Learning from Observations – Decision Trees

Decision Trees

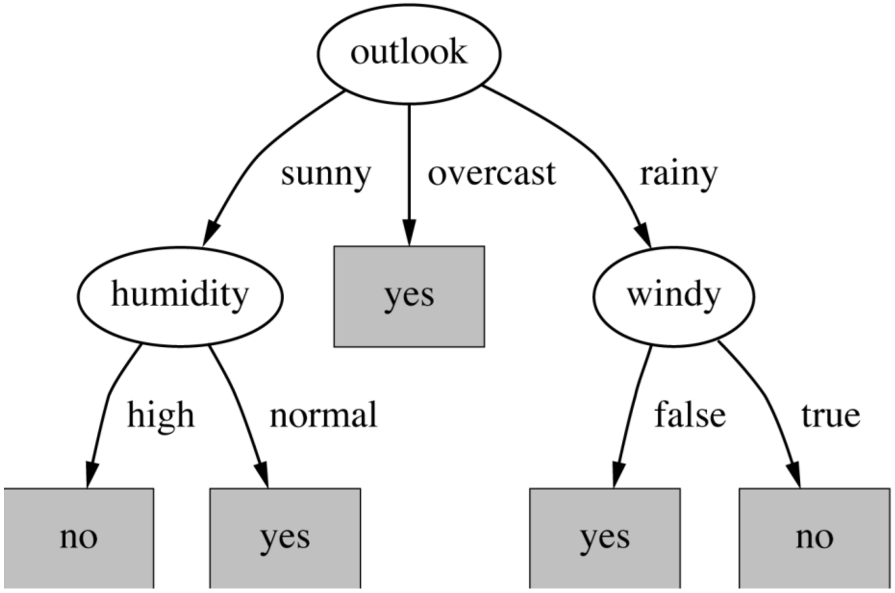
- Extending ID3:
  - To permit numeric attributes: *straightforward*
  - To deal sensibly with missing values: *trickier*
  - Stability for noisy data: *requires pruning mechanism*
- End result: C4.5 (Quinlan)
  - Best-known and (probably) most widely-used learning algorithm
  - Commercial successor: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



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Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool			
…	…			

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
…	…	…	…	…

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

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**

Missing Values

- 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
- During classification, split the instance into pieces in the same way
  - Merge probability distribution using weights

Pruning

- Prevent overfitting to noise in the 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 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
- 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

- 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
  - Prepruning won't expand the root node
- But: XOR-type problems rare in practice
- And: prepruning faster than postpruning

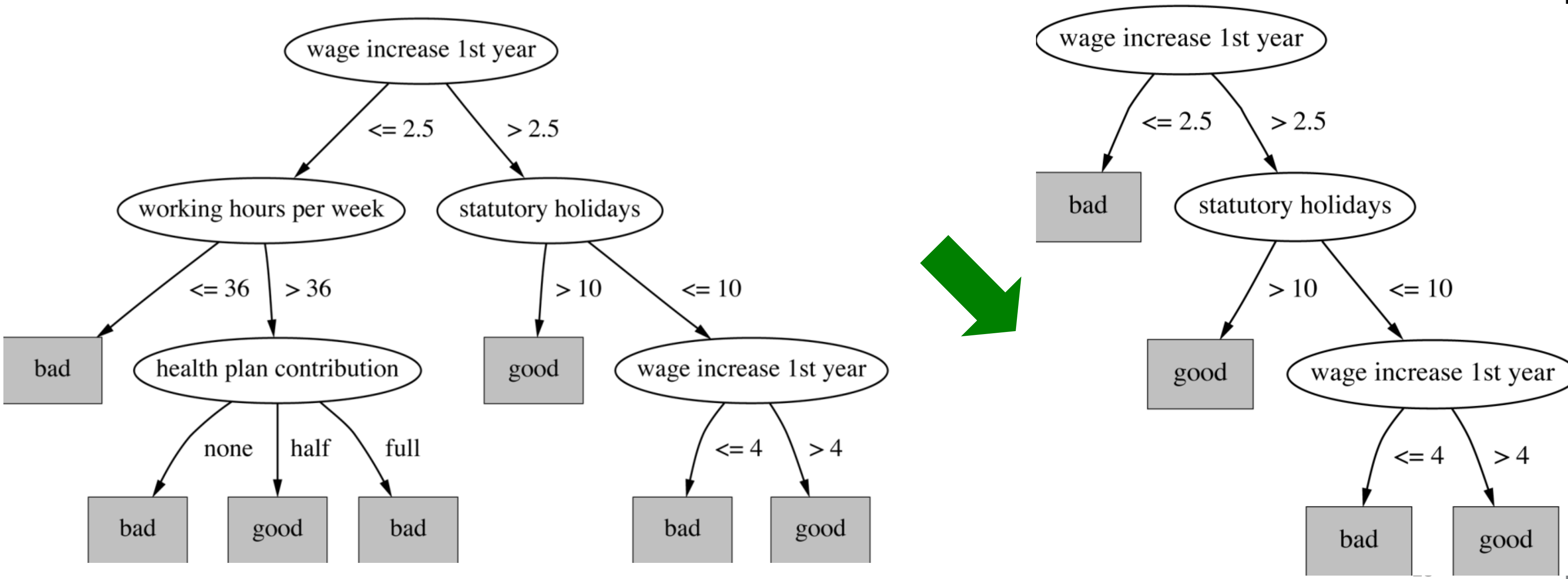
	a	b	class
1	0	0	0
2	0	1	1
3	1	0	1
4	1	1	0

Postpruning

- First, build full tree
- Then, prune it
    - Fully-grown tree shows all attribute interactions
- Two pruning operations:
    - *Subtree replacement*
    - *Subtree raising*
- Possible strategies:
    - Error estimation
    - Significance testing
    - MDL principle

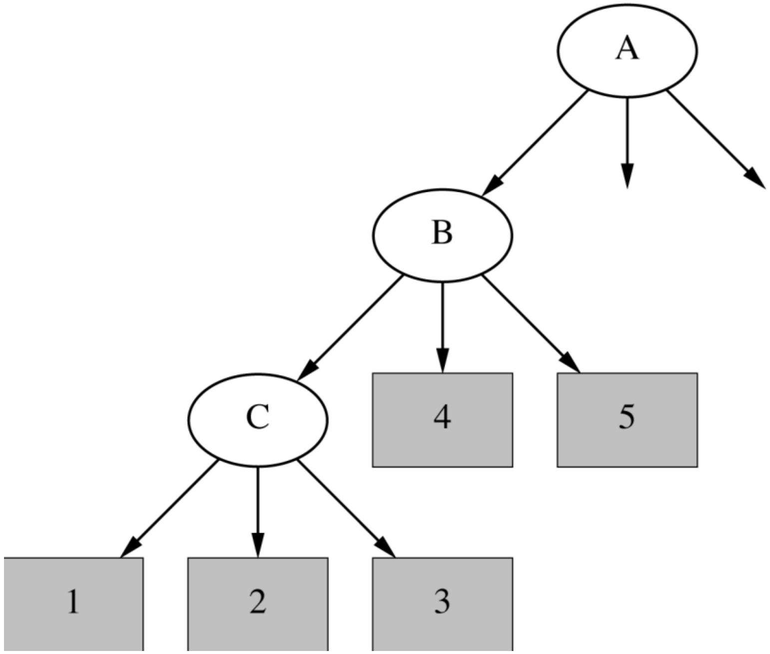
Subtree Replacement

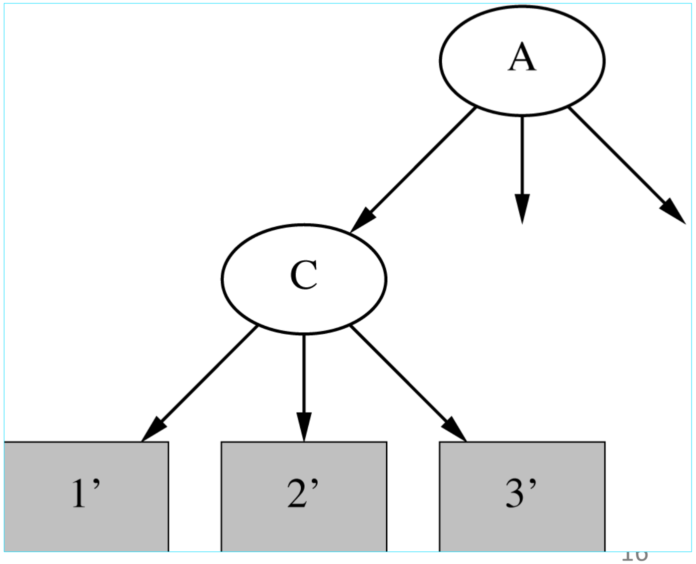
- *Bottom-up*
- Consider replacing a tree only after considering all its subtrees



Subtree Raising

- Delete node
- Redistribute instances
- Slower than subtree replacement





Estimating Error Rates

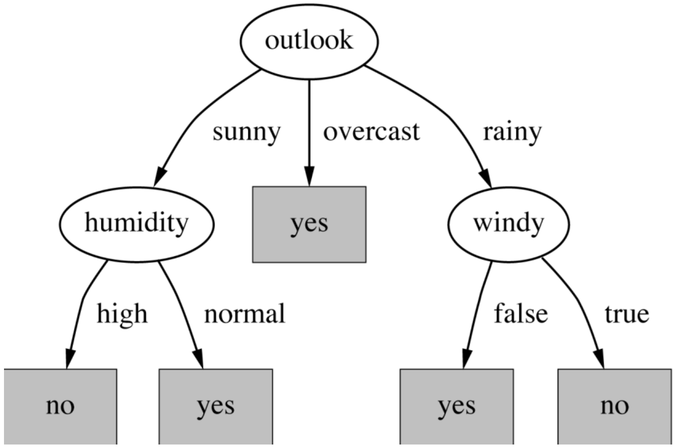
- Prune only if it does not increase the estimated error
- Error on the training data is NOT a useful estimator *(would result in almost no pruning)*
- Use hold-out set for pruning (“reduced-error pruning”)

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
- Commercial version C5.0 rules use 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)

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
  - 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

Cost-Complexity Pruning

- 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
  - Pruning 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 of each

Discussion

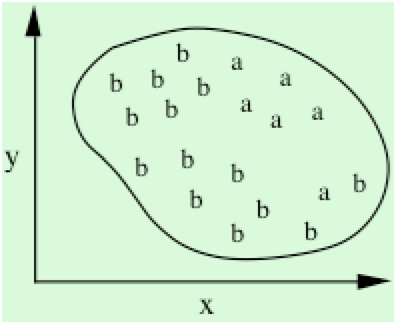
- The most extensively studied method of machine learning used in inductive learning
- Different criteria for attribute/test selection rarely make a large difference
- Different pruning methods mainly change the size of the resulting pruned tree

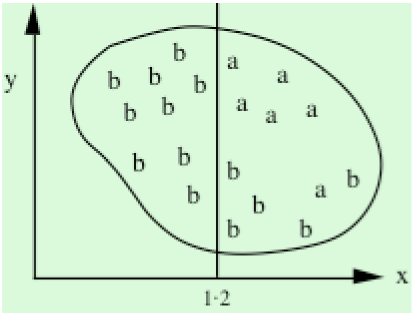
Learning from Observations – Rules

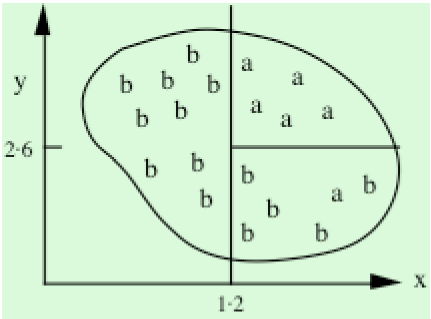
Covering Algorithms

- Can convert decision tree into a rule set
  - Straightforward, but rule set overly complex
  - More effective conversions are not trivial
- Instead, can generate rule set directly
  - For each class in turn find rule set that covers all instances in it (excluding instances not in the class)
- Called a *covering* approach:
  - At each stage a rule is identified that "covers" some of the instances

Example: Generating a Rule







If ???
then class = a

If x > 1.2
then class = a

If x > 1.2 and y > 2.6
then class = a

- Possible rule set for class “b”:

  If x ≤ 1.2 then class = b

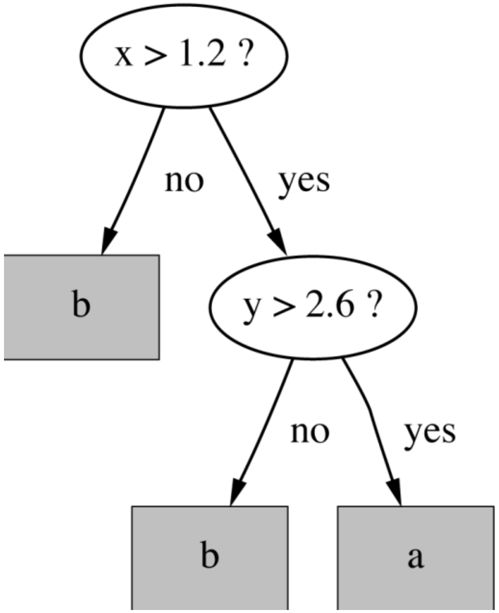
  If x > 1.2 and y ≤ 2.6 then class = b

- Could add more rules, get “perfect” rule set

Rules vs. Trees

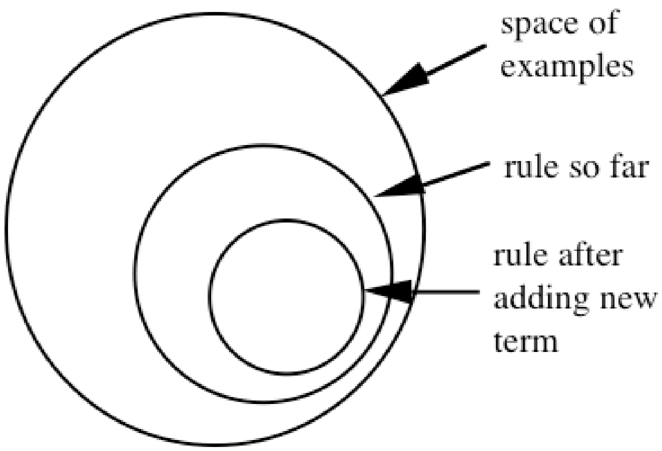
Corresponding decision tree:
(produces exactly the same predictions)

- But rule sets *can* be clearer when decision trees suffer from replicated subtrees
- Also, in multiclass situations, covering algorithm concentrates on one class at a time whereas decision tree learner takes all classes into account



Simple Covering Algorithm

- Generates a rule by adding tests that maximize rule's accuracy
- Similar to situation in decision trees: problem of selecting an attribute to split on
  - But decision tree inducer maximizes overall purity
- Each new test reduces rule's coverage



Selecting a Test

- Goal: Maximize Accuracy
  - t total number of instances covered by rule
  - p positive examples of the class covered by rule
  - $t - p$ number of errors made by rule

  ⇒Select test that maximizes the ratio p/t
- We are finished when $p/t = 1$ or the set of instances can't be split any further

Example: Contact Lens Data

- Rule we seek:

```
If ?
    then recommendation = hard
```

- Possible tests:

Age = Young	2/8
Age = Pre-presbyopic	1/8
Age = Presbyopic	1/8
Spectacle prescription = Myope	3/12
Spectacle prescription = Hypermetrope	1/12
Astigmatism = no	0/12
Astigmatism = yes	4/12
Tear production rate = Reduced	0/12
Tear production rate = Normal	4/12

Modified Rule and Resulting Data

- Rule with best test added:

```
If astigmatism = yes
    then recommendation = hard
```

- Instances covered by modified rule

Age	Spectacle prescription	Astigmatism	Tear production rate	Recommended lenses
Young	Myope	Yes	Reduced	None
Young	Myope	Yes	Normal	Hard
Young	Hypermetrope	Yes	Reduced	None
Young	Hypermetrope	Yes	Normal	hard
Pre-presbyopic	Myope	Yes	Reduced	None
Pre-presbyopic	Myope	Yes	Normal	Hard
Pre-presbyopic	Hypermetrope	Yes	Reduced	None
Pre-presbyopic	Hypermetrope	Yes	Normal	None
Presbyopic	Myope	Yes	Reduced	None
Presbyopic	Myope	Yes	Normal	Hard
Presbyopic	Hypermetrope	Yes	Reduced	None
Presbyopic	Hypermetrope	Yes	Normal	None

Further Refinement

- Current state:

```
If astigmatism = yes
    and ?
  then recommendation = hard
```

- Possible tests:

Age = Young	2/4
Age = Pre-presbyopic	1/4
Age = Presbyopic	1/4
Spectacle prescription = Myope	3/6
Spectacle prescription = Hypermetrope	1/6
Tear production rate = Reduced	0/6
Tear production rate = Normal	4/6

Modified Rule and Resulting Data

- Rule with best test added:

```
If astigmatism = yes
    and tear production rate = normal
then recommendation = hard
```

- Instances covered by modified rule:

Age	Spectacle prescription	Astigmatism	Tear production rate	Recommended lenses
Young	Myope	Yes	Normal	Hard
Young	Hypermetrope	Yes	Normal	hard
Pre-presbyopic	Myope	Yes	Normal	Hard
Pre-presbyopic	Hypermetrope	Yes	Normal	None
Presbyopic	Myope	Yes	Normal	Hard
Presbyopic	Hypermetrope	Yes	Normal	None

Further Refinement

- Current state:

```
If astigmatism = yes
     and tear production rate = normal
     and ?
   then recommendation = hard
```

- Possible tests:

Age = Young	2/2
Age = Pre-presbyopic	1/2
Age = Presbyopic	1/2
Spectacle prescription = Myope	3/3
Spectacle prescription = Hypermetrope	1/3

- Tie between the first and the fourth test
  - We choose the one with greater coverage

The Result

- Final rule:

```
If astigmatism = yes
   and tear production rate = normal
   and spectacle prescription = myope
   then recommendation = hard
```

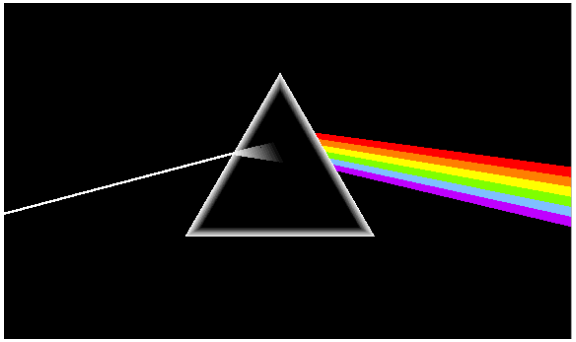
- Second rule for recommending “hard lenses”:
(built from instances not covered by first rule)

```
If age = young and astigmatism = yes
   and tear production rate = normal
   then recommendation = hard
```

- These two rules cover all “hard lenses”:
  - The process is then repeated with other two classes

Pseudo-Code for PRISM

```
For each class C
  Initialize E to the instance set
  While E contains instances in class C
    Create a rule R with an empty left-hand side that predicts class C
    Until R is perfect (or there are no more attributes to use) do
      For each attribute A not mentioned in R, and each value v,
        Consider adding the condition A = v to the left-hand side of R
        Select A and v to maximize the accuracy p/t
          (break ties by choosing the condition with the largest p)
      Add A = v to R
    Remove the instances covered by R from E
```



Rules vs. Decision Lists

- PRISM with outer loop removed generates a decision list for one class
  - Subsequent rules are designed for rules that are not covered by previous rules
  - But: order doesn’t matter because all rules predict the same class
- Outer loop considers all classes separately
  - No order dependence implied
- Problems: overlapping rules, default rule required

Separate and Conquer

- Methods like PRISM (for dealing with one class) are *separate-and-conquer* algorithms:
  - First, identify a useful rule
  - Then, separate out all the instances it covers
  - Finally, "conquer" the remaining instances
- Difference to divide-and-conquer methods:
  - Subset covered by rule doesn't need to be explored any further

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

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

Variations

- Generating rules for classes in order
  - Start with the smallest class
  - Leave the largest class covered by the default rule
- Stopping criterion
  - Stop rule production if accuracy becomes too low
- Rule learner RIPPER:
  - Uses MDL-based stopping criterion
  - Employs post-processing step to modify rules guided by MDL criterion

Using Global Optimization

- RIPPER: *Repeated Incremental Pruning to Produce Error Reduction* (does global optimization in an efficient way)
    - Classes are processed in order of increasing size
    - Initial rule set for each class is generated using IREP
- An MDL-based stopping condition is used
- Once a rule set has been produced for each class, each rule is re-considered and two variants are produced
    - One is an extended version, one is grown from scratch
    - Chooses among three candidates according to *DL*
- Final clean-up step greedily deletes rules to minimize DL

PART

- Avoids global optimization step used in C4.5rules and RIPPER
- Builds a *partial* decision tree to obtain a rule
- Uses C4.5's procedures to build a tree

Notes on PART

- Make leaf with maximum coverage into a rule
- Treat missing values just as C4.5 does
  - i.e. split instance into pieces
- Time taken to generate a rule:
  - Worst case: same as for building a pruned tree
    - Occurs when data is noisy
  - Best case: same as for building a single rule
    - Occurs when data is noise free

Rules with Exceptions

1. Given: a way of generating a single good rule
2. Then it's easy to generate rules with exceptions
3. Select default class for top-level rule
4. Generate a good rule for one of the remaining classes
5. Apply this method recursively to the two subsets produced by the rule (i.e. instances that are covered/not covered)