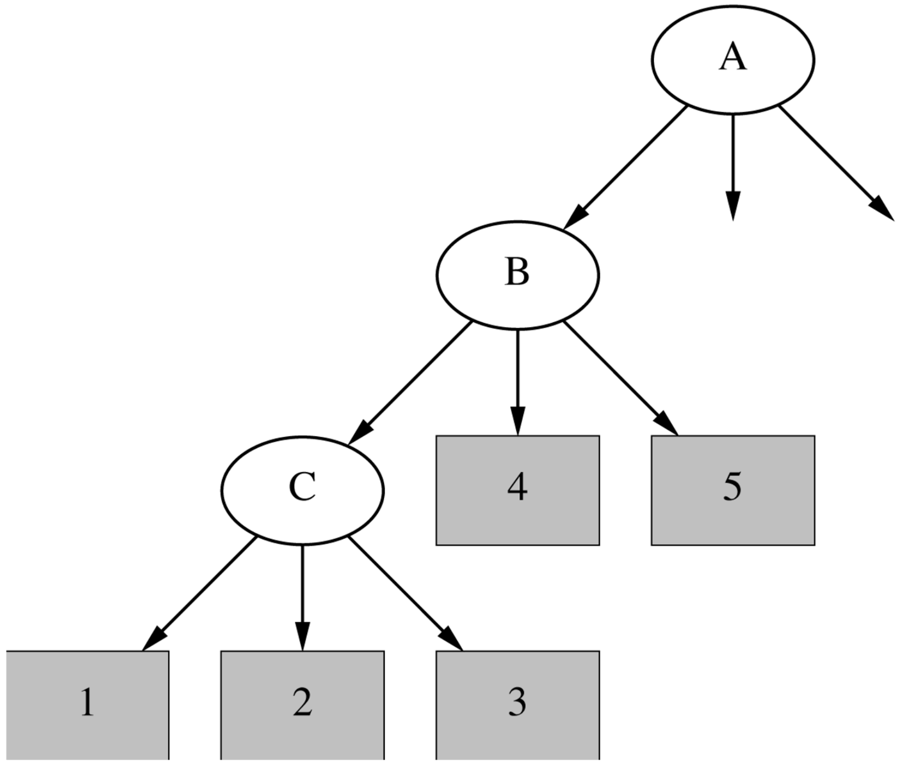
Subtree replacement

- Bottom-up
- Consider replacing a tree only after considering all its subtrees

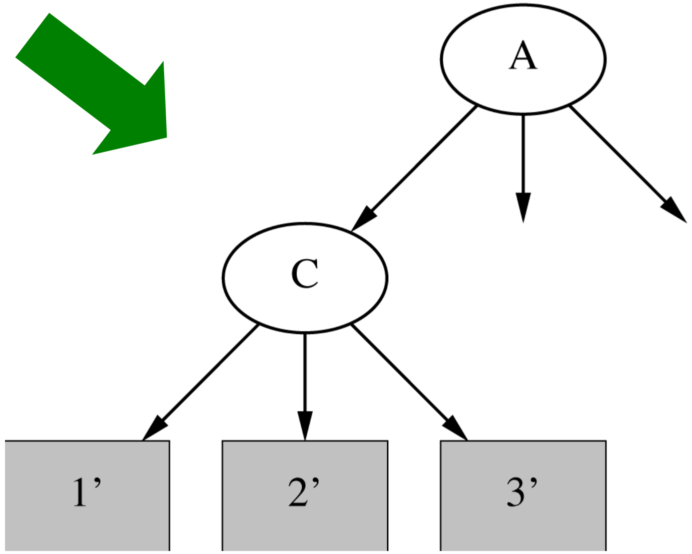




Subtree raising



- Delete node
- Redistribute instances
- Slower than subtree replacement
  (Worthwhile?)



Estimating error rates

- Prune only if it does not increase the estimated error
- Error on the training data is NOT a useful estimator (would result in almost no pruning)
- One possibility: use hold-out set for pruning (yields “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)

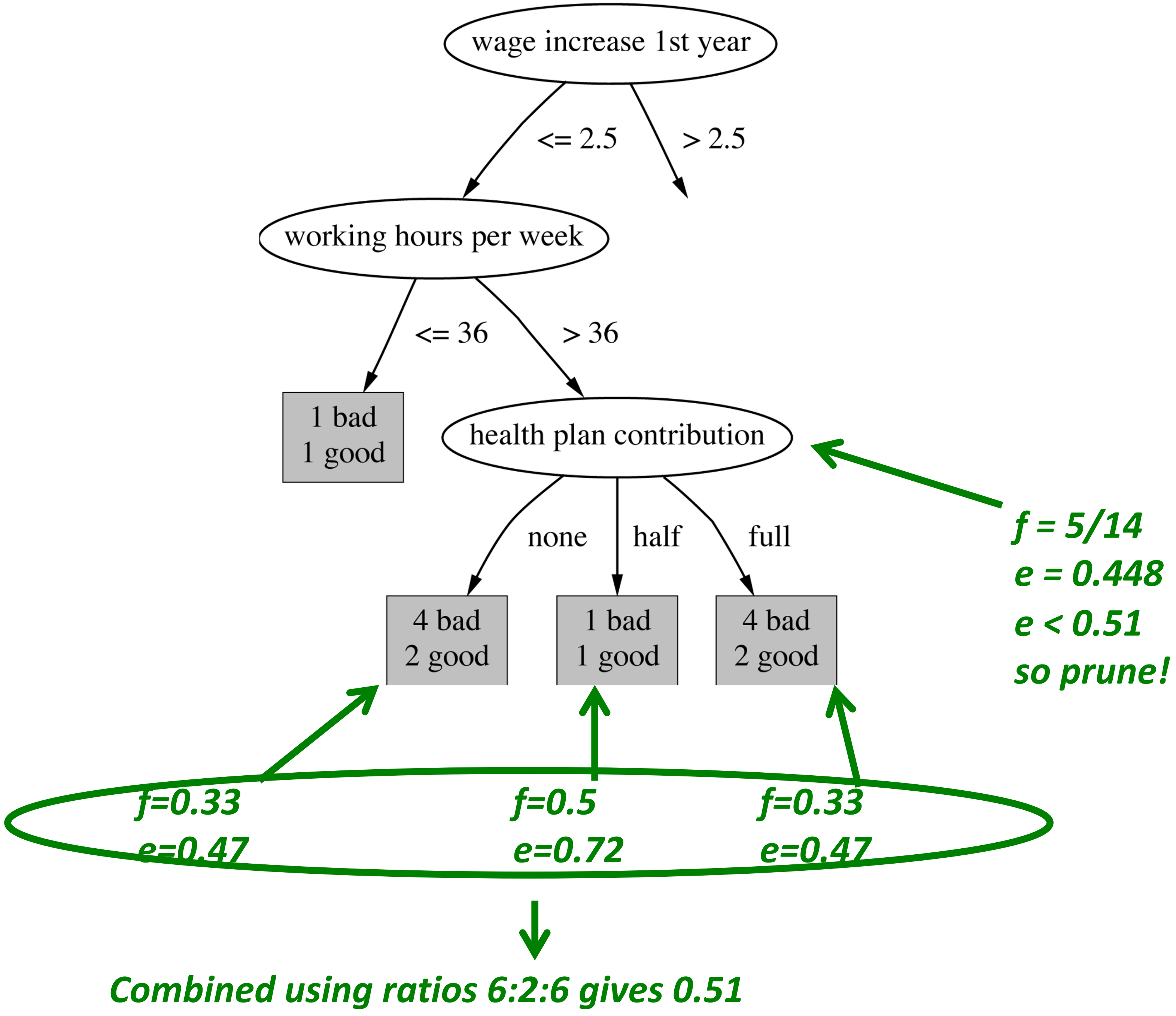
C4.5's method

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

$$e = \frac{f + \frac{z^2}{2N} + z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}}}{1 + \frac{z^2}{N}}$$

- 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



wage increase 1st year
<= 2.5
> 2.5
working hours per week
<= 36
> 36
1 bad
1 good
health plan contribution
none
half
full
4 bad
2 good
1 bad
1 good
4 bad
2 good
f = 5/14
e = 0.448
e < 0.51
so prune!
f=0.33
e=0.47
f=0.5
e=0.72
f=0.33
e=0.47
Combined using ratios 6:2:6 gives 0.51

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

C4.5: choices and options

- C4.5rules slow for large and noisy datasets
- Successor algorithm 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)
- Time complexity of C4.5 is actually greater than what was stated above:
  - For each numeric split point that has been identified, the *entire* training set is scanned to find the closest actual point

Cost-complexity pruning

- C4.5's postpruning often does not prune enough
  - Tree size continues to grow when more instances are added even if performance on independent data does not improve
  - But: it is very fast and popular in practice
- Can be worthwhile in some cases to strive for a more compact tree at the expense of more computational effort
  - *Cost-complexity pruning* method from the CART (Classification and Regression Trees) learning system achieves this
  - Applies cross-validation or a hold-out set to choose an appropriate tree size for the final tree

Cost-complexity pruning details

- Basic idea:
  - First prune subtrees that, relative to their size, lead to the smallest increase in error on the training data
  - Increase in error (α): average error increase per leaf of subtree
  - Bottom-up pruning based on this criterion generates a *sequence* of successively smaller trees
  - Each candidate tree in the sequence corresponds to one particular threshold value α_i
- Which tree to chose as the final model?
  - Use either a hold-out set or cross-validation to estimate the error for each α_i
  - Rebuild tree on entire training set using chosen value of α

Discussion

TDIDT: Top-Down Induction of Decision Trees

- The most extensively studied method of machine learning used in data mining
- Different criteria for attribute/test selection rarely make a large difference
- Different pruning methods mainly change the size of the resulting pruned tree
- C4.5 builds *univariate* decision trees: each node tests a single attribute
- Some TDITDT systems can build *multivariate* trees (e.g., the famous CART tree learner)

Discussion and Bibliographic Notes

- CART’s pruning method (Breiman et al. 1984) can often produce smaller trees than C4.5’s method
- C4.5’s overfitting problems have been investigated empirically by Oates and Jensen (1997). Hall (2003) showed reducing c took care of issues raised.
- A complete description of C4.5, the early 1990s version, appears as a excellent and readable book (Quinlan 1993)
- An MDL-based heuristic for C4.5 Release 8 that combats overfitting of numeric attributes is described by Quinlan (1998)
- The more recent version of Quinlan’s tree learner, C5.0, is also available as open-source code

Classification Rules

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
- Accuracy 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 measures interact with the pruning mechanism used

Missing values, numeric attributes

- Common treatment of missing values:
  for any test, they fail
- This means the algorithm must either
  - use other tests to separate out positive instances
  - leave them uncovered until later in the process
- In some cases it is better to treat "missing" as a separate value (i.e., if "missing" has a special significance"
- Numeric attributes are treated just like they are in decision trees, with binary split points
  - Split points are found by optimizing test selection criterion, similar to what happens when finding a split 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

RIPPER

William Cohen, Fast Effective Rule Induction, Proceedings of the 12th International Conference on Machine Learning

IREP-Based

- Based on incremental reduced error pruning (IREP).
- Grow rules one at a time.
- Have a growing set of 2/3 of the examples for building the rule and a pruning set of 1/3.
- Build rules for 2 class problems. Order classes by size from smallest to largest.
- Build rules for smallest class vs. all other examples first.

Using a pruning set

- For statistical validity, must evaluate measure on data not used for training:
  - This requires a *growing set* and a *pruning set*
- *Reduced-error pruning* :
  build full rule set and then prune it
- *Incremental reduced-error pruning* : simplify each rule as soon as it is built
  - Can re-split data after rule has been pruned
- Stratification advantageous

Incremental reduced-error pruning

```
Initialize E to the instance set
Until E is empty do
   Split E into Grow and Prune in the ratio 2:1
   For each class C for which Grow contains an instance
      Use basic covering algorithm to create best perfect rule
         for C
      Calculate w(R):  worth of rule on Prune
            and w(R-): worth of rule with final condition
                       omitted
      If w(R) < w(R-), prune rule and repeat previous step
   From the rules for the different classes, select the one
      that's worth most (i.e. with largest w(R))
   Print the rule
   Remove the instances covered by rule from E
Continue
```

Incremental reduced-error pruning Modified for RIPPER

- Order classes according to increasing prevalence
  $(C_1, \ldots, C_k)$
  find rule set to separate C_1 from other classes
  `IREP(Pos=`C_1`,Neg=`$C_2, \ldots, C_k$`)`
  remove all instances learned by rule set
  find rule set to separate C_2 from $C_3, \ldots, C_k$
  ...
  C_k remains as default class

Question

- The requirement in RIPPER of a pruning set
  - a) reflects the belief that learning on all training data may overfit
  - b) is done to minimize accuracy
  - c) will work better for large training sets, avoiding starving the learning system for data
  - d) uses the idea of just pruning a test when it does not improve performance on the test data.

Incremental reduced-error pruning Modified for RIPPER

```
procedure IREP(Pos,Neg)
begin
    Ruleset := ∅
    while Pos≠ ∅ do
        /* grow and prune a new rule */
        split (Pos,Neg) into (GrowPos,GrowNeg)
          and (PrunePos,PruneNeg)
        Rule := GrowRule(GrowPos,GrowNeg)
        Rule := PruneRule(Rule,PrunePos,PruneNeg)
        if the error rate of Rule on
          (PrunePos,PruneNeg) exceeds 50% then
            return Ruleset
        else
            add Rule to Ruleset
            remove examples covered by Rule
              from (Pos,Neg)
        endif
    endwhile
    return Ruleset
end
```

Growing a Rule

- To grow a rule, we have a training set of positive and negative examples.

- We add a test to a rule of the form
  - $\text{atttribute}_i = v$ for a valid nominal value or $\text{atttribute}_i < x$ or $\text{atttribute}_i >= x$ for a continuous attribute with x in the range of values (usually x is an observed value)

Choosing a test to Grow a Rule

- Foil gain is used:

$$Foil\_Gain(Test, R) = t(\log_2 \frac{p_1}{p_1 + n_1} - \log_2 \frac{p_0}{p_0 + n_0})$$

- Where p_0 is the number of positive examples covered by R and n_0 is the number of negative examples covered by R
- p_1 is the number of positive examples covered by the R+ Test and n_1 is the number of negative examples covered.
- t is the number of positive bindings of R also covered by R+ Test.

Measures used in IREP

- $[p + (N - n)] / T$
  - (N is total number of negatives, p (n) positive (negative) examples covered, T total number of examples)
  - Counterintuitive:
    - p = 2000 and n = 1000 vs. p = 1000 and n = 1
- Success rate p / t
  - Problem: p = 1 and t = 1

  vs. p = 1000 and t = 1001
- $(p - n) / t$
  - Same effect as success rate because it equals $2p/t - 1$
- Seems hard to find a simple measure of a rule's worth that corresponds with intuition

Improvements to get RIPPER

$$v(Rule, PrunePos, PruneNeg) \equiv \frac{p-n}{p+n},$$

Where P (N) is the total number of examples in PrunePos (PruneNeg) and p (n) is the number of examples in PrunePos (PruneNeg) covered by Rule.

Improvements to get RIPPER

- Find total description length of rule set and examples computed.
- Stop adding rules when this description length is more that d bits larger than the smallest description length found thus far. (d=64).
- For a rule set R_i, …, R_k consider each rule in turn in order learned. Create replacement and revision rules.

Replacement and Revision Rules

- Replacement for R_i, R_i' is formed by growing and then pruning a rule with pruning guided to minimize error of entire rule set as measured on the pruning set.

$$R_1, \ldots, R_i', \ldots, R_k$$

- The revision is created by greedily adding conditions to R_i, rather than the empty rule.
- The final theory can contain only one of the original, replacement or revision rules based on MDL.

Question

- Ripper growing a replacement rule is based on the idea that
  - a) searching too much is bad
  - b) there are no good rules unless you use all data
  - c) all train/prune splits are equal
  - d) the random split into a training and pruning set may affect the quality of the rules obtained
  - e) a different rule may be built when looking at a full rule sets accuracy

Optimization

- Can add more rules from IREP* to get RIPPER2 and in general can get RIPPERk for k optimizations.
- Let a rule have k conditions of n possible conditions, pr be known by the message recipient (pr=k/n here) and ||k|| be the number of bits needed to send integer k. Equation for bits for rule is below.

$$S(n,k,pr) \equiv (k\log_2\frac{1}{pr} + (n-k)\log_2\frac{1}{1-pr} + \|k\|) \times 0.5 = bits$$

Optimization

- Rule accuracy can be encoded by exceptions (false positives and false negatives).
- Let a rule cover p of P cases with fp – false positives and fn - false negatives, the bits required to encode exceptions are:

$$bits = \log_2(\binom{p}{fp}) + \log_2(\binom{P-p}{fn})$$

- To get the MDL you must sum all rules and exceptions for them.

Results

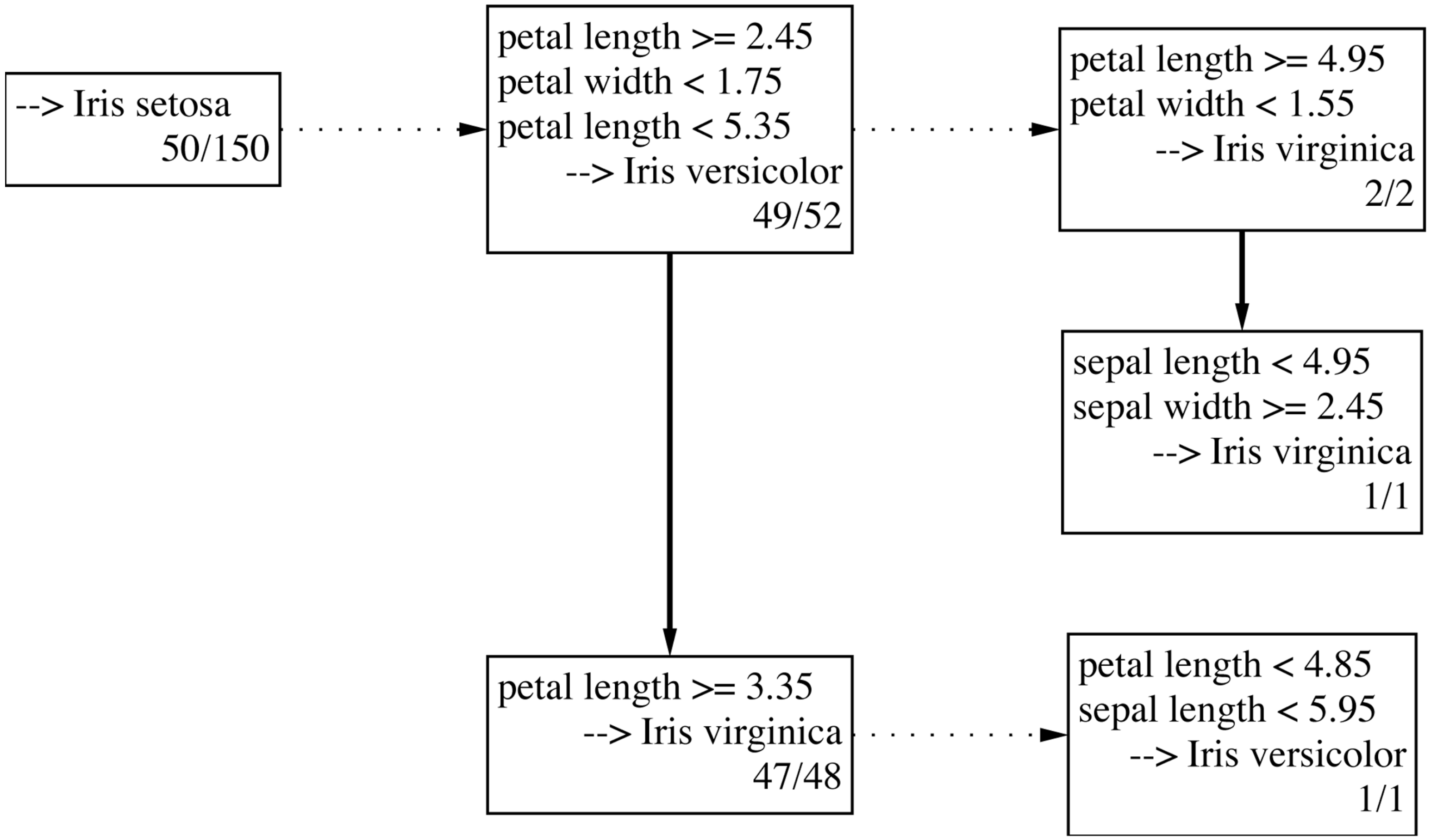
- RIPPER is much better than IREP* (28-7-2) for won, loss and tie on 37 data sets.
- Faster and better than C4.5 rules (20-15-2)

Rules with exceptions

- Assume we have a way of generating a single good rule
- Then, in principle, it is easy to generate rules with exceptions
- Algorithm for building a tree of rules:

1. Select default class for top-level rule
2. Generate a good rule for one of the remaining classes
3. Apply this method recursively to the two subsets produced by the rule
   (i.e., instances that are covered/not covered)

Iris data example



Discussion and Bibliographic Notes

- The idea of incremental reduced-error pruning is due to Fürnkranz and Widmer (1994)
- The RIPPER rule learner is due to Cohen (1995)
  - What we have presented here is the basic idea of the algorithm; there are many more details in the implementation
- An extensive theoretical study of various test selection criteria for rules has been performed by Fürnkranz and Flach (2005)
- The rule-learning scheme based on partial decision trees was developed by Frank and Witten (1998)
- The procedure for generating rules with exceptions was part of Gaines and Compton's *Induct* system (1995)
  - They called rules with exceptions *ripple-down* rules
  - Richards and Compton (1998) describe their role as an alternative to classic knowledge engineering

Association Rules

Association rules

- The Apriori algorithm finds frequent item sets via a generate-and-test methodology
  - Successively longer item sets are formed from shorter ones
  - Each different size of candidate item set requires a full scan of the dataset
  - Combinatorial nature of generation process is costly – particularly if there are many item sets, or item sets are large
- Appropriate data structures can help
- The *FP-growth* algorithm for finding frequent item sets employs an extended prefix tree (FP-tree)

FP-growth

- FP-growth uses a Frequent Pattern Tree (FP-tree) to store a compressed version of the data
- Only two passes through a dataset are required to map the data into an FP-tree
- The tree is then processed recursively to “grow” large item sets directly
  - Avoids generating and testing candidate item sets against the entire database

Building a frequent pattern tree

1) First pass over the data: count the number times individual items occur
2) Second pass over the data: before inserting each instance into the FP-tree, sort its items in descending order of their frequency of occurrence
    1) Individual items that do not meet the minimum support are not inserted into the tree
    2) Ideally, many instances will share items that occur frequently individually, resulting in a high degree of compression close to the root of the tree

An example using the weather data

Frequency of individual items (minimum support = 6)

play = yes	**9**
windy = false	**8**
humidity = normal	**7**
humidity = high	**7**
windy = true	**6**
temperature = mild	**6**
play = no	5
outlook = sunny	5
outlook = rainy	5
temperature = hot	4
temperature = cool	4
outlook = overcast	4

An example using the weather data

- Instances with items sorted

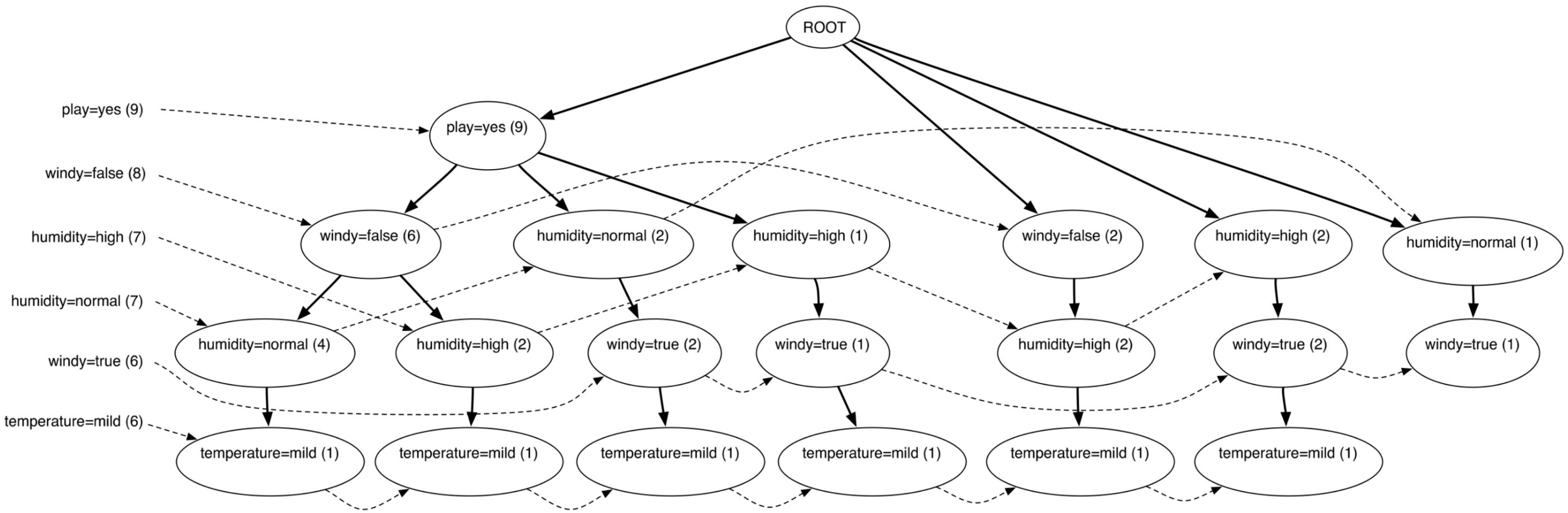
```
1 windy=false, humidity=high, play=no, outlook=sunny, temperature=hot
2 humidity=high, windy=true, play=no, outlook=sunny, temperature=hot
3 play=yes, windy=false, humidity=high, temperature=hot, outlook=overcast
4 play=yes, windy=false, humidity=high, temperature=mild, outlook=rainy
.
.
.
14 humidity=high, windy=true, temperature=mild, play=no, outlook=rainy
```

- Final answer: six single-item sets (previous slide) plus two multiple-item sets that meet minimum support

```
play=yes and windy=false             6
play=yes and
humidity=normal      6
```

Finding large item sets

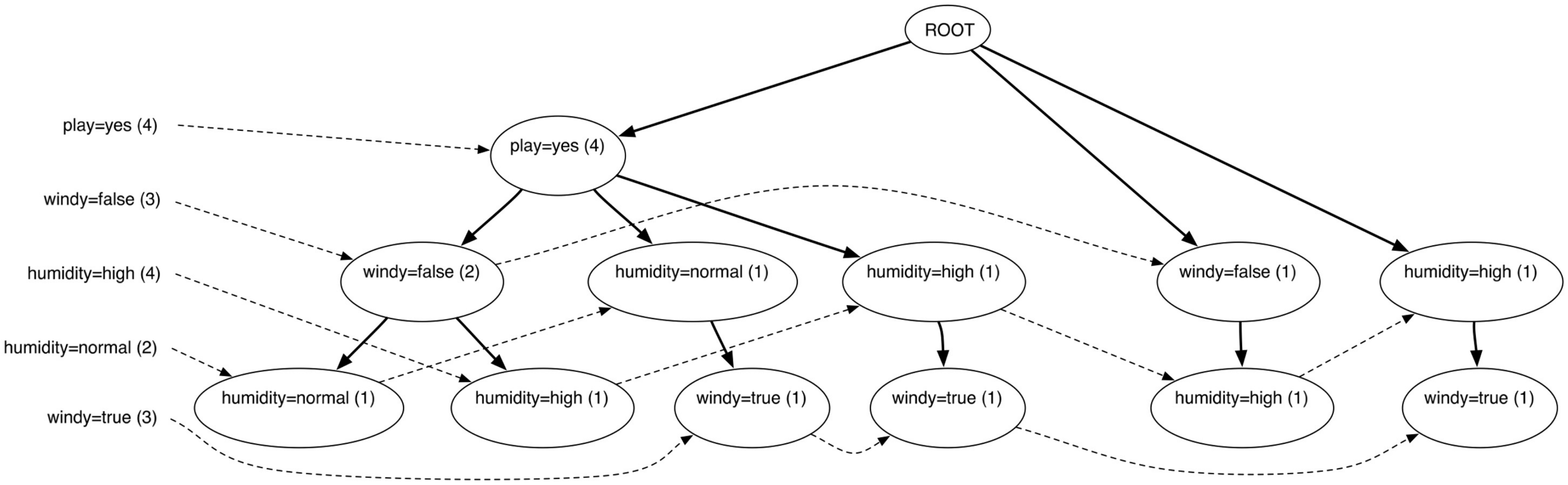
- FP-tree for the weather data (min support 6)



- Process header table (shown on left) from bottom
  - Add *temperature=mild* to the list of large item sets
  - Are there any item sets containing temperature=mild that meet the minimum support?

Finding large item sets cont.

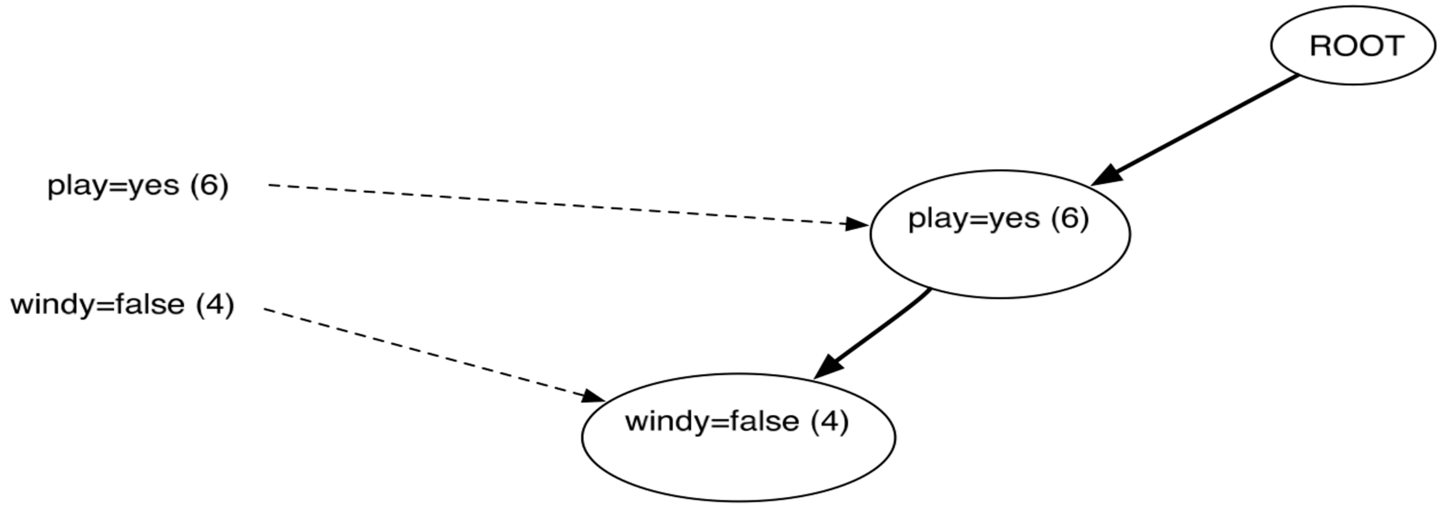
- FP-tree for the data conditioned on *temperature=mild*



- Created by scanning the first (original) tree
  - Follow *temperature=mild* link from header table to find all instances that contain *temperature=mild*
  - Project counts from original tree
- Header table shows that *temperature=mild* cannot be grown any longer

Finding large item sets cont.

- FP-tree for the data conditioned on *humidity=normal*



- Created by scanning the first (original) tree
  - Follow *humidity=normal* link from header table to find all instances that contain *humidity=normal*
  - Project counts from original tree
- Header table shows that *humidty=normal* **can** be grown to include *play=yes*

Finding large item sets cont.

- All large item sets have now been found
- However, in order to be sure it is necessary to process the entire header link table from the original tree
- Association rules are formed from large item sets in the same way as for Apriori
- FP-growth can be up to an order of magnitude faster than Apriori for finding large item sets

Discussion and Bibliographic Notes

- The FP-tree and the FP-growth algorithm were introduced by Han et al. (2000) following pioneering work by Zaki et al. (1997)
- Han et al. (2004) give a more comprehensive description; the algorithm has been extended in various ways
- Wang et al. (2003) develop an algorithm called CLOSET+ to mine *closed* item sets
  - Close item sets are sets for which there is no proper superset that has the same support
  - Produces few redundant rules and thus eases the task that users face when examining the output of the mining process
- GSP, for Generalized Sequential Patterns, is a method for mining patterns in event sequences (Srikant and Agrawal, 1996)
- An approach like FP-growth is used for event sequences by PrefixSpan (Pei et al., 2004) and CloSpan (Yan et al., 2003)
- For graph patterns, there is gSpan (Yan and Han, 2002) and CloseGraph (Yan and Han, 2003)

You have reached the end of the lecture.

Reference:

I. H. Witten, E. Frank,M. A. Hall and C. J. Pal(2016).*Data Mining: Practical Machine Learning Tools and Techniques.* Morgan Kaufmann