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Data Mining

Practical Machine Learning Tools and Techniques

Slides for Chapter 6 of *Data Mining* by I. H. Witten, E. Frank and M. A. Hall

Implementation:
Real machine learning schemes

- Decision trees
  - From ID3 to C4.5 (pruning, numeric attributes, ...)
- Classification rules
  - From PRISM to RIPPER and PART (pruning, numeric data, …)
- Association Rules
  - Frequent-pattern trees
- Extending linear models
  - Support vector machines and neural networks
- Instance-based learning
  - Pruning examples, generalized exemplars, distance functions

Implementation:
Real machine learning schemes

- Numeric prediction
  - Regression/model trees, locally weighted regression
- Bayesian networks
  - Learning and prediction, fast data structures for learning
- Clustering: hierarchical, incremental, probabilistic
  - Hierarchical, incremental, probabilistic, Bayesian
- Semisupervised learning
  - Clustering for classification, co-training
- Multi-instance learning
  - Converting to single-instance, upgrading learning algorithms, dedicated multi-instance methods

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

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
…	…	…	…	…

```
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				
Overcast				
Rainy				
Rainy				
Rainy				
…				

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
```

```
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
- 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

- 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 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
- 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

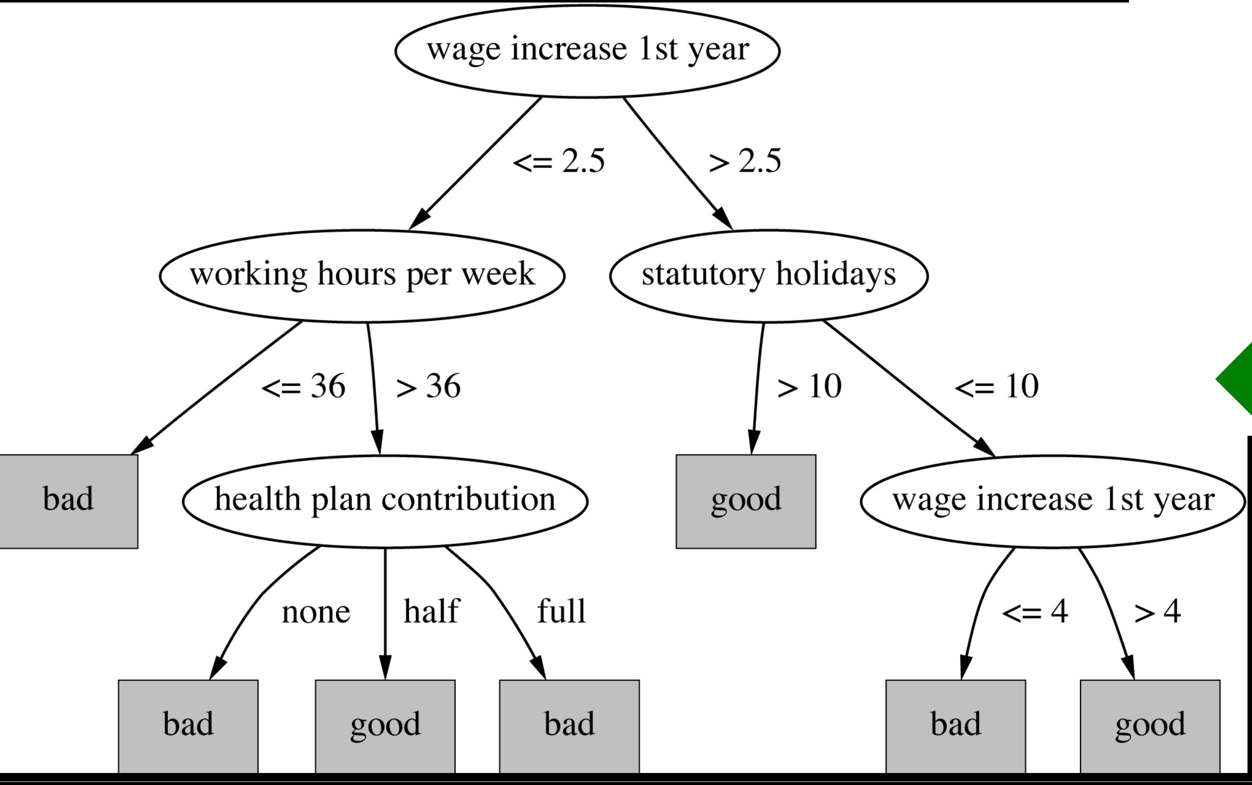
- Pre-pruning may stop the growth process prematurely: *early stopping*
- Classic example: XOR/Parity-problem
  - No *individual* attribute exhibits any significant association to the class
  - Structure is only visible in fully expanded tree
  - Prepruning won't expand the root node
- But: XOR-type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

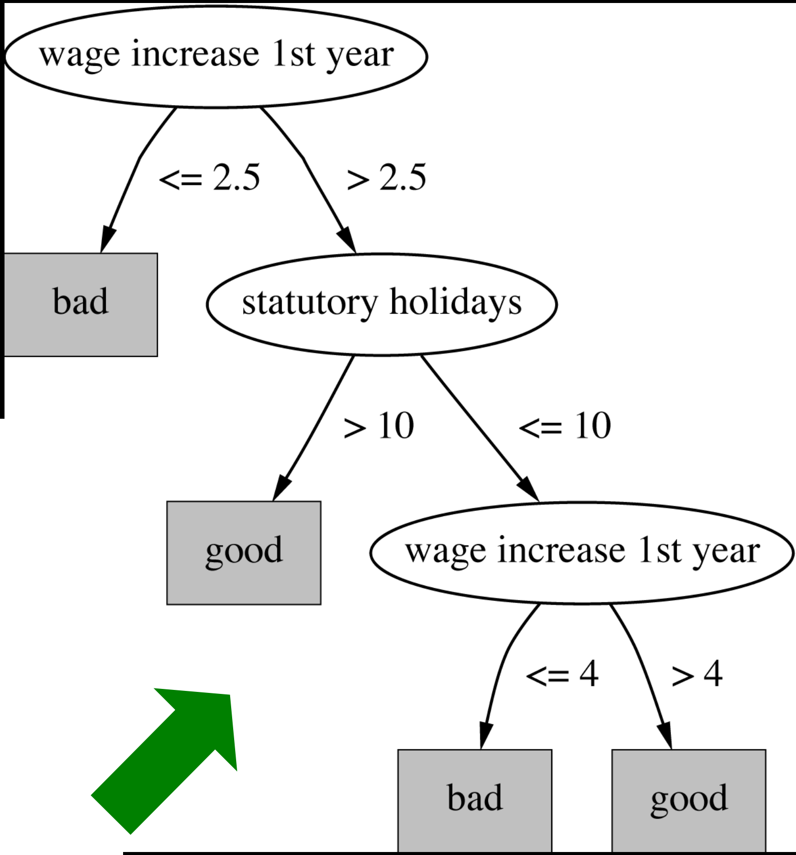
Postpruning

- 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

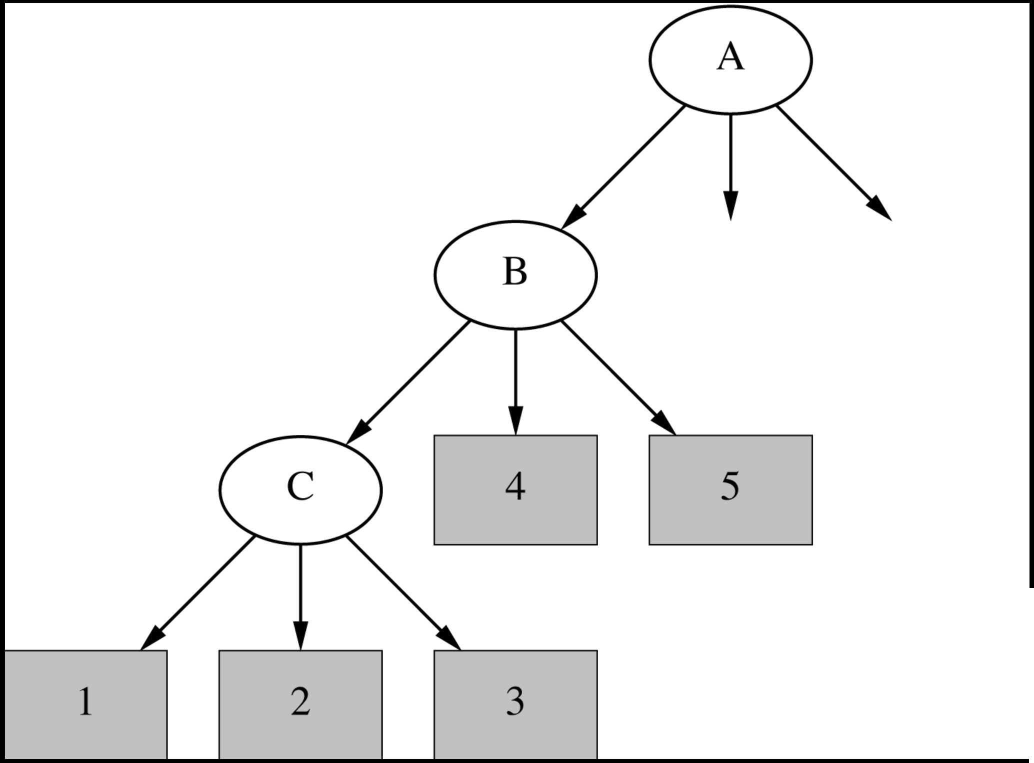
Subtree replacement

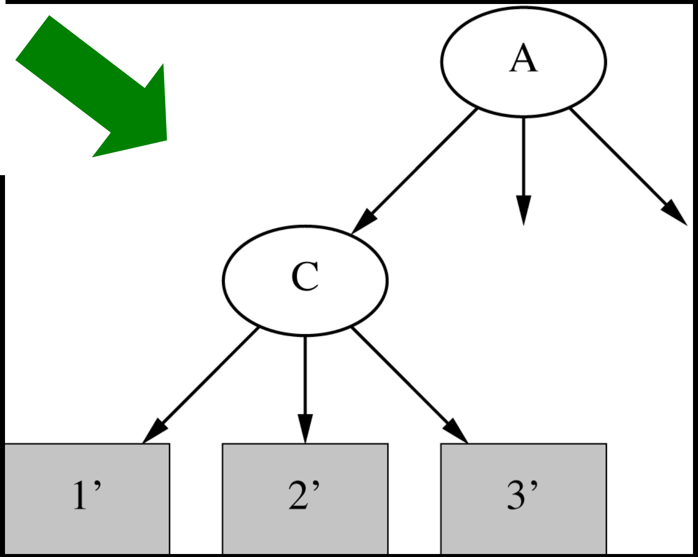
- *Bottom-up*
- Consider replacing a tree only after considering all its subtrees





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)
- 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)

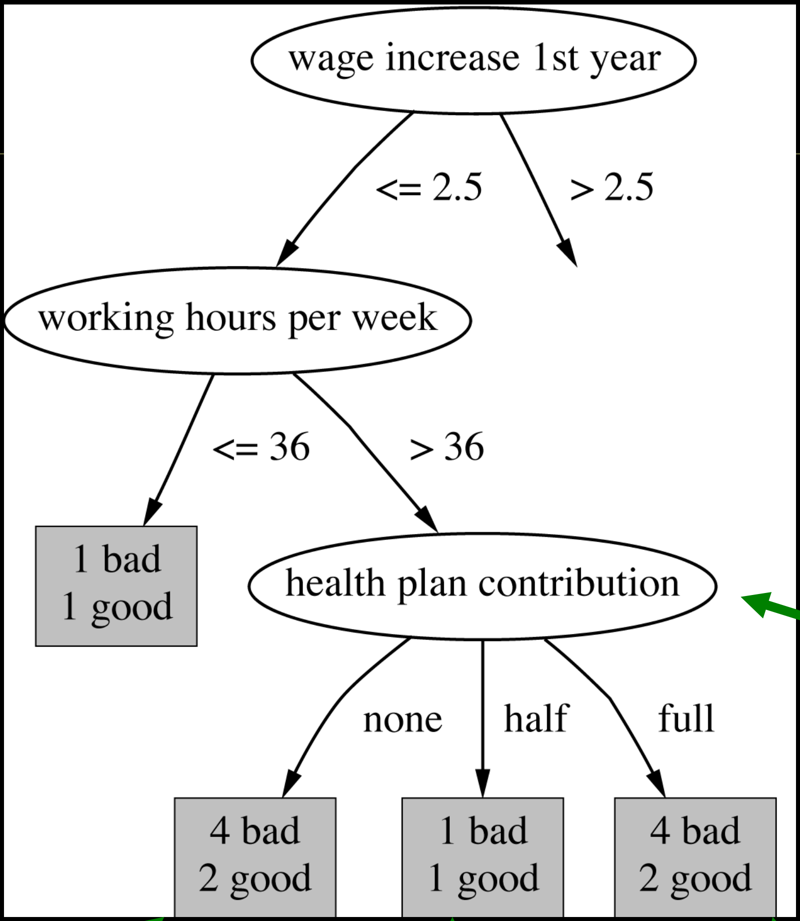
C4.5's method

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

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

- 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



f = 5/14
e = 0.46
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
- 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)

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

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
- Some TDITDT systems can build *multivariate* trees (e.g. CART)

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

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
```

Measures used in IREP

- $[p + (N - n)] / T$
  - (N is total number of negatives)
  - 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

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
  - *DL*: bits needs to send examples wrt set of rules, bits needed to send *k* tests, and bits for *k*
- 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

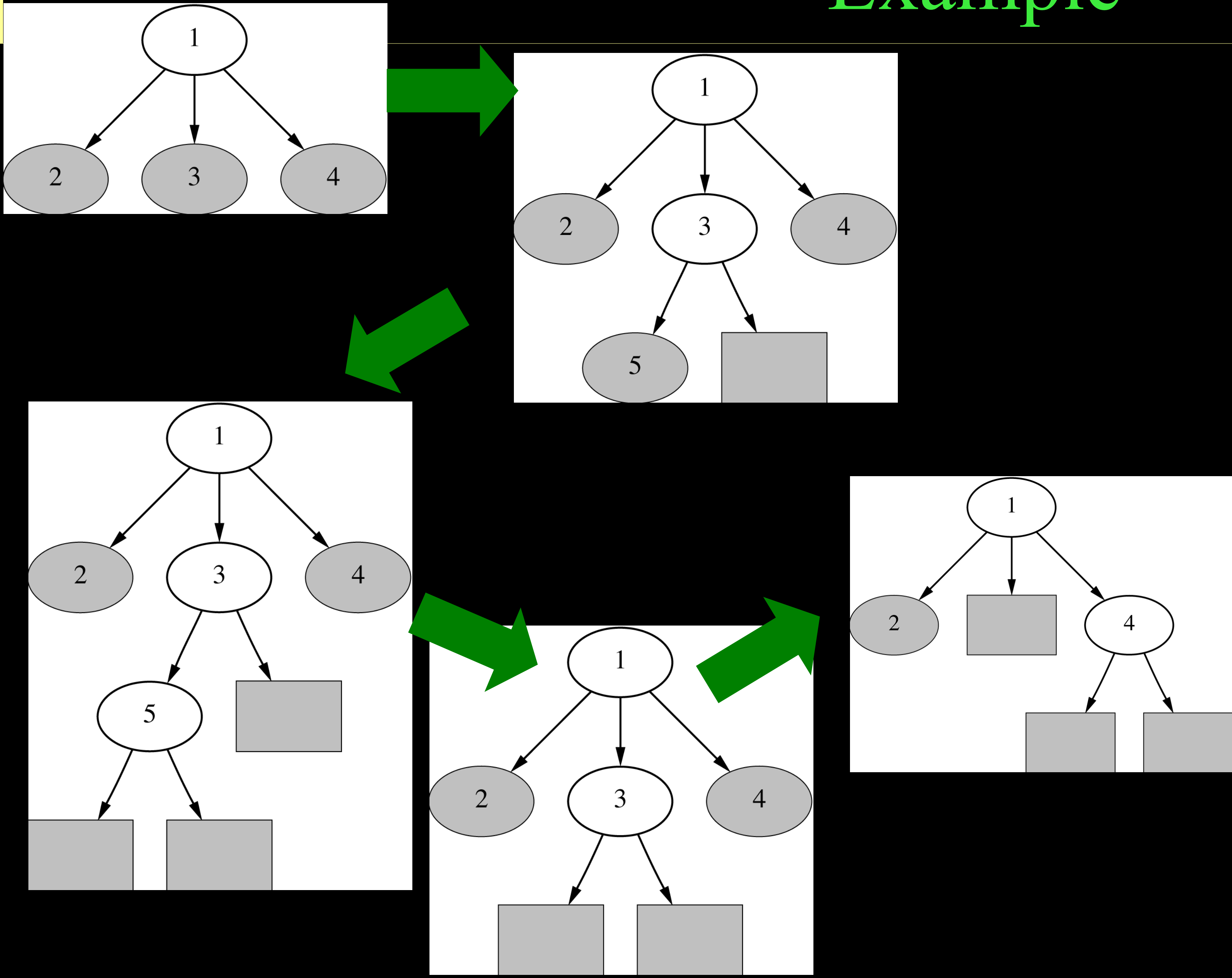
PART

- Avoids global optimization step used in C4.5rules and RIPPER
- Generates an unrestricted decision list using basic separate-and-conquer procedure
- Builds a *partial* decision tree to obtain a rule
  - A rule is only pruned if all its implications are known
  - Prevents *hasty generalization*
- Uses C4.5's procedures to build a tree

Building a partial tree

```
Expand-subset (S):
  Choose test T and use it to split set of examples
    into subsets
  Sort subsets into increasing order of average
    entropy
  while
      there is a subset X not yet been expanded
      AND   all subsets expanded so far are leaves
    expand-subset(X)
  if
      all subsets expanded are leaves
      AND estimated error for subtree
             ≥ estimated error for node
    undo expansion into subsets and make node a leaf
```

Example



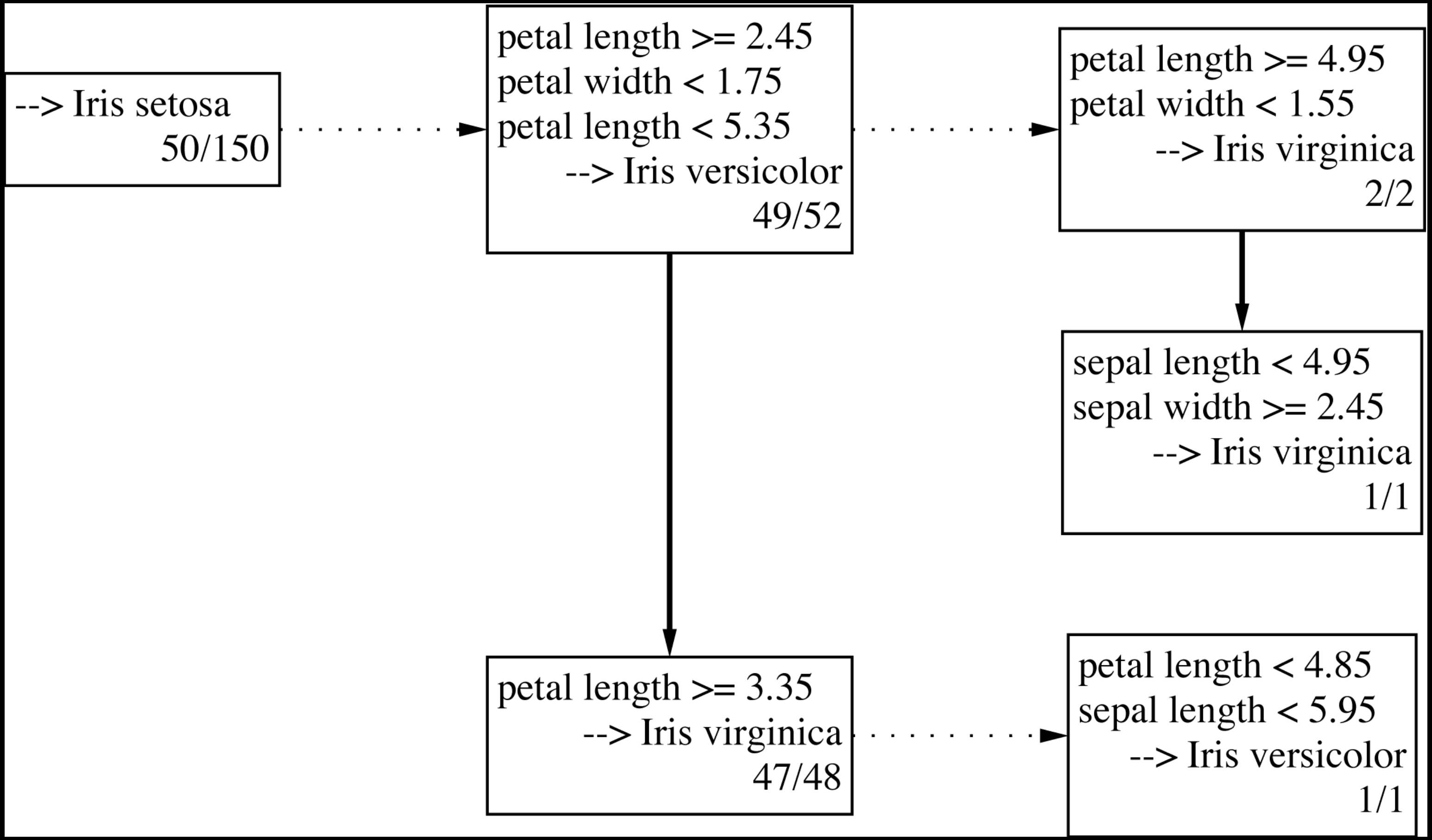
Notes on PART

- 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)

Iris data example



Association rules

- 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 data
  - Combinatorial nature of generation process is costly – particularly if there are many item sets, or item sets are large
- Appropriate data structures can help
- FP-growth 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 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, as found in step 1

   - Individual items that do not meet the minimum support are not inserted into the tree
   - Hopefully 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

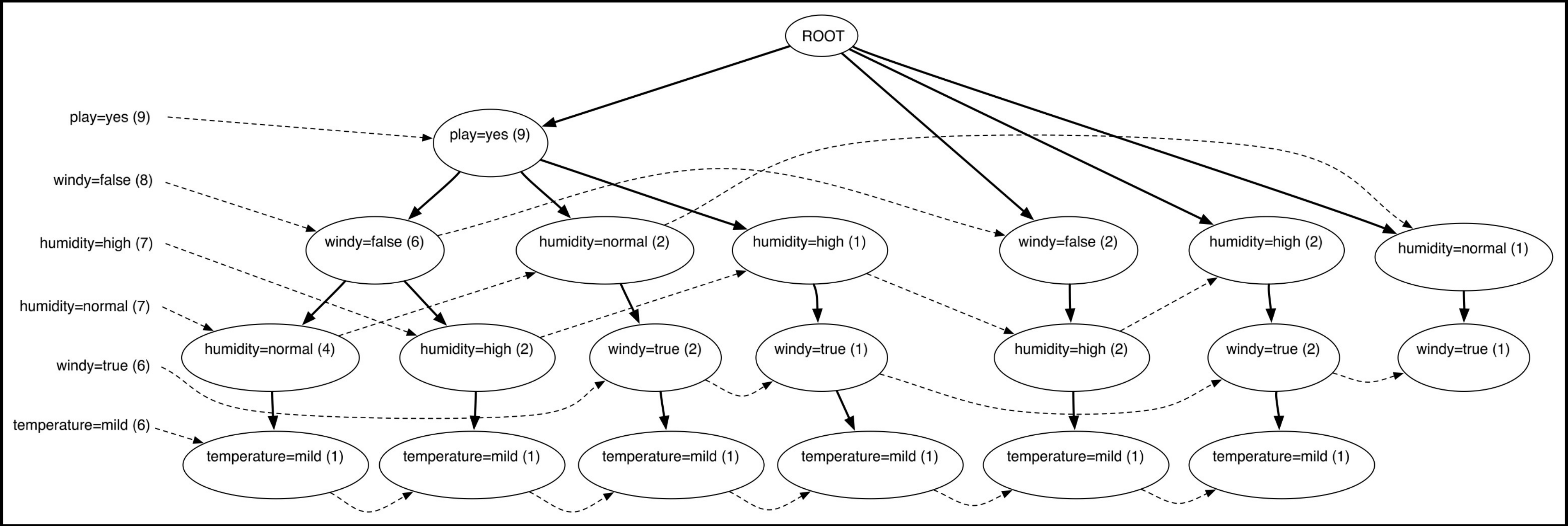
```
1 windy=false, humidity=high, play=no, outlook=sunny, temperature=hot
2 humidity=high, windy=true, play=no, outlook=sunny, temperature=hot
3 play=yes, windy=false, humidity=high, temperature=hot, outlook=overcast
4 play=yes, windy=false, humidity=high, temperature=mild, outlook=rainy
.
.
.
14 humidity=high,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

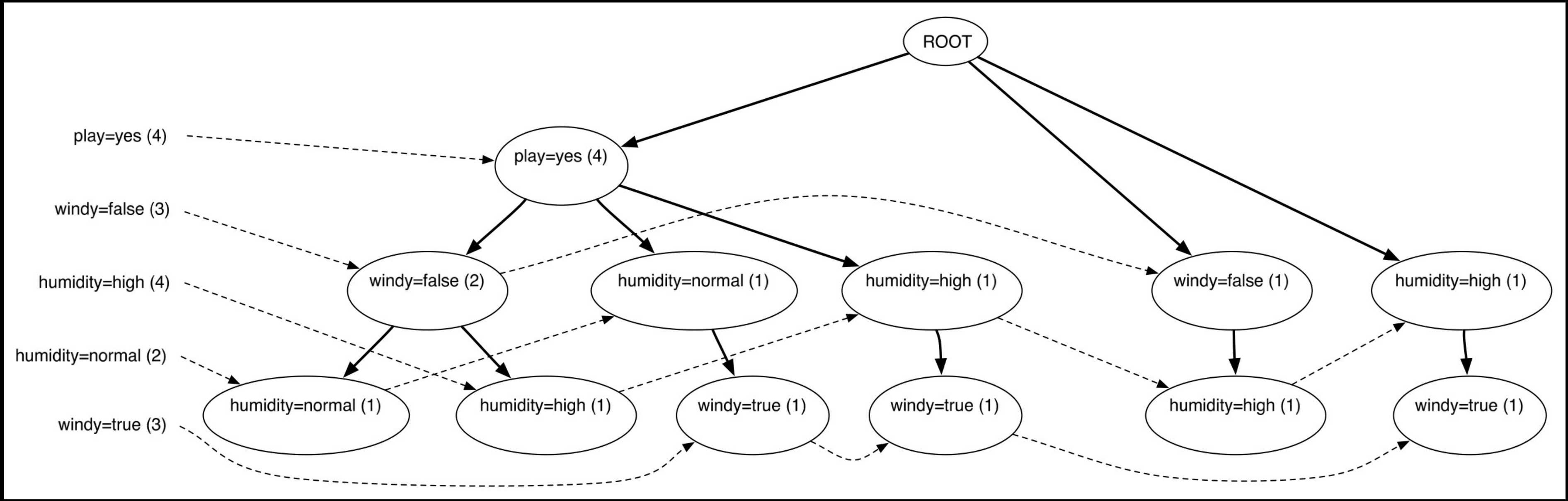
- FP-tree for the weather data (min support 6)



- Process header table from bottom
  - Add *temperature=mild* to the list of large item sets
  - Are there any item sets containing temperature=mild that meet min support?

Finding large item sets cont.

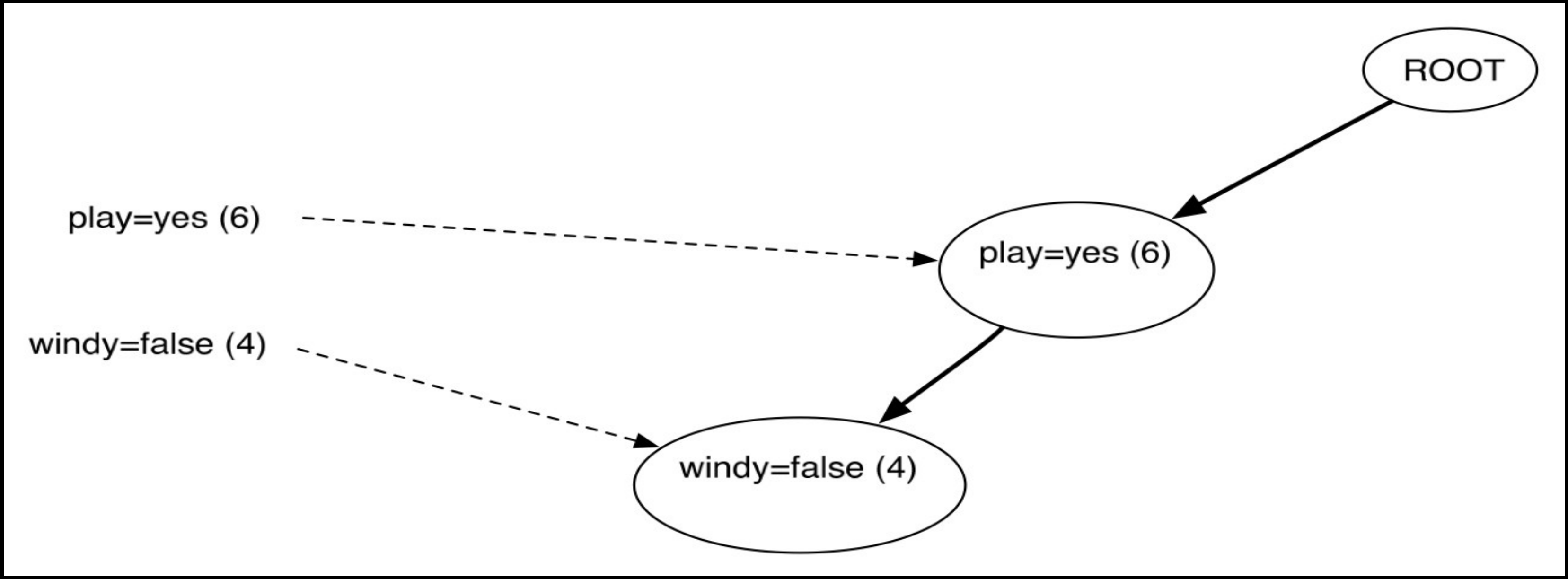
- FP-tree for the data conditioned on *temperature=mild*



- 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* can't 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

Extending linear classification

- Linear classifiers can’t model nonlinear class boundaries
- Simple trick:
  - Map attributes into new space consisting of combinations of attribute values
  - E.g.: all products of *n* factors that can be constructed from the attributes
- Example with two attributes and $n = 3$:

$$x = w_1 a_1^3 + w_2 a_1^2 a_2 + w_3 a_1 a_2^2 + w_4 a_2^3$$

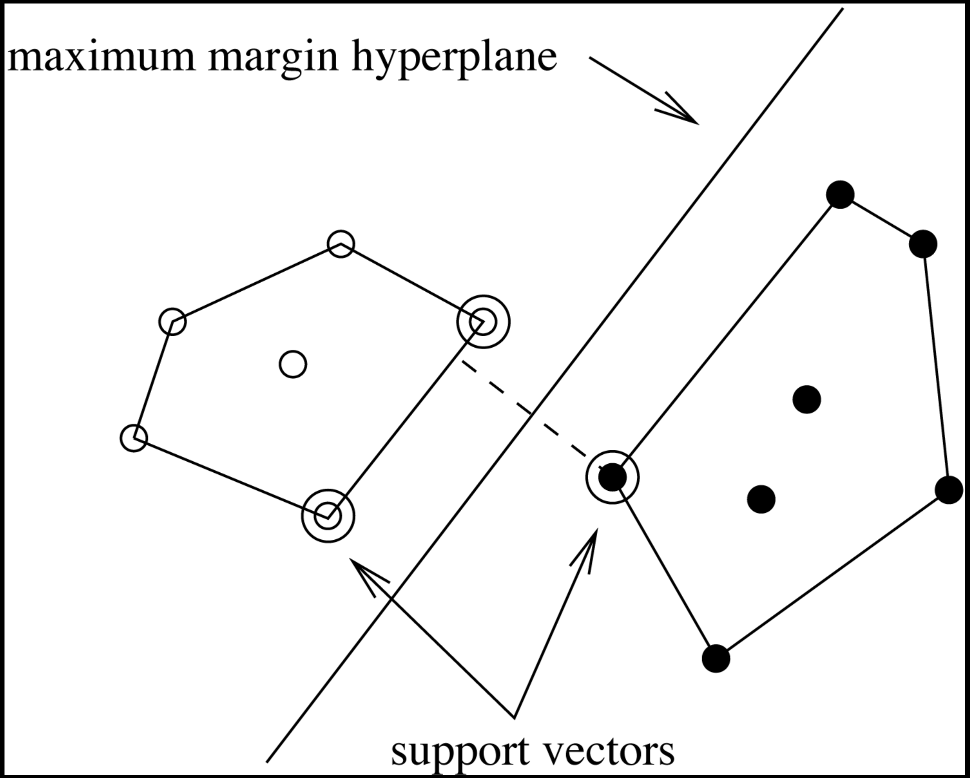
Problems with this approach

- 1st problem: speed
  - 10 attributes, and $n = 5 \Rightarrow$ >2000 coefficients
  - Use linear regression with attribute selection
  - Run time is cubic in number of attributes
- 2nd problem: overfitting
  - Number of coefficients is large relative to the number of training instances
  - *Curse of dimensionality* kicks in

Support vector machines

- *Support vector machines* are algorithms for learning linear classifiers
- Resilient to overfitting because they learn a particular linear decision boundary:
  - The *maximum margin hyperplane*
- Fast in the nonlinear case
  - Use a mathematical trick to avoid creating "pseudo-attributes"
  - The nonlinear space is created implicitly

The maximum margin hyperplane



- The instances closest to the maximum margin hyperplane are called *support vectors*

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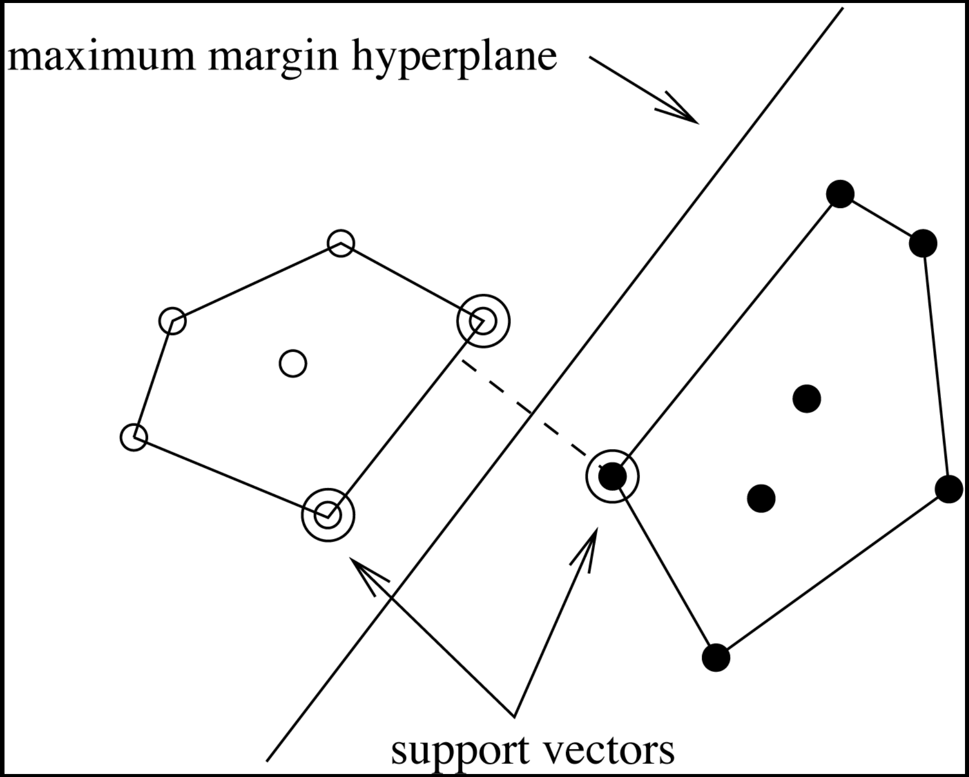
Support vectors

- The support vectors define the maximum margin hyperplane
  - **All other instances can be deleted without changing its position and orientation**



- This means the hyperplane can be written as

$$x = w_0 + w_1 a_1 + w_2 a_2$$
$$x = b + \sum_{\text{i is supp. vector}} \alpha_i y_i \vec{a}(i) \cdot \vec{a}$$

Finding support vectors

$$x = b + \sum_{\text{i is supp. vector}} \alpha_i y_i \vec{a}(i) \cdot \vec{a}$$

- Support vector: training instance for which $\alpha_i > 0$
- Determine α_i and b ?—
  A *constrained quadratic optimization* problem
  - Off-the-shelf tools for solving these problems
  - However, special-purpose algorithms are faster
  - Example: Platt's *sequential minimal optimization* algorithm (implemented in WEKA)
- Note: all this assumes separable data!

Nonlinear SVMs

- "Pseudo attributes" represent attribute combinations
- Overfitting not a problem because the maximum margin hyperplane is stable
    - There are usually few support vectors relative to the size of the training set
- Computation time still an issue
    - Each time the dot product is computed, all the "pseudo attributes" must be included

A mathematical trick

- Avoid computing the “pseudo attributes”
- Compute the dot product before doing the nonlinear mapping
- Example:

$$x = b + \sum_{\text{i is supp. vector}} \alpha_i y_i (\vec{a}(i) \cdot \vec{a})^n$$

- Corresponds to a map into the instance space spanned by all products of *n* attributes

Other kernel functions

- Mapping is called a "kernel function"
- Polynomial kernel

$$x = b + \sum_{\text{i is supp. vector}} \alpha_i y_i (\vec{a}(i) \cdot \vec{a})^n$$

- We can use others:

$$x = b + \sum_{\text{i is supp. vector}} \alpha_i y_i K(\vec{a}(i) \cdot \vec{a})$$

- Only requirement:

$$K(\vec{x}_i, \vec{x}_j) = \phi(\vec{x}_i) \cdot \phi(\vec{x}_j)$$

- Examples:

$$K(\vec{x}_i, \vec{x}_j) = (\vec{x}_i \cdot \vec{x}_j + 1)^d$$

$$K(\vec{x}_i, \vec{x}_j) = \exp\left(\frac{-(\vec{x}_i - \vec{x}_j)^2}{2\sigma^2}\right)$$

$$K(\vec{x}_i, \vec{x}_j) = \tanh(\beta \vec{x}_i \cdot \vec{x}_j + b) \quad *$$

Noise

- Have assumed that the data is separable (in original or transformed space)
- Can apply SVMs to noisy data by introducing a "noise" parameter *C*
- *C* bounds the influence of any one training instance on the decision boundary
  - Corresponding constraint: $0 \le \alpha_i \le C$
- Still a quadratic optimization problem
- Have to determine *C* by experimentation

Sparse data

- SVM algorithms speed up dramatically if the data is *sparse* (i.e. many values are 0)
- Why? Because they compute lots and lots of dot products
- Sparse data $\Rightarrow$
  compute dot products very efficiently
  - Iterate only over non-zero values
- SVMs can process sparse datasets with 10,000s of attributes

Applications

- Machine vision: e.g face identification
  - Outperforms alternative approaches (1.5% error)
- Handwritten digit recognition: USPS data
  - Comparable to best alternative (0.8% error)
- Bioinformatics: e.g. prediction of protein secondary structure
- Text classifiation
- Can modify SVM technique for numeric prediction problems

Support vector regression

- Maximum margin hyperplane only applies to classification
- However, idea of support vectors and kernel functions can be used for regression
- Basic method same as in linear regression: want to minimize error
    - Difference A: ignore errors smaller than ε and use absolute error instead of squared error
    - Difference B: simultaneously aim to maximize flatness of function
- User-specified parameter ε defines "tube"

More on SVM regression

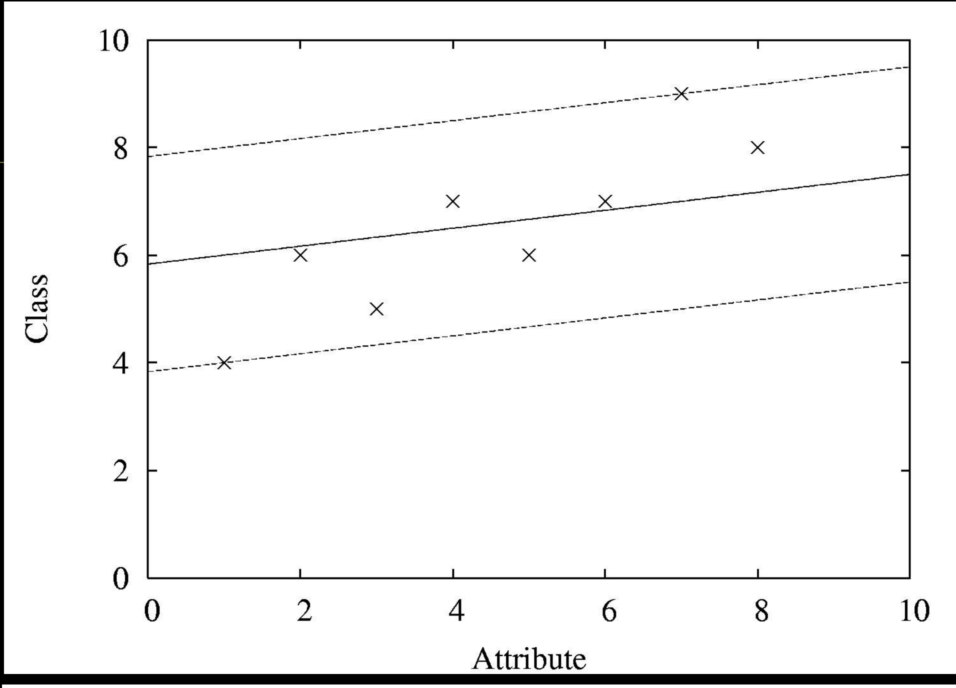
- If there are tubes that enclose all the training points, the flattest of them is used
  - Eg.: mean is used if $2\varepsilon >$ range of target values
- Model can be written as:

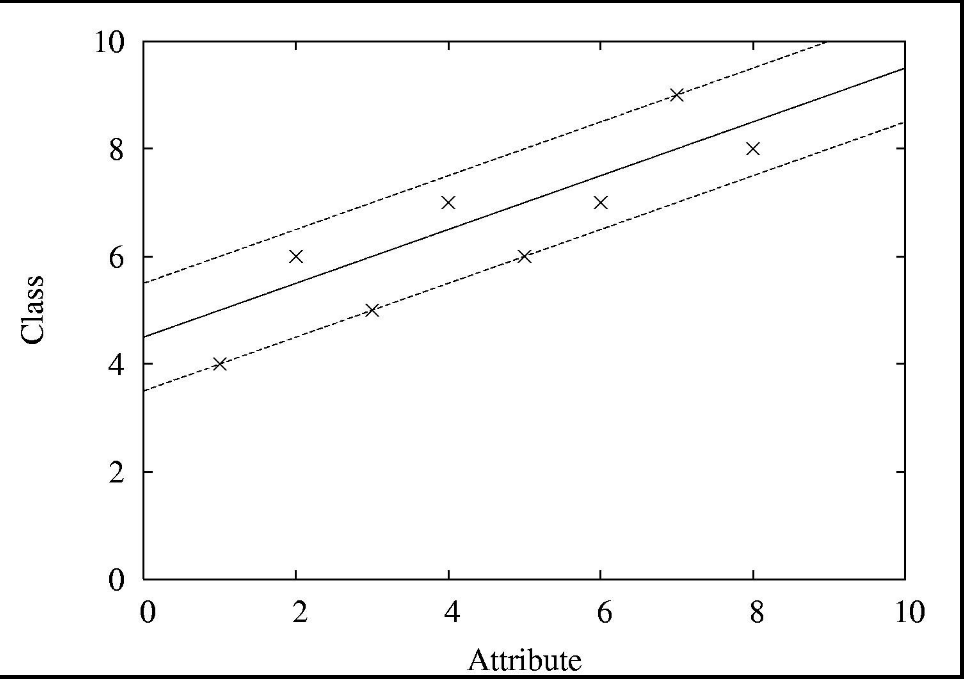
$$x = b + \sum_{\text{i is supp. vector}} \alpha_i \vec{a}(i) \cdot \vec{a}$$

  - Support vectors: points on or outside tube
  - Dot product can be replaced by kernel function
  - Note: coefficients α_i may be negative
- No tube that encloses all training points?
  - Requires trade-off between error and flatness
  - Controlled by upper limit *C* on absolute value of coefficients α_i

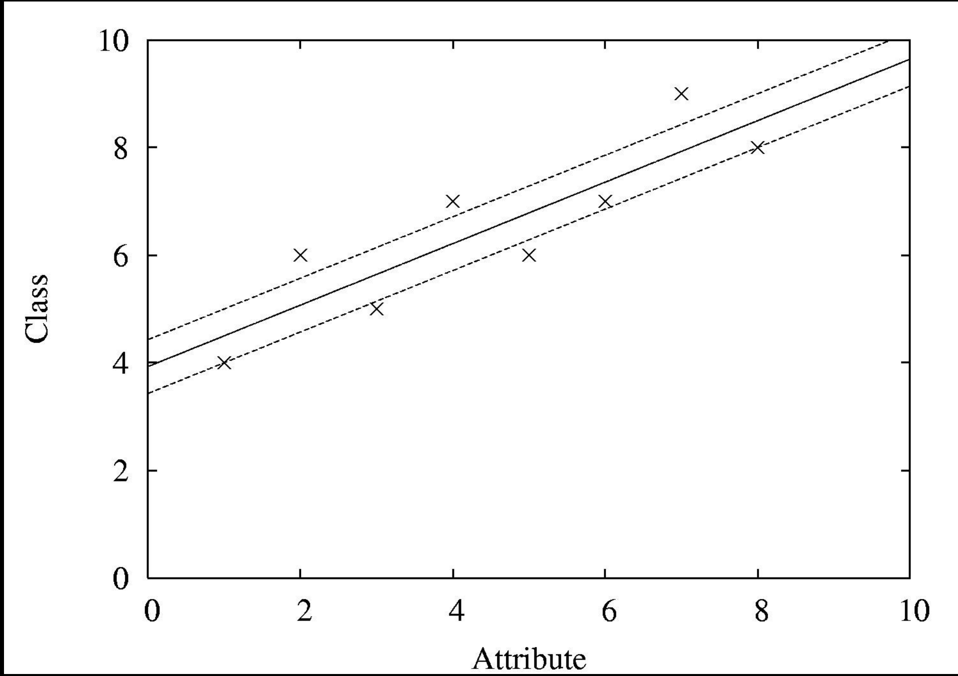
Examples

ε = 2





ε = 1



ε = 0.5

Kernel Ridge Regression

- For classic linear regression using squared loss, only simple matrix operations are need to find the model
  - Not the case for support vector regression with user-specified loss ε
- Combine the power of the kernel trick with simplicity of standard least-squares regression?
  - Yes! *Kernel ridge regression*

Kernel Ridge Regression

- Like SVM, predicted class value for a test instance a is expressed as a weighted sum over the dot product of the test instance with training instances
- Unlike SVM, **all** training instances participate – not just support vectors
  - No sparseness in solution (no support vectors)
- Does not ignore errors smaller than ε
- Uses squared error instead of absolute error

Kernel Ridge Regression

- More computationally expensive than standard linear regresion when #instances > #attributes
  - Standard regression – invert an $m \times m$ matrix ($O(m^3)$), m = #attributes
  - Kernel ridge regression – invert an $n \times n$ matrix ($O(n^3)$), n = #instances
- Has an advantage if
  - A non-linear fit is desired
  - There are more attributes than training instances

The kernel perceptron

- Can use "kernel trick" to make non-linear classifier using perceptron rule
- Observation: weight vector is modified by adding or subtracting training instances
- Can represent weight vector using all instances that have been misclassified:
    - Can use $\sum_i \sum_j y(j) a'(j)_i a_i$
      instead of $\sum_i w_i a_i$
      (where *y* is either -1 or +1)
- Now swap summation signs: $\sum_j y(j) \sum_i a'(j)_i a_i$
    - Can be expressed as: $\sum_j y(j) \vec{a}'(j) \cdot \vec{a}$
- Can replace dot product by kernel: $\sum_j y(j) K(\vec{a}'(j), \vec{a})$

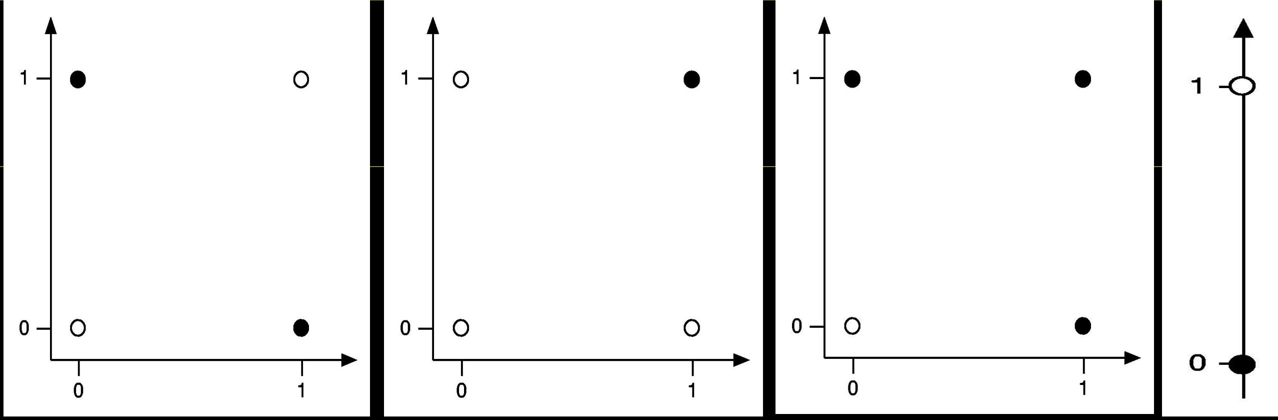
Comments on kernel perceptron

- Finds separating hyperplane in space created by kernel function (if it exists)
  - But: doesn't find maximum-margin hyperplane
- Easy to implement, supports incremental learning
- Linear and logistic regression can also be upgraded using the kernel trick
  - But: solution is not “sparse”: every training instance contributes to solution
- Perceptron can be made more stable by using all weight vectors encountered during learning, not just last one (*voted perceptron*)
  - Weight vectors vote on prediction (vote based on number of successful classifications since inception)

Multilayer perceptrons

- Using kernels is only one way to build nonlinear classifier based on perceptrons
- Can create network of perceptrons to approximate arbitrary target concepts
- *Multilayer perceptron* is an example of an artificial neural network
    - Consists of: input layer, hidden layer(s), and output layer
- Structure of MLP is usually found by experimentation
- Parameters can be found using *backpropagation*

Examples


1
0
0
1
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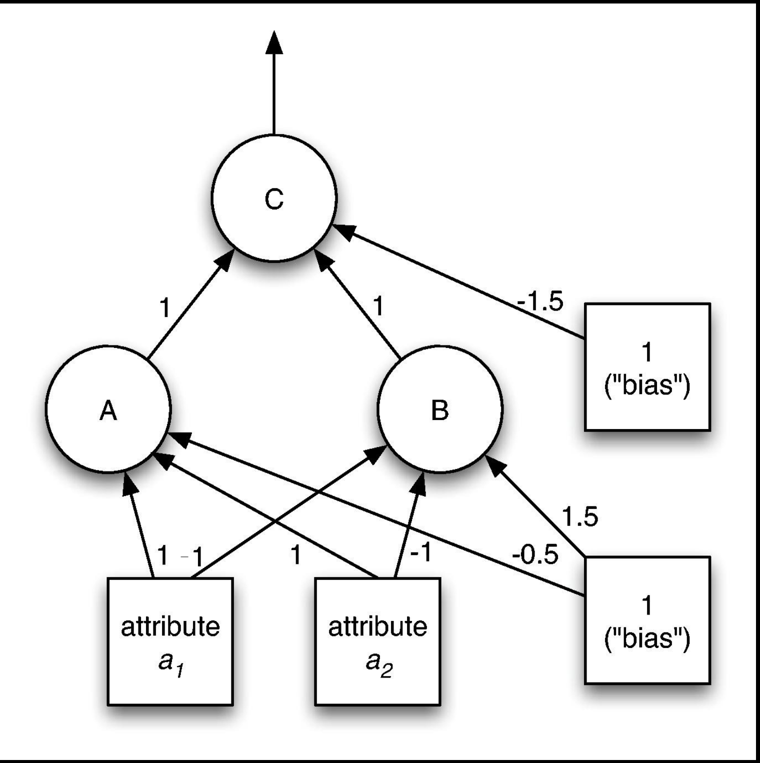
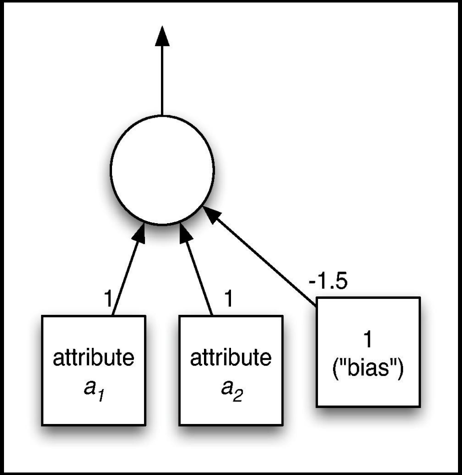
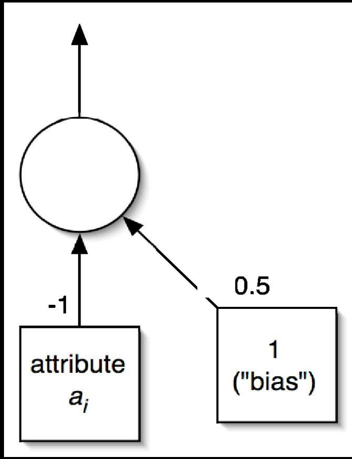
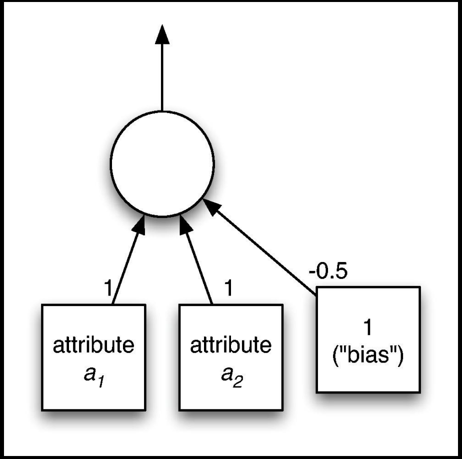
0
1
1
0
0
1
1
0


C
A
B
1
1
-1.5
1 -1
1
-1
1.5
-0.5
1
("bias")
attribute
a_1
attribute
a_2
1
("bias")


1
1
-1.5
attribute
a_1
attribute
a_2
1
("bias")


-1
0.5
attribute
a_i
1
("bias")


1
1
-0.5
attribute
a_1
attribute
a_2
1
("bias")

Backpropagation

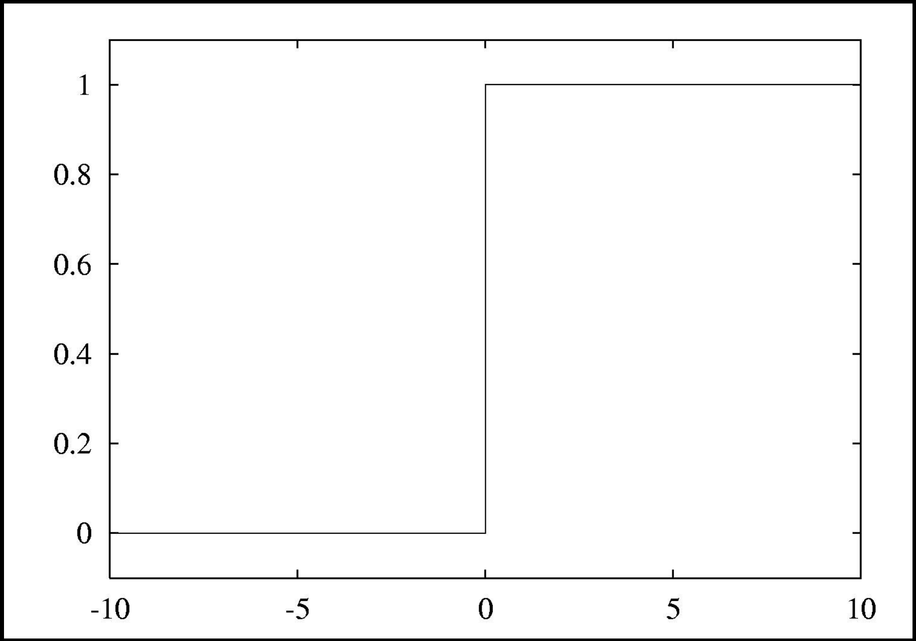
- How to learn weights given network structure?
  - Cannot simply use perceptron learning rule because we have hidden layer(s)
  - Function we are trying to minimize: error
  - Can use a general function minimization technique called *gradient descent*
    - Need differentiable *activation function*: use *sigmoid function* instead of threshold function

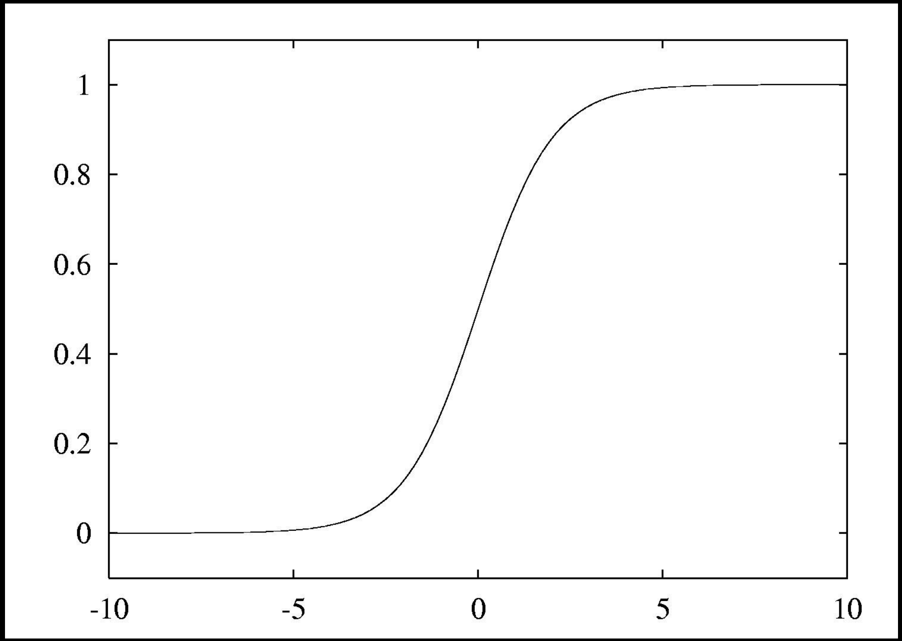
$$f(x)=\frac{1}{1+\exp(-x)}$$

    - Need differentiable error function: can't use zero-one loss, but can use squared error

$$E=\frac{1}{2}(y-f(x))^2$$

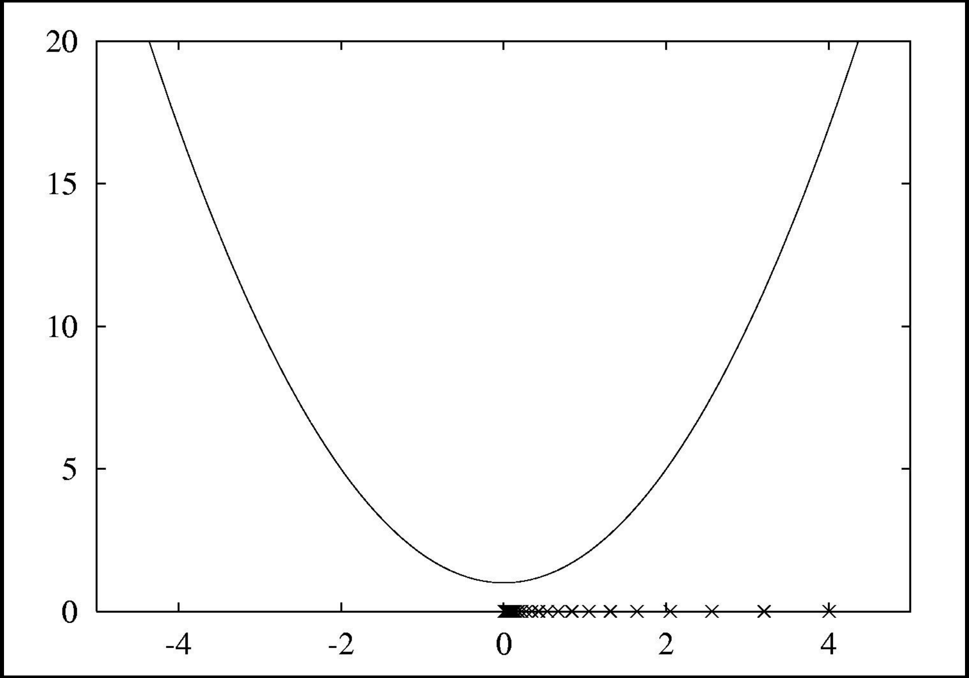
The two activation functions





Gradient descent example

- Function: x^2+1
- Derivative: $2x$
- Learning rate: 0.1
- Start value: 4



Can only find a local minimum!

Minimizing the error I

- Need to find partial derivative of error function for each parameter (i.e. weight)

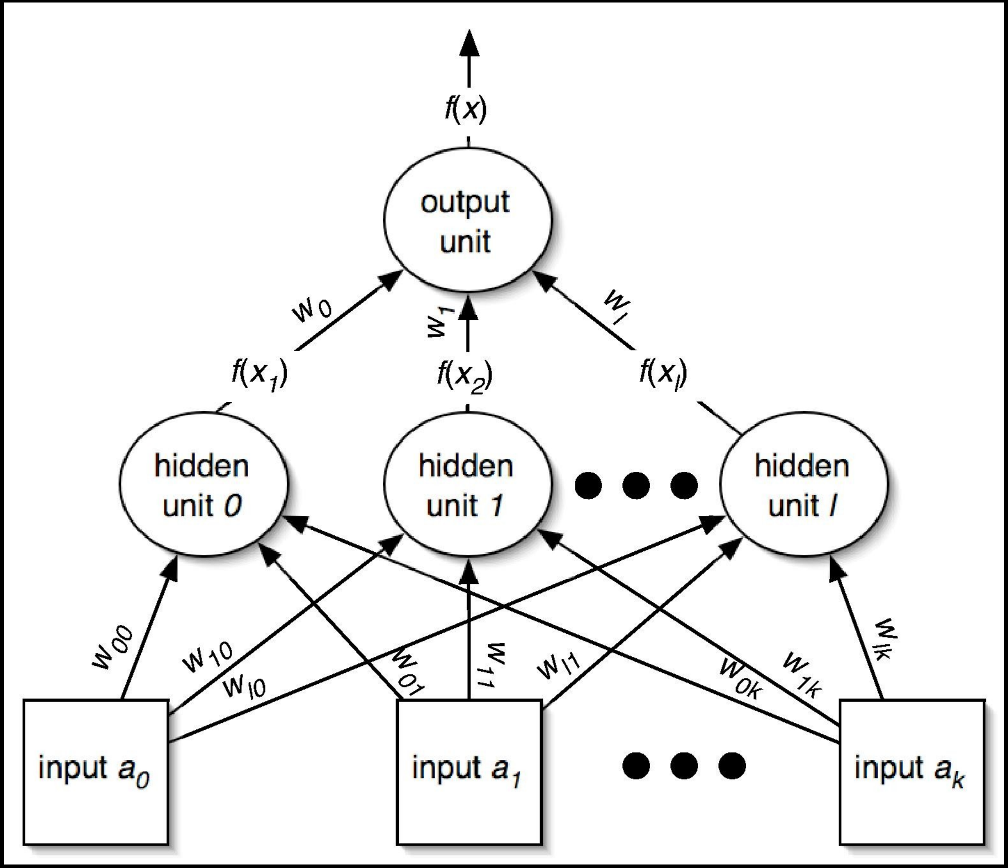
$$\frac{dE}{dw_i} = (y - f(x))\frac{df(x)}{dw_i}$$

$$\frac{df(x)}{dx} = f(x)(1 - f(x))$$

$$x = \sum_i w_i f(x_i)$$

$$\frac{df(x)}{dw_i} = f'(x) f(x_i)$$

$$\frac{dE}{dw_i} = (y - f(x)) f'(x) f(x_i)$$



Minimizing the error II

- What about the weights for the connections from the input to the hidden layer?

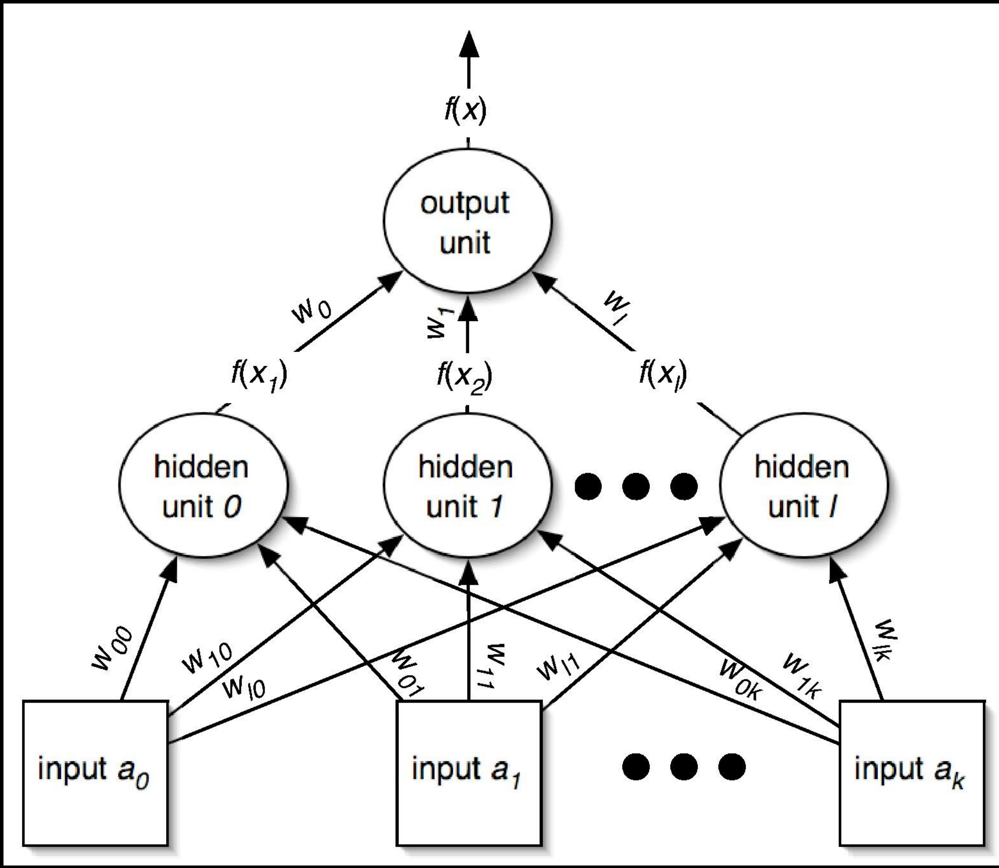
$$\frac{dE}{dw_{ij}} = \frac{dE}{dx}\frac{dx}{dw_{ij}} = (y - f(x))f'(x)\frac{dx}{dw_{ij}}$$

$$x = \sum_i w_i f(x_i)$$

$$\frac{dx}{dw_{ij}} = w_i \frac{df(x_i)}{dw_{ij}}$$

$$\frac{df(x_i)}{dw_{ij}} = f'(x_i)\frac{dx_i}{dw_{ij}} = f'(x_i)a_i$$

$$\frac{dE}{dw_{ij}} = (y - f(x))f'(x)w_i f'(x_i)a_i$$



Remarks

- Same process works for multiple hidden layers and multiple output units (eg. for multiple classes)
- Can update weights after all training instances have been processed or incrementally:
    - *batch learning* vs. *stochastic backpropagation*
    - Weights are initialized to small random values
- How to avoid overfitting?
    - *Early stopping*: use validation set to check when to stop
    - *Weight decay*: add penalty term to error function
- How to speed up learning?
    - *Momentum*: re-use proportion of old weight change
    - Use optimization method that employs 2nd derivative

Radial basis function networks

- Another type of *feedforward network* with two layers (plus the input layer)
- Hidden units represent points in instance space and activation depends on distance
  - To this end, distance is converted into similarity: Gaussian activation function
    - Width may be different for each hidden unit
  - Points of equal activation form hypersphere (or hyperellipsoid) as opposed to hyperplane
- Output layer same as in MLP

Learning RBF networks

- Parameters: centers and widths of the RBFs + weights in output layer
- Can learn two sets of parameters independently and still get accurate models
  - Eg.: clusters from *k*-means can be used to form basis functions
  - Linear model can be used based on fixed RBFs
  - Makes learning RBFs very efficient
- Disadvantage: no built-in attribute weighting based on relevance
- RBF networks are related to RBF SVMs

Stochastic gradient descent

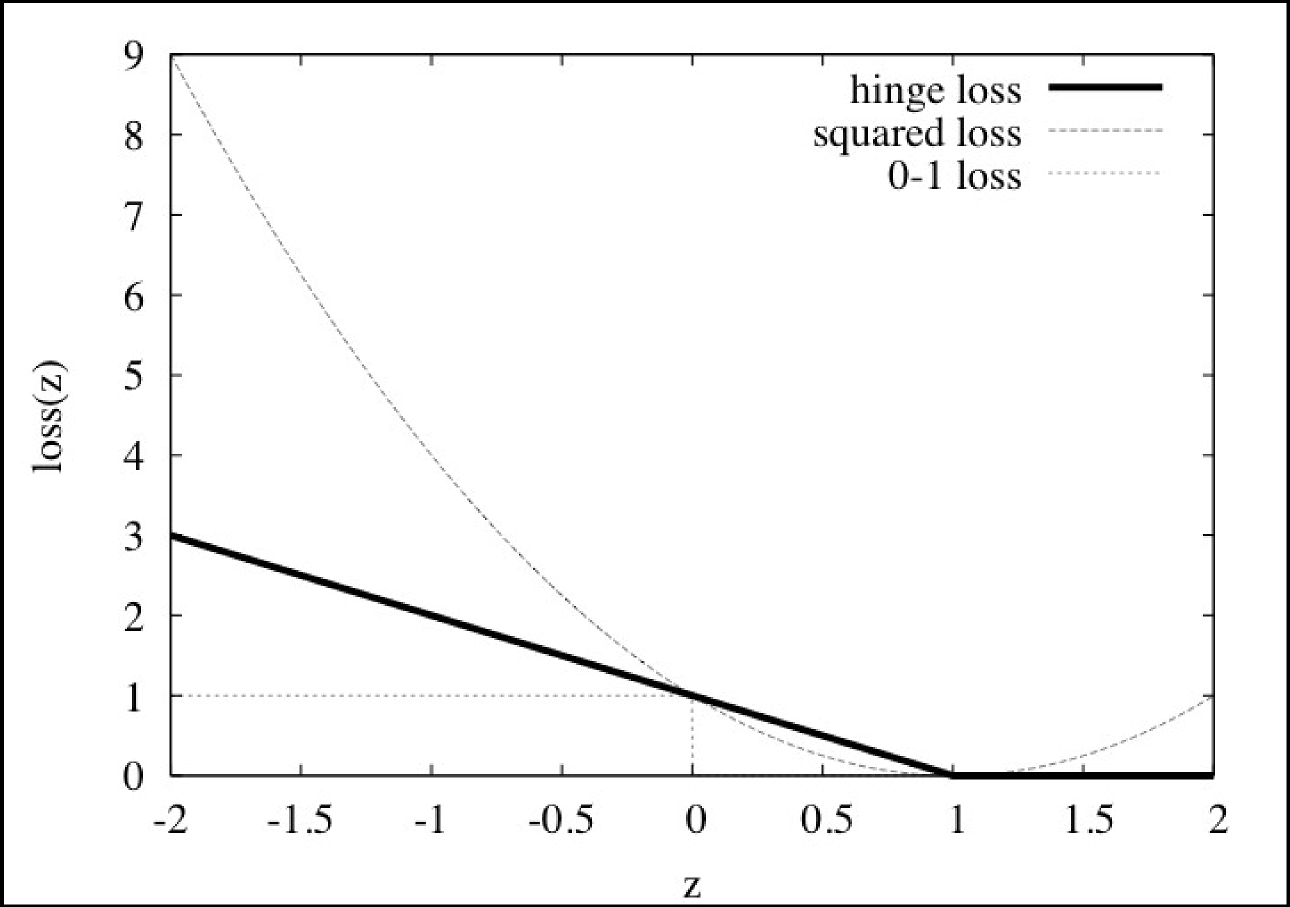
- Have seen gradient descent + stochastic backpropagation for learning weights in a neural network
- Gradient descent is a general-purpose optimization technique
    - Can be applied whenever the objective function is *differentiable*
    - Actually, can be used even when the objective function is not completely differentiable!
        - Subgradients
- One application: learn linear models – e.g. linear SVMs or logistic regression

Stochastic gradient descent cont.

- Learning linear models using gradient descent is easier than optimizing non-linear NN
  - Objective function has global minimum rather than many local minima
- Stochastic gradient descent is fast, uses little memory and is suitable for incremental online learning

Stochastic gradient descent cont.

- For SVMs, the error function (to be minimized) is called the *hinge loss*



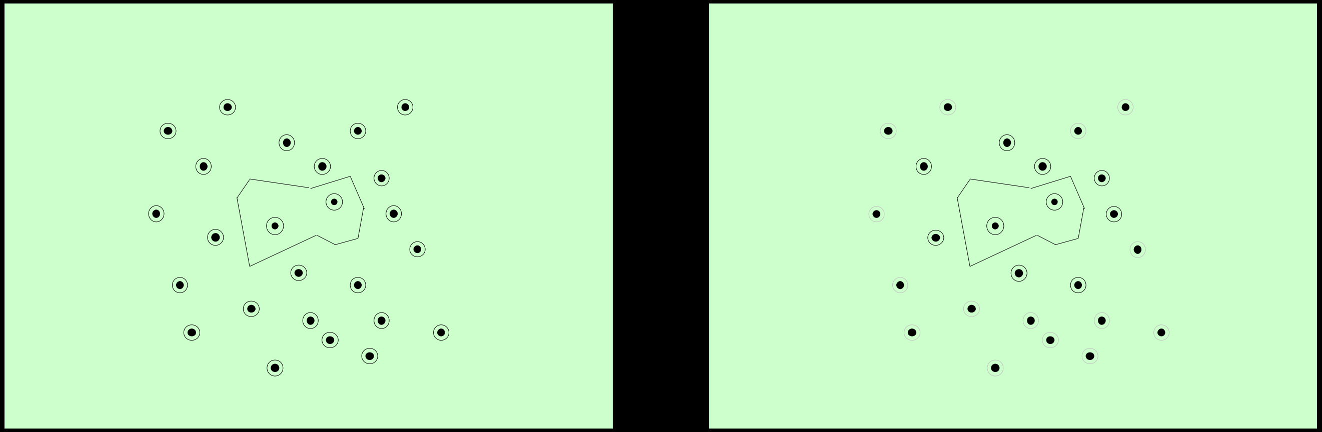
Stochastic gradient descent cont.

- In the linearly separable case, the hinge loss is 0 for a function that successfully separates the data
  - The *maximum margin* hyperplane is given by the **smallest** weight vector that achieves 0 hinge loss
- Hinge loss is not differentiable at $z = 1$; cant compute gradient!
  - *Subgradient* – something that resembles a gradient
  - Use 0 at $z = 1$
  - In fact, loss is 0 for $z \geq 1$, so can focus on $z < 1$ and proceed as usual

Instance-based learning

- Practical problems of 1-NN scheme:
  - Slow (but: fast tree-based approaches exist)
    - Remedy: remove irrelevant data
  - Noise (but: *k* -NN copes quite well with noise)
    - Remedy: remove noisy instances
  - All attributes deemed equally important
    - Remedy: weight attributes (or simply select)
  - Doesn’t perform explicit generalization
    - Remedy: rule-based NN approach

Learning prototypes



- Only those instances involved in a decision need to be stored
- Noisy instances should be filtered out
- Idea: only use *prototypical* examples

Speed up, combat noise

- IB2: save memory, speed up classification
  - Work incrementally
  - Only incorporate misclassified instances
  - Problem: noisy data gets incorporated
- IB3: deal with noise
  - Discard instances that don't perform well
  - Compute confidence intervals for
    - 1. Each instance's success rate
    - 2. Default accuracy of its class
  - Accept/reject instances
    - Accept if lower limit of 1 exceeds upper limit of 2
    - Reject if upper limit of 1 is below lower limit of 2

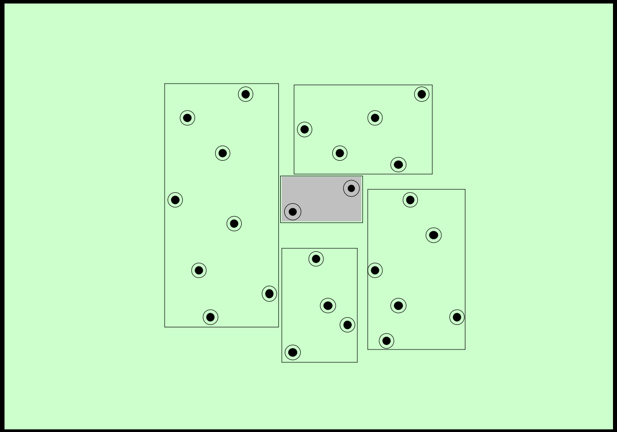
Weight attributes

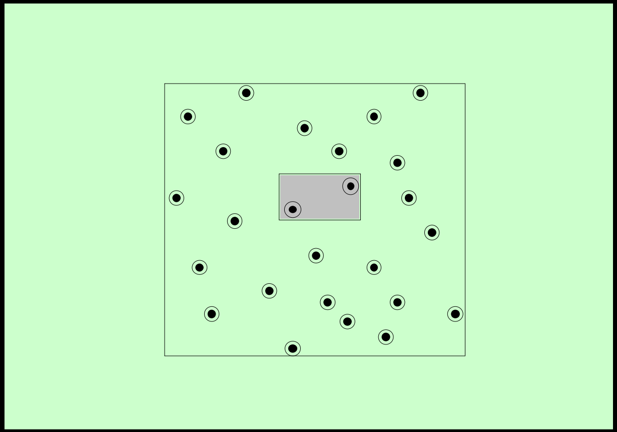
- IB4: weight each attribute
  (weights can be class-specific)
- Weighted Euclidean distance:

$$\sqrt{(w_1^2(x_1-y_1)^2+\ldots+w_n^2(x_n-y_n)^2)}$$

- Update weights based on nearest neighbor
  - Class correct: increase weight
  - Class incorrect: decrease weight
  - Amount of change for *i* th attribute depends on $|x_i - y_i|$

Rectangular generalizations



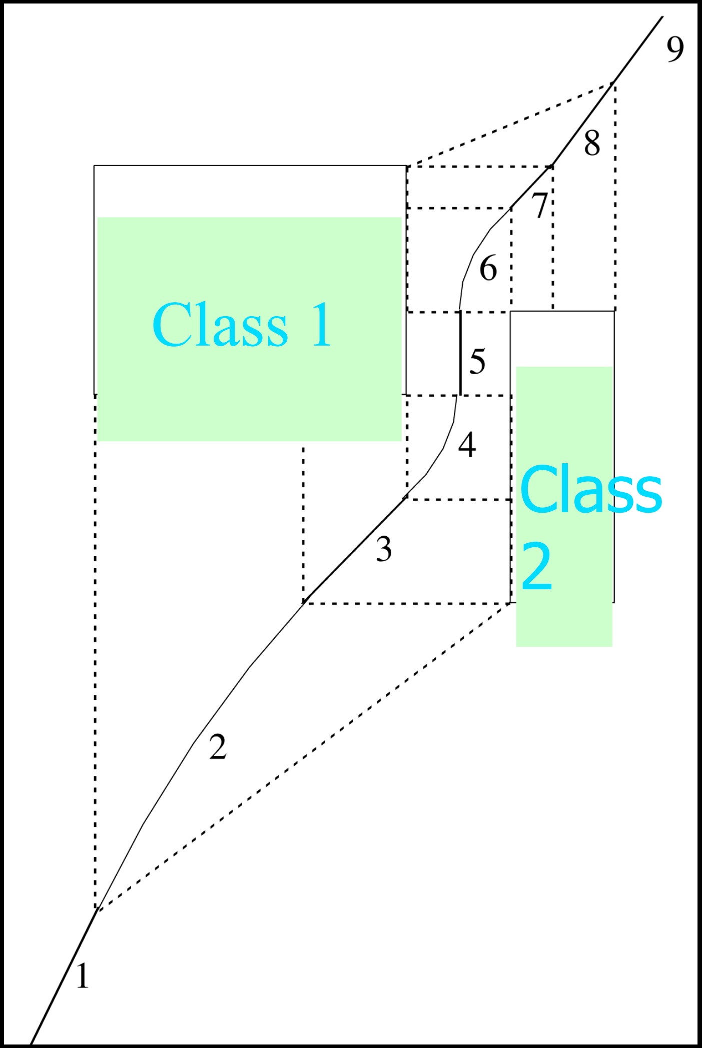


- Nearest-neighbor rule is used outside rectangles
- Rectangles are rules! (But they can be more conservative than “normal” rules.)
- Nested rectangles are rules with exceptions

Generalized exemplars

- Generalize instances into *hyperrectangles*
  - Online: incrementally modify rectangles
  - Offline version: seek small set of rectangles that cover the instances
- Important design decisions:
  - Allow overlapping rectangles?
    - Requires conflict resolution
  - Allow nested rectangles?
  - Dealing with uncovered instances?

Separating generalized exemplars



Separation line

Generalized distance functions

- Given: some transformation operations on attributes
- K*: similarity = probability of transforming instance A into B by chance
  - Average over all transformation paths
  - Weight paths according their probability *(need way of measuring this)*
- Uniform way of dealing with different attribute types
- Easily generalized to give distance between *sets* of instances

Numeric prediction

- Counterparts exist for all schemes previously discussed
  - Decision trees, rule learners, SVMs, etc.
- (Almost) all classification schemes can be applied to regression problems using discretization
  - Discretize the class into intervals
  - Predict weighted average of interval midpoints
  - Weight according to class probabilities

Regression trees

- Like decision trees, but:
  - Splitting criterion: minimize intra-subset variation
  - Termination criterion: std dev becomes small
  - Pruning criterion: based on numeric error measure
  - Prediction: Leaf predicts average class values of instances
- Piecewise constant functions
- Easy to interpret
- More sophisticated version: *model trees*

Model trees

- Build a regression tree
- Each leaf $\Rightarrow$ linear regression function
- Smoothing: factor in ancestor's predictions
  - Smoothing formula: $p' = \frac{np+kq}{n+k}$
  - Same effect can be achieved by incorporating ancestor models into the leaves
- Need linear regression function at each *node*
- At each node, use only a subset of attributes
  - Those occurring in subtree
  - (+maybe those occurring in path to the root)
- Fast: tree usually uses only a small subset of the attributes

Building the tree

- Splitting: standard deviation reduction

$$SDR = sd(T) - \sum_i \left|\frac{T_i}{T}\right| \times sd(T_i)$$

- Termination:
  - Standard deviation < 5% of its value on full training set
  - Too few instances remain (e.g. < 4)

Pruning:

- Heuristic estimate of absolute error of LR models:

$$\frac{n+\nu}{n-\nu} \times \text{average\_absolute\_error}$$

- Greedily remove terms from LR models to minimize estimated error
- Heavy pruning: single model may replace whole subtree
- Proceed bottom up: compare error of LR model at internal node to error of subtree

Nominal attributes

- Convert nominal attributes to binary ones
  - Sort attribute by average class value
  - If attribute has k values, generate $k - 1$ binary attributes
    - i th is 0 if value lies within the first i , otherwise 1
- Treat binary attributes as numeric
- Can prove: best split on one of the new attributes is the best (binary) split on original

Missing values

- Modify splitting criterion:

$$SDR = \frac{m}{|T|} \times [sd(T) - \sum_i |\frac{T_i}{T}| \times sd(T_i)]$$

- To determine which subset an instance goes into, use *surrogate splitting*
  - Split on the attribute whose correlation with original is greatest
  - Problem: complex and time-consuming
  - Simple solution: always use the class
- Test set: replace missing value with average

Surrogate splitting based on class

- Choose split point based on instances with known values
- Split point divides instances into 2 subsets
  - *L* (smaller class average)
  - *R* (larger)
- *m* is the average of the two averages
- For an instance with a missing value:
  - Choose *L* if class value $< m$
  - Otherwise *R*
- Once full tree is built, replace missing values with averages of corresponding leaf nodes

Pseudo-code for M5'

- Four methods:
  - Main method: *MakeModelTree*
  - Method for splitting: *split*
  - Method for pruning: *prune*
  - Method that computes error: *subtreeError*
- We'll briefly look at each method in turn
- Assume that linear regression method performs attribute subset selection based on error

MakeModelTree

```
MakeModelTree (instances)
{
  SD = sd(instances)
  for each k-valued nominal attribute
    convert into k-1 synthetic binary attributes
  root = newNode
  root.instances = instances
  split(root)
  prune(root)
  printTree(root)
}
```

split

```
split(node)
{
  if sizeof(node.instances) < 4 or
     sd(node.instances) < 0.05*SD
    node.type = LEAF
  else
    node.type = INTERIOR
    for each attribute
      for all possible split positions of attribute
        calculate the attribute's SDR
    node.attribute = attribute with maximum SDR
    split(node.left)
    split(node.right)
}
```

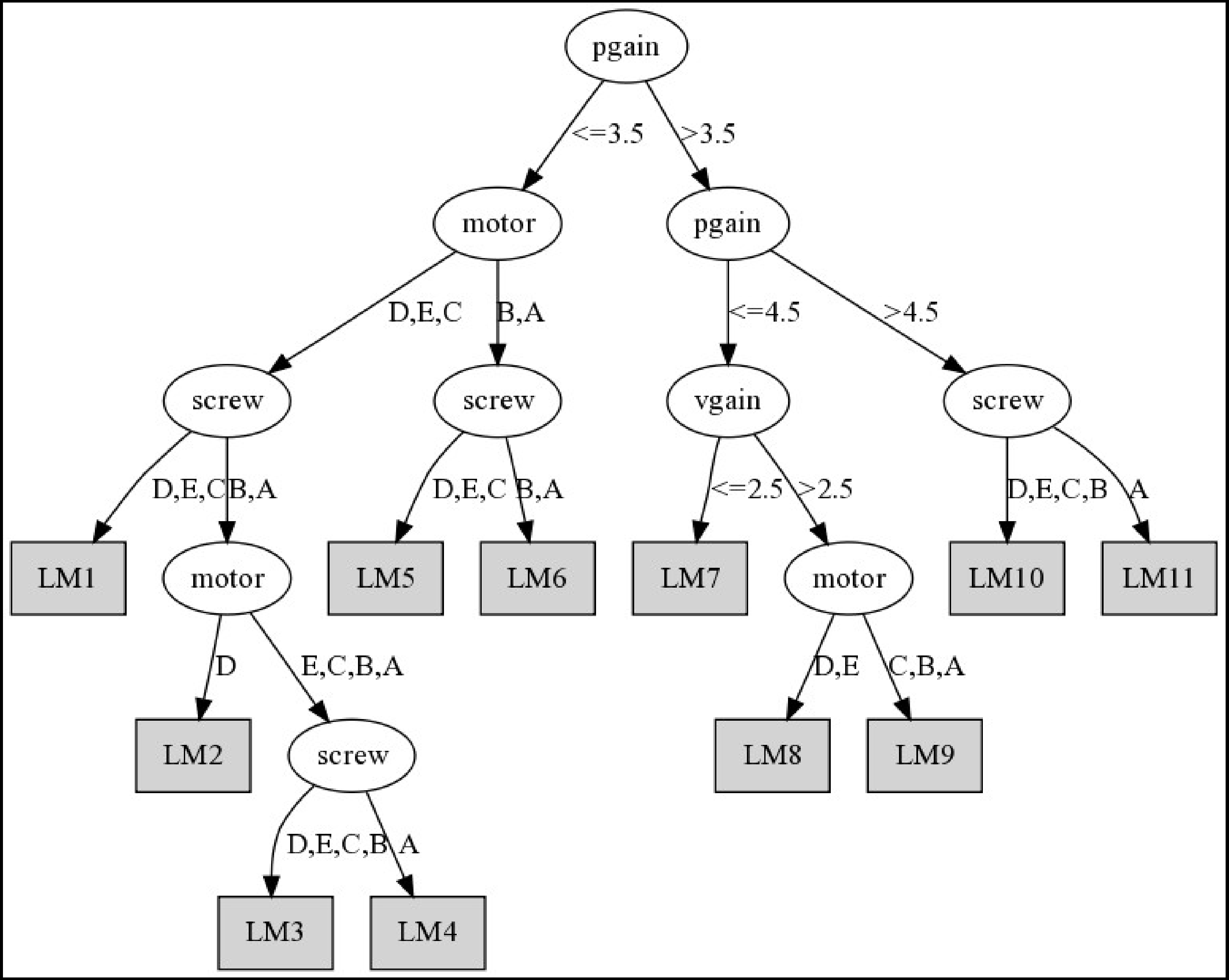
prune

```
prune(node)
{
  if node = INTERIOR then
    prune(node.leftChild)
    prune(node.rightChild)
    node.model = linearRegression(node)
    if subtreeError(node) > error(node) then
      node.type = LEAF
}
```

subtreeError

```
subtreeError(node)
{
  l = node.left; r = node.right
  if node = INTERIOR then
    return (sizeof(l.instances)*subtreeError(l)
            + sizeof(r.instances)*subtreeError(r))
              /sizeof(node.instances)
  else return error(node)
}
```

Model tree for servo data



Rules from model trees

- PART algorithm generates classification rules by building partial decision trees
- Can use the same method to build rule sets for regression
    - Use model trees instead of decision trees
    - Use variance instead of entropy to choose node to expand when building partial tree
- Rules will have linear models on right-hand side
- Caveat: using smoothed trees may not be appropriate due to separate-and-conquer strategy

Locally weighted regression

- Numeric prediction that combines
  - instance-based learning
  - linear regression
- "Lazy":
  - computes regression function at prediction time
  - works incrementally
- Weight training instances
  - according to distance to test instance
  - needs weighted version of linear regression
- Advantage: nonlinear approximation
- But: slow

Design decisions

- Weighting function:
  - Inverse Euclidean distance
  - Gaussian kernel applied to Euclidean distance
  - Triangular kernel used the same way
  - etc.
- *Smoothing parameter* is used to scale the distance function
  - Multiply distance by inverse of this parameter
  - Possible choice: distance of *k* th nearest training instance (makes it data dependent)

Discussion

- Regression trees were introduced in CART
- Quinlan proposed model tree method (M5)
- M5’: slightly improved, publicly available
- Quinlan also investigated combining instance-based learning with M5
- CUBIST: Quinlan’s commercial rule learner for numeric prediction
- Interesting comparison: neural nets vs. M5

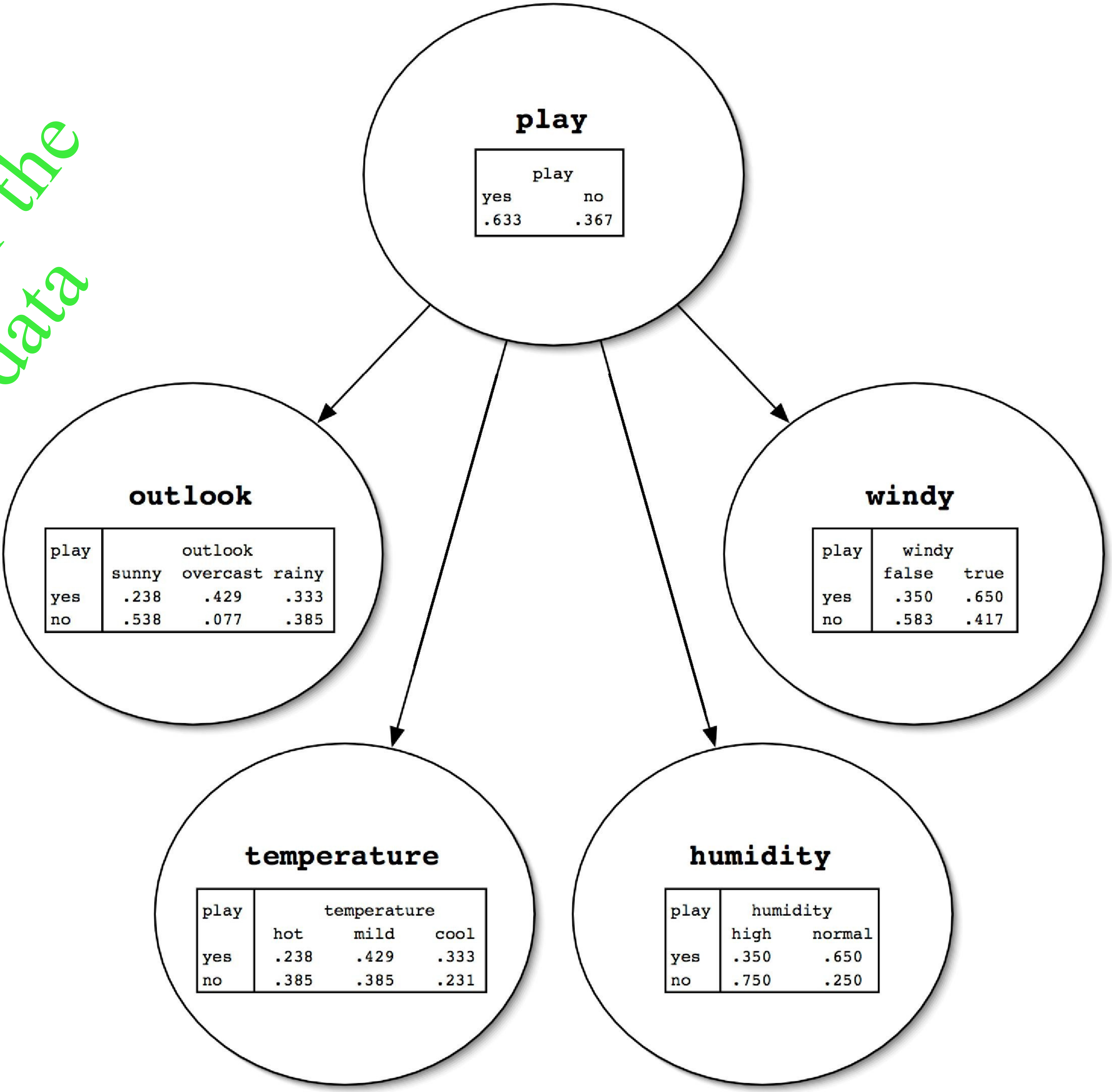
From naïve Bayes to Bayesian Networks

- Naïve Bayes assumes:
  attributes conditionally independent given the class
- Doesn’t hold in practice but classification accuracy often high
- However: sometimes performance much worse than e.g. decision tree
- Can we eliminate the assumption?

Enter Bayesian networks

- Graphical models that can represent any probability distribution
- Graphical representation: directed acyclic graph, one node for each attribute
- Overall probability distribution factorized into component distributions
- Graph’s nodes hold component distributions (conditional distributions)

Network for the weather data



play

play	
yes	no
.633	.367

outlook

play	outlook		
	sunny	overcast	rainy
yes	.238	.429	.333
no	.538	.077	.385

temperature

play	temperature		
	hot	mild	cool
yes	.238	.429	.333
no	.385	.385	.231

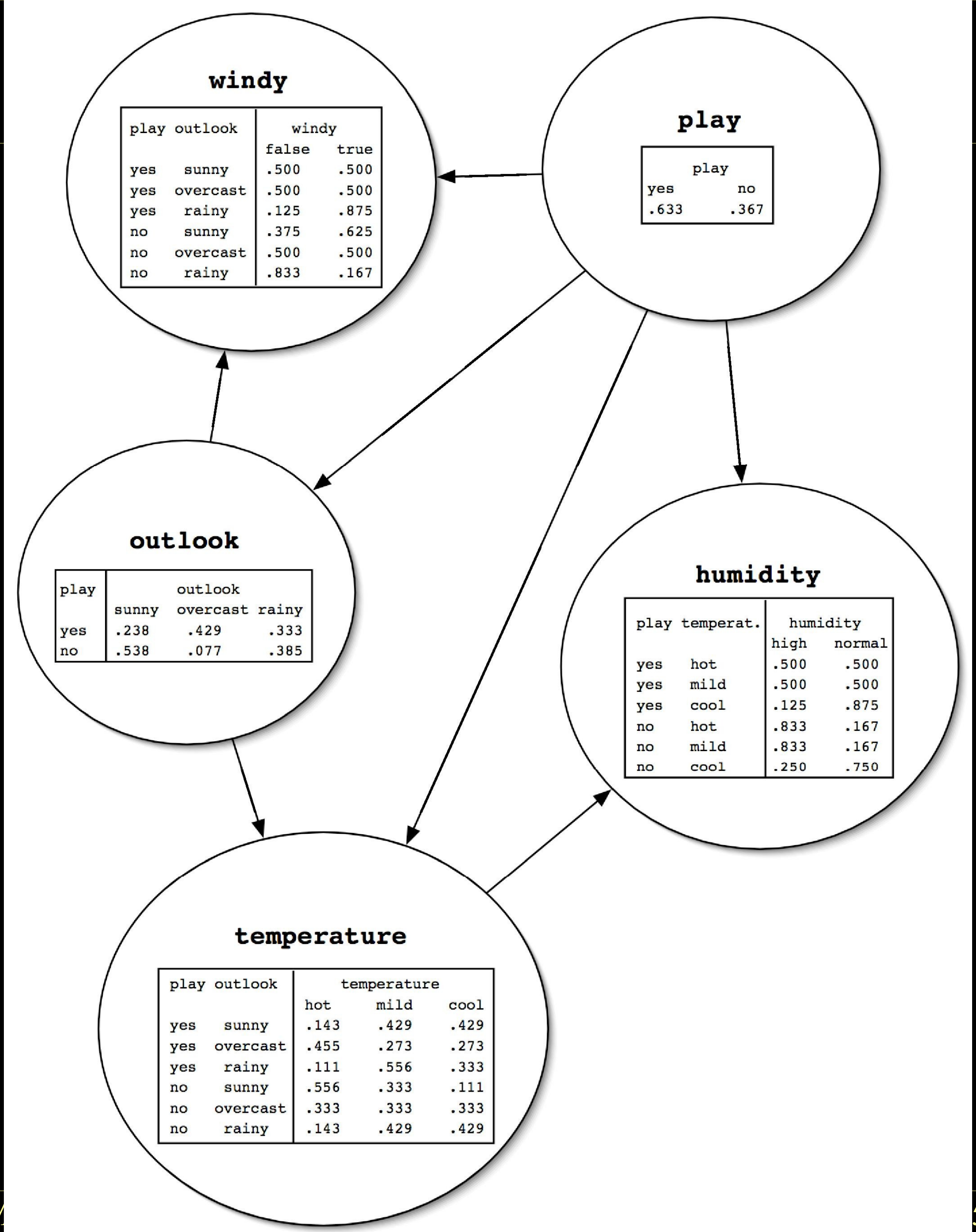
humidity

play	humidity	
	high	normal
yes	.350	.650
no	.750	.250

windy

play	windy	
	false	true
yes	.350	.650
no	.583	.417

Network for the weather data



play

play	
yes	no
.633	.367

windy

play	outlook	windy	
		false	true
yes	sunny	.500	.500
yes	overcast	.500	.500
yes	rainy	.125	.875
no	sunny	.375	.625
no	overcast	.500	.500
no	rainy	.833	.167

outlook

play	outlook		
	sunny	overcast	rainy
yes	.238	.429	.333
no	.538	.077	.385

humidity

play	temperat.	humidity	
		high	normal
yes	hot	.500	.500
yes	mild	.500	.500
yes	cool	.125	.875
no	hot	.833	.167
no	mild	.833	.167
no	cool	.250	.750

temperature

play	outlook	temperature		
		hot	mild	cool
yes	sunny	.143	.429	.429
yes	overcast	.455	.273	.273
yes	rainy	.111	.556	.333
no	sunny	.556	.333	.111
no	overcast	.333	.333	.333
no	rainy	.143	.429	.429

Computing the class probabilities

- Two steps: computing a product of probabilities for each class and normalization
  - For each class value
    - Take all attribute values and class value
    - Look up corresponding entries in conditional probability distribution tables
    - Take the product of all probabilities
  - Divide the product for each class by the sum of the products (normalization)

Why can we do this? (Part I)

- Single assumption: values of a node’s parents completely determine probability distribution for current node

$$Pr[\text{node}|\text{ancestors}] = Pr[\text{node}|\text{parents}]$$

Means that node/attribute is conditionally independent of other ancestors given parents

Why can we do this? (Part II)

- Chain rule from probability theory:

$$Pr[a_{1,} a_{2,} \ldots, a_n] = \prod_{i=1}^{n} Pr[a_i | a_{i-1}, \ldots, a_1]$$

Because of our assumption from the previous slide:

$$Pr[a_{1,} a_{2,} \ldots, a_n] = \prod_{i=1}^{n} Pr[a_i | a_{i-1}, \ldots, a_1] = \prod_{i=1}^{n} Pr[a_i | a_i's\, parents]$$

WEKA
The University of Waikato

Learning Bayes nets

- Basic components of algorithms for learning Bayes nets:
  - Method for evaluating the goodness of a given network
    - Measure based on probability of training data given the network (or the logarithm thereof)
  - Method for searching through space of possible networks
    - Amounts to searching through sets of edges because nodes are fixed

Problem: overfitting

- Can’t just maximize probability of the training data
  - Because then it’s always better to add more edges (fit the training data more closely)
- Need to use cross-validation or some penalty for complexity of the network

AIC measure:

$$AIC\,score = -\mathrm{LL} + K$$

MDL measure:

$$MDL\,score = -\mathrm{LL} + \frac{K}{2}\log N$$

LL: log-likelihood (log of probability of data), *K*: number of free parameters, *N*: #instances

Another possibility: Bayesian approach with prior distribution over networks

Searching for a good structure

- Task can be simplified: can optimize each node separately
  - Because probability of an instance is product of individual nodes' probabilities
  - Also works for AIC and MDL criterion because penalties just add up
- Can optimize node by adding or removing edges from other nodes
- Must not introduce cycles!

The K2 algorithm

- Starts with given ordering of nodes (attributes)
- Processes each node in turn
- Greedily tries adding edges from previous nodes to current node
- Moves to next node when current node can’t be optimized further
- Result depends on initial order

Some tricks

- Sometimes it helps to start the search with a naïve Bayes network
- It can also help to ensure that every node is in Markov blanket of class node
    - Markov blanket of a node includes all parents, children, and children's parents of that node
    - Given values for Markov blanket, node is conditionally independent of nodes outside blanket
    - I.e. node is irrelevant to classification if not in Markov blanket of class node

Other algorithms

- Extending K2 to consider greedily adding or deleting edges between any pair of nodes
    - Further step: considering inverting the direction of edges
- TAN (Tree Augmented Naïve Bayes):
    - Starts with naïve Bayes
    - Considers adding second parent to each node (apart from class node)
    - Efficient algorithm exists

Likelihood vs. conditional likelihood

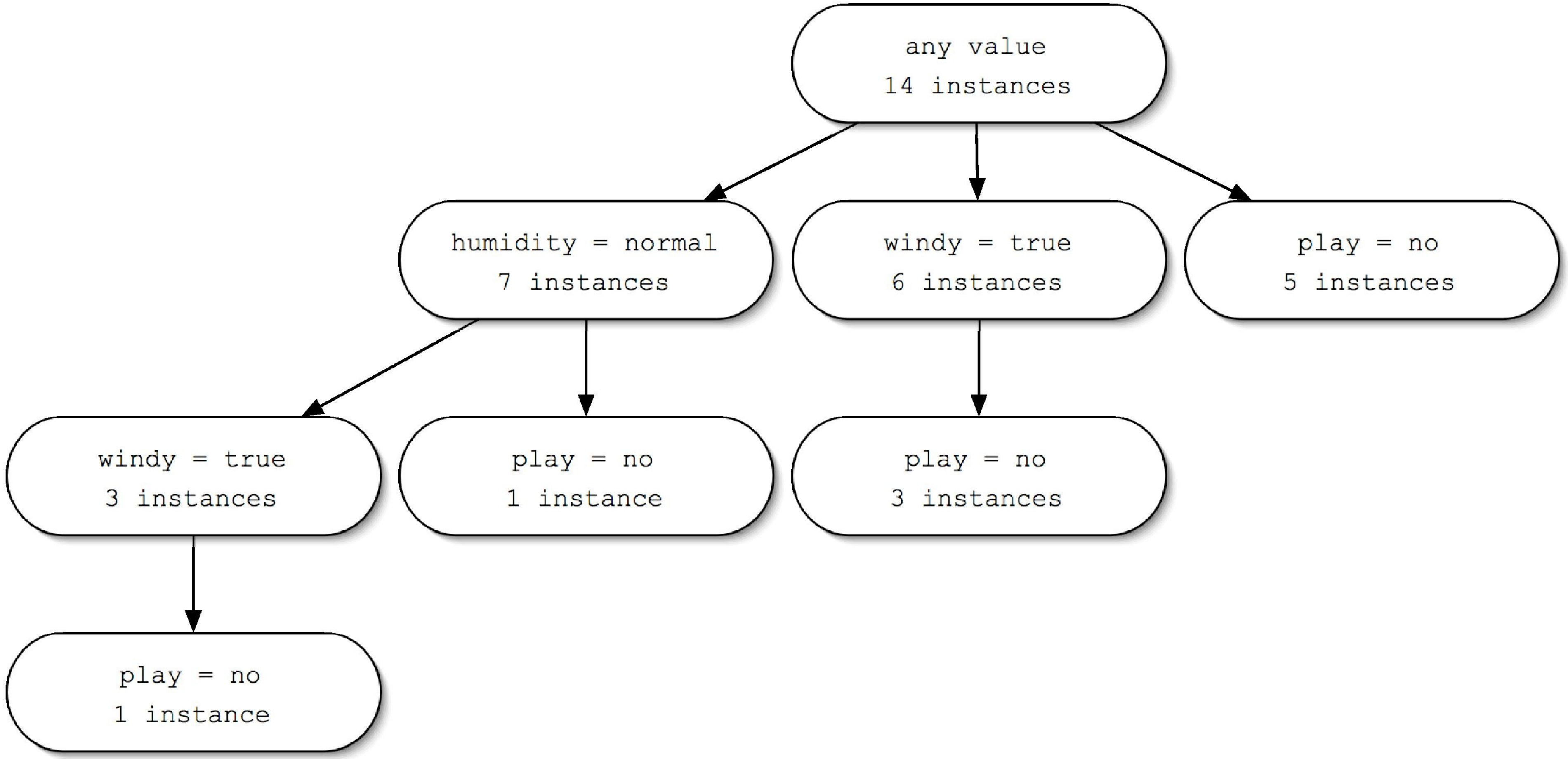
- In classification what we really want is to maximize probability of class given other attributes
  - *Not* probability of the instances
- But: no closed-form solution for probabilities in nodes' tables that maximize this
- However: can easily compute conditional probability of data based on given network
- Seems to work well when used for network scoring

Data structures for fast learning

- Learning Bayes nets involves a lot of counting for computing conditional probabilities
- Naïve strategy for storing counts: hash table
    - Runs into memory problems very quickly
- More sophisticated strategy: *all-dimensions (AD) tree*
    - Analogous to *k*D-tree for numeric data
    - Stores counts in a tree but in a clever way such that redundancy is eliminated
    - Only makes sense to use it for large datasets

AD tree example

humidity	windy	play	count
high	true	yes	1
high	true	no	2
high	false	yes	2
high	false	no	2
normal	true	yes	2
normal	true	no	1
normal	false	yes	4
normal	false	no	0



Building an AD tree

- Assume each attribute in the data has been assigned an index
- Then, expand node for attribute *i* with the values of all attributes *j* > *i*
    - Two important restrictions:
        - Most populous expansion for each attribute is omitted (breaking ties arbitrarily)
        - Expansions with counts that are zero are also omitted
- The root node is given index zero

Discussion

- We have assumed: discrete data, no missing values, no new nodes
- Different method of using Bayes nets for classification: *Bayesian multinets*
  - I.e. build one network for each class and make prediction using Bayes' rule
- Different class of learning methods for Bayes nets: testing conditional independence assertions
- Can also build Bayes nets for regression tasks

Clustering: how many clusters?

- How to choose *k* in *k*-means? Possibilities:
  - Choose *k* that minimizes cross-validated squared distance to cluster centers
  - Use penalized squared distance on the training data (eg. using an MDL criterion)
  - Apply *k*-means recursively with *k* = 2 and use stopping criterion (eg. based on MDL)
    - Seeds for subclusters can be chosen by seeding along direction of greatest variance in cluster
      (one standard deviation away in each direction from cluster center of parent cluster)
    - Implemented in algorithm called *X*-means (using Bayesian Information Criterion instead of MDL)

Hierarchical clustering

- Recursively splitting clusters produces a hierarchy that can be represented as a *dendogram*
  - Could also be represented as a Venn diagram of sets and subsets (without intersections)
  - Height of each node in the dendogram can be made proportional to the dissimilarity between its children

Agglomerative clustering

- Bottom-up approach
- Simple algorithm
  - Requires a distance/similarity measure
  - Start by considering each instance to be a cluster
  - Find the two closest clusters and merge them
  - Continue merging until only one cluster is left
  - The record of mergings forms a hierarchical clustering structure – a *binary dendogram*

Distance measures

- *Single-linkage*
  - Minimum distance between the two clusters
  - Distance between the clusters closest two members
  - Can be sensitive to outliers
- *Complete-linkage*
  - Maximum distance between the two clusters
  - Two clusters are considered close only if all instances in their union are relatively similar
  - Also sensitive to outliers
  - Seeks compact clusters

Distance measures cont.

- Compromise between the extremes of minimum and maximum distance
- Represent clusters by their centroid, and use distance between centroids – *centroid linkage*
    - Works well for instances in multidimensional Euclidean space
    - Not so good if all we have is pairwise similarity between instances
- Calculate average distance between each pair of members of the two clusters – *average-linkage*
- Technical deficiency of both: results depend on the numerical scale on which distances are measured

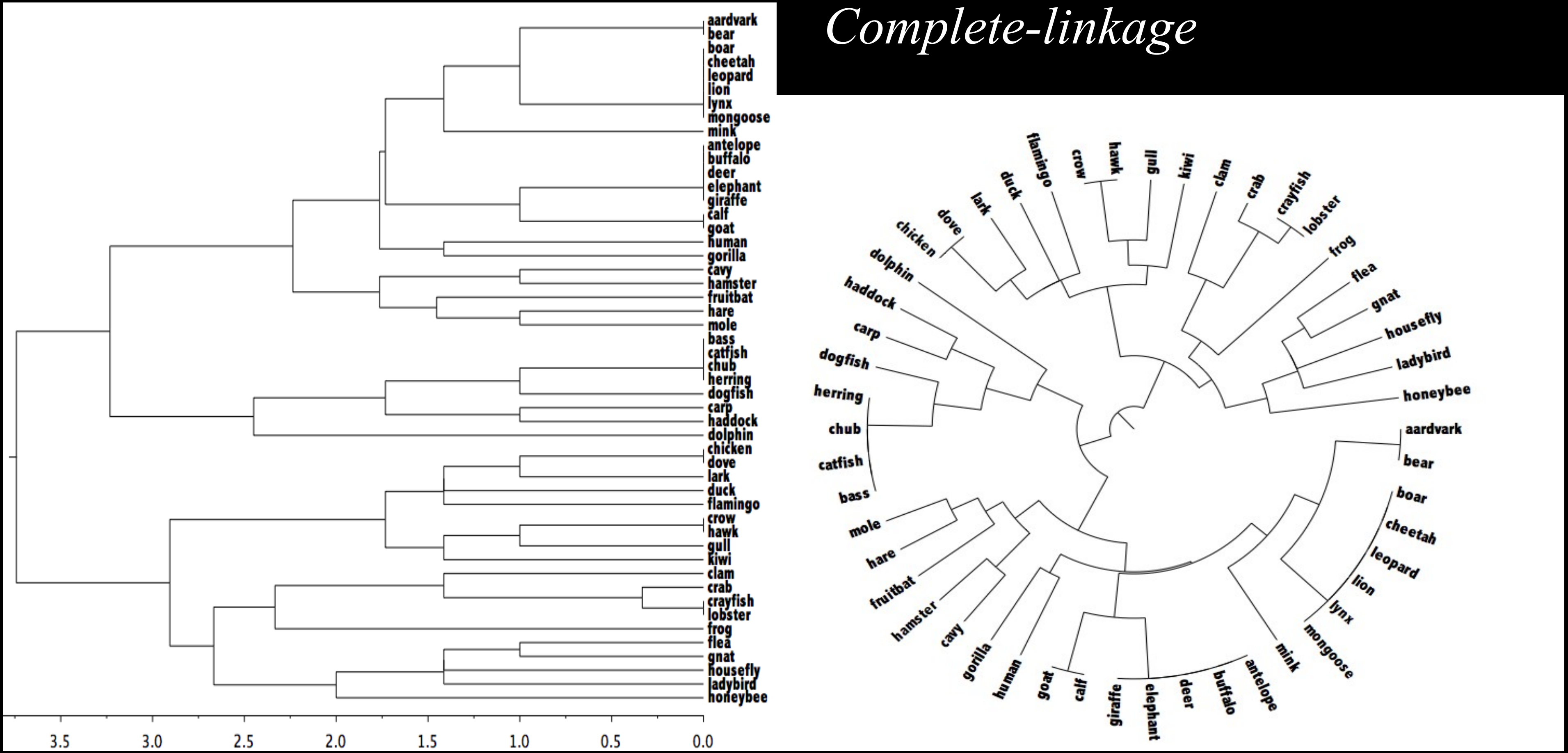
More distance measures

- *Group-average* clustering
  - Uses the average distance between all members of the merged cluster
  - Differs from average-linkage because it includes pairs from the same original cluster
- *Ward's* clustering method
  - Calculates the increase in the sum of squares of the distances of the instances from the centroid before and after fusing two clusters
  - Minimize the increase in this squared distance at each clustering step
- **All** measures will produce the same result if the clusters are compact and well separated

Example hierarchical clustering

- 50 examples of different creatures from the zoo data

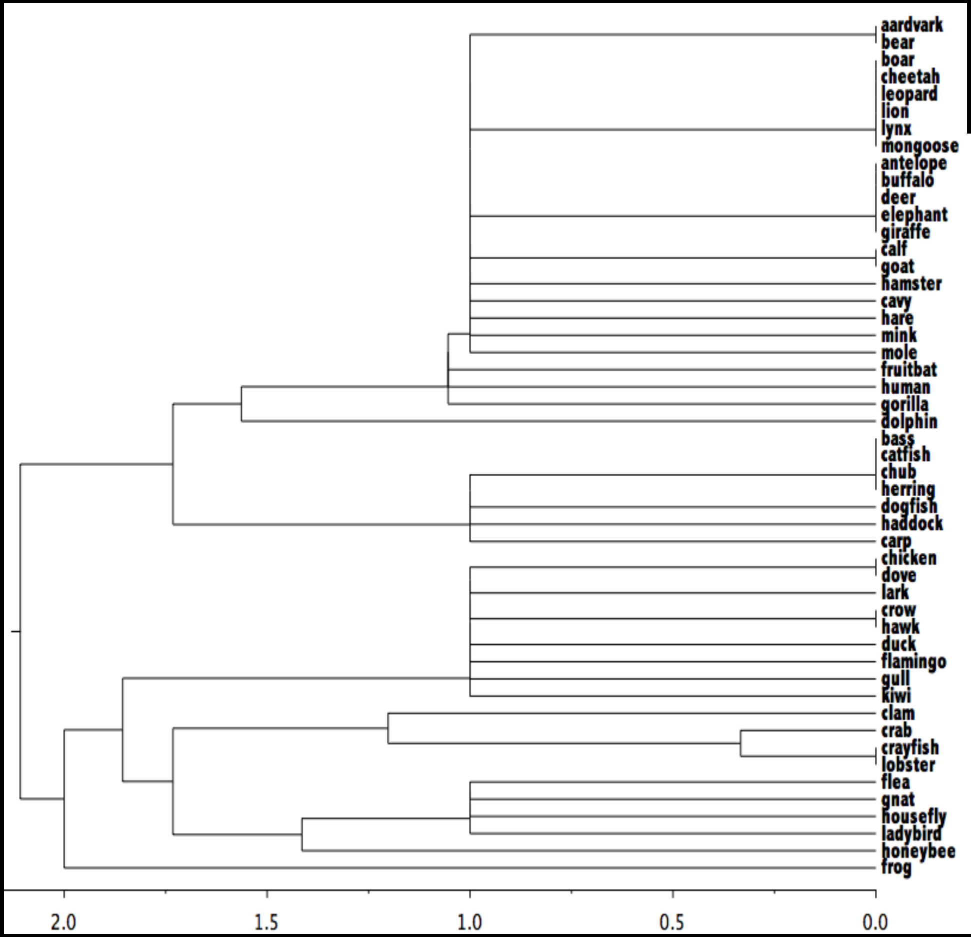
Complete-linkage



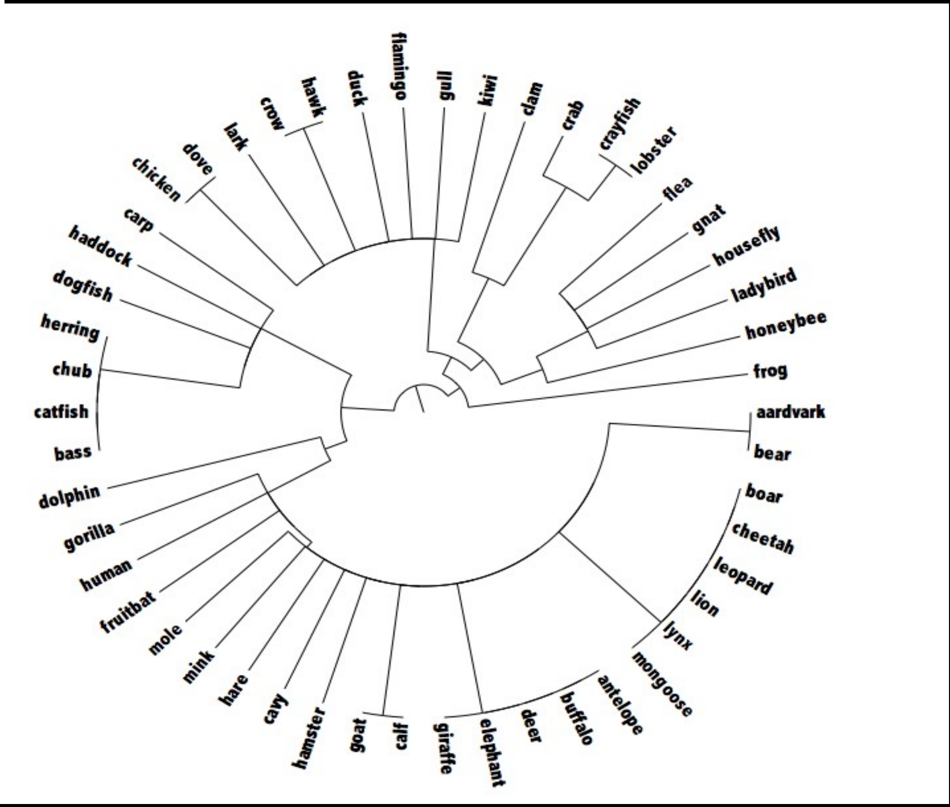
Dendogram

Polar plot

Example hierarchical clustering 2



Single-linkage



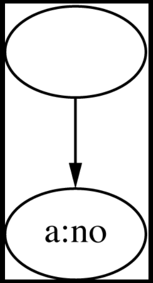
Incremental clustering

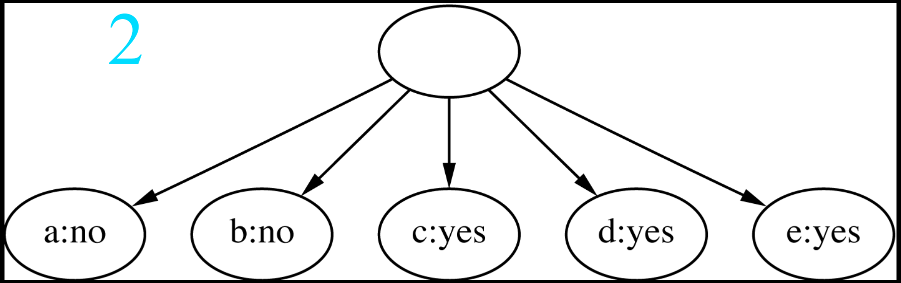
- Heuristic approach (COBWEB/CLASSIT)
- Form a hierarchy of clusters incrementally
- Start:
  - tree consists of empty root node
- Then:
  - add instances one by one
  - update tree appropriately at each stage
  - to update, find the right leaf for an instance
  - May involve restructuring the tree
- Base update decisions on *category utility*

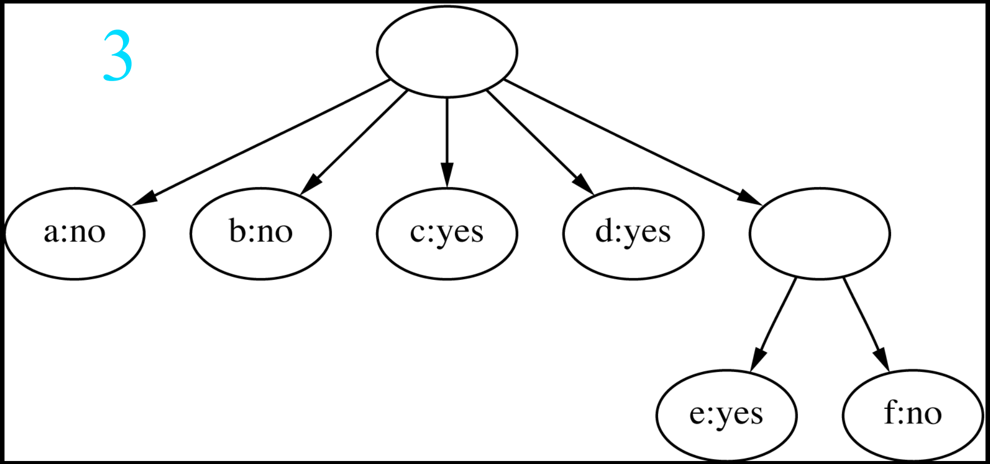
Clustering weather data

ID	Outlook	Temp.	Humidity	Windy
A	Sunny	Hot	High	False
B	Sunny	Hot	High	True
C	Overcast	Hot	High	False
D	Rainy	Mild	High	False
E	Rainy	Cool	Normal	False
F	Rainy	Cool	Normal	True
G	Overcast	Cool	Normal	True
H	Sunny	Mild	High	False
I	Sunny	Cool	Normal	False
J	Rainy	Mild	Normal	False
K	Sunny	Mild	Normal	True
L	Overcast	Mild	High	True
M	Overcast	Hot	Normal	False
N	Rainy	Mild	High	True

1







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L	Overcast	Mild	High	True
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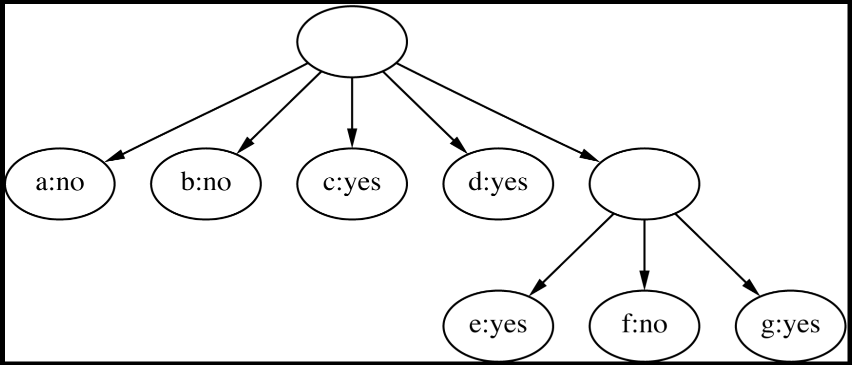
4



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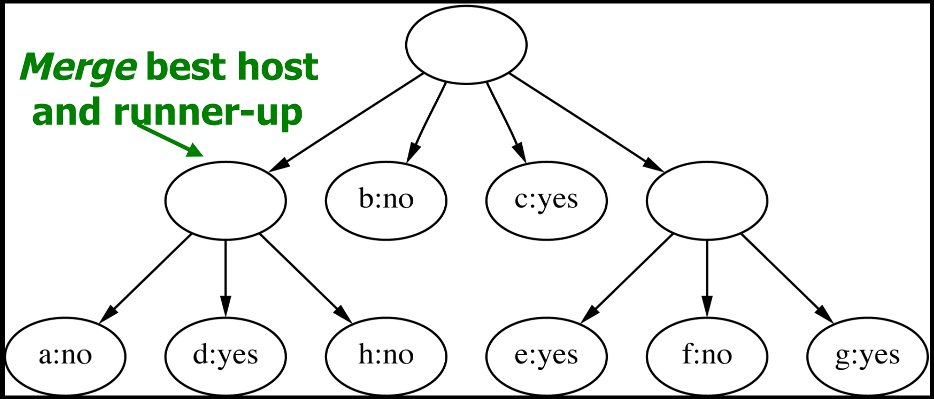
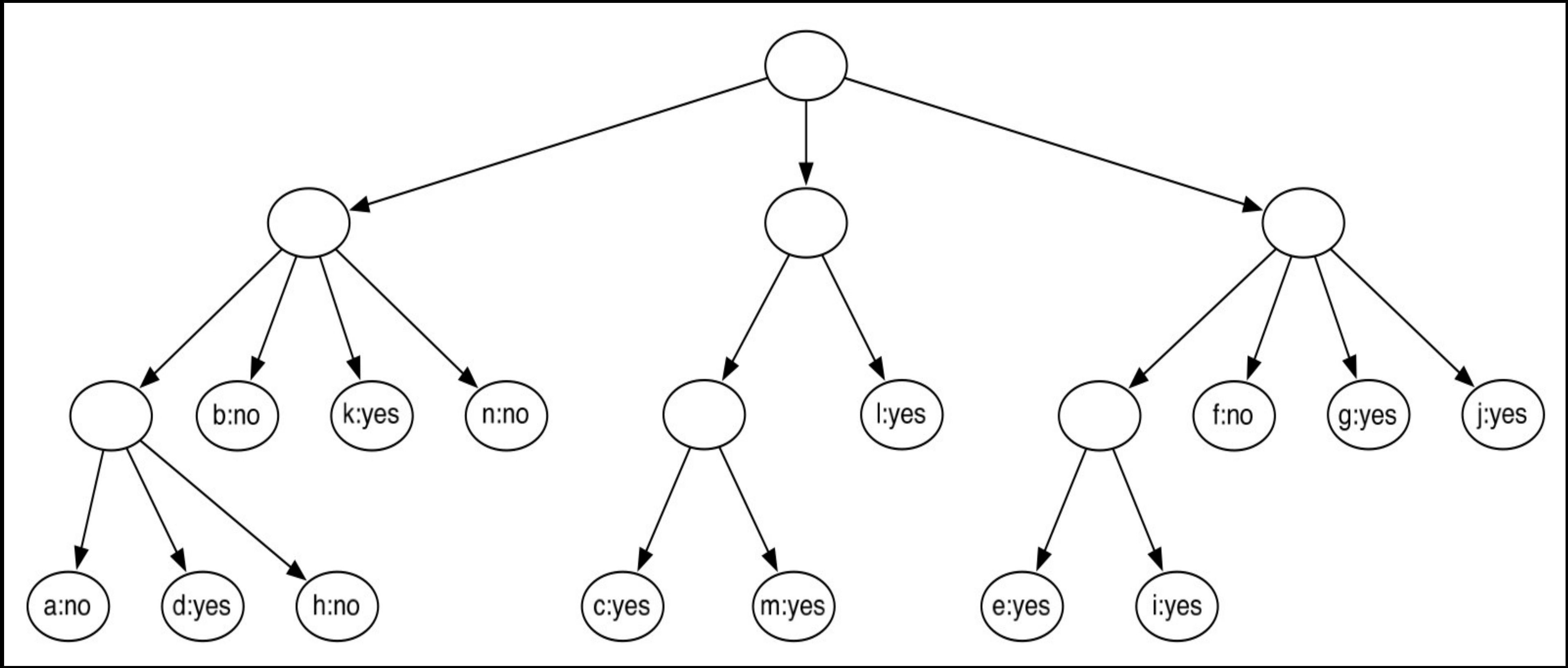
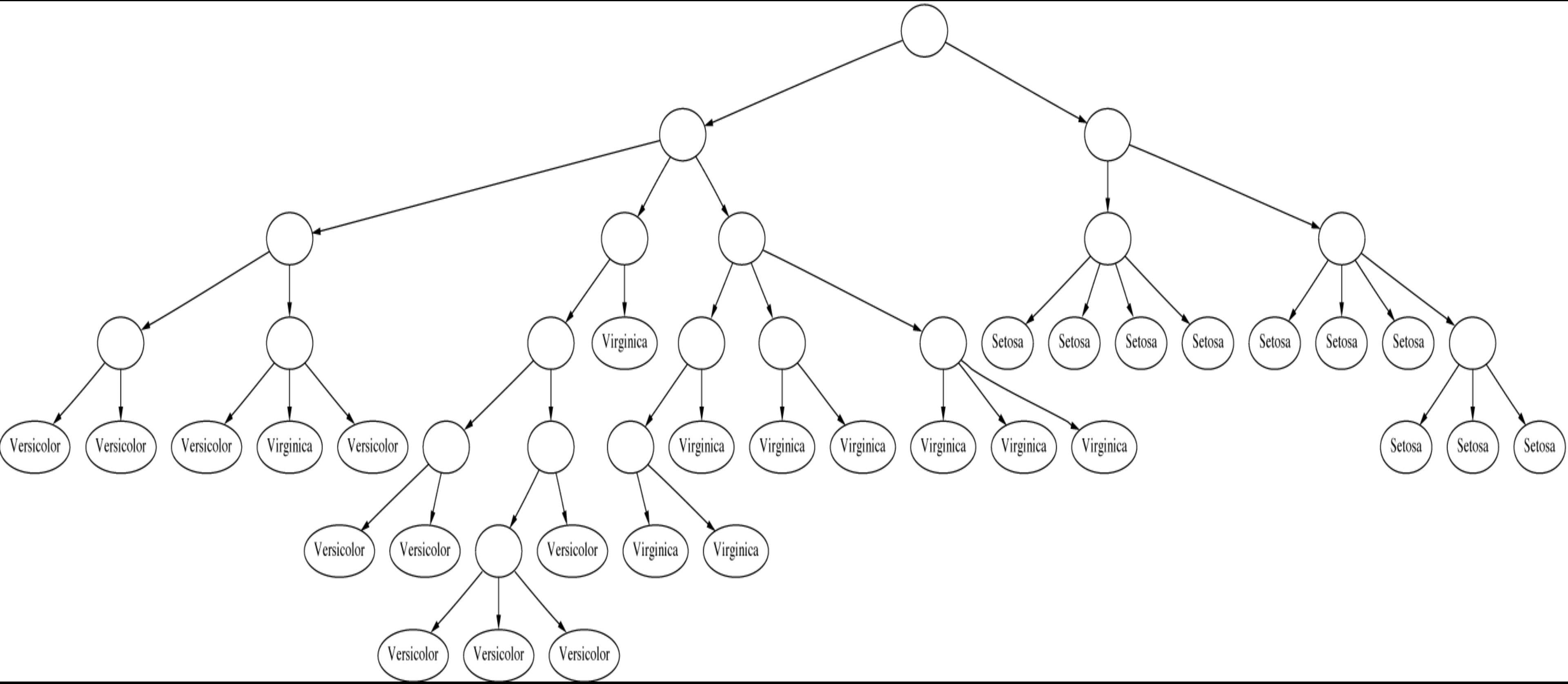


Consider *splitting* the best host if merging doesn't help

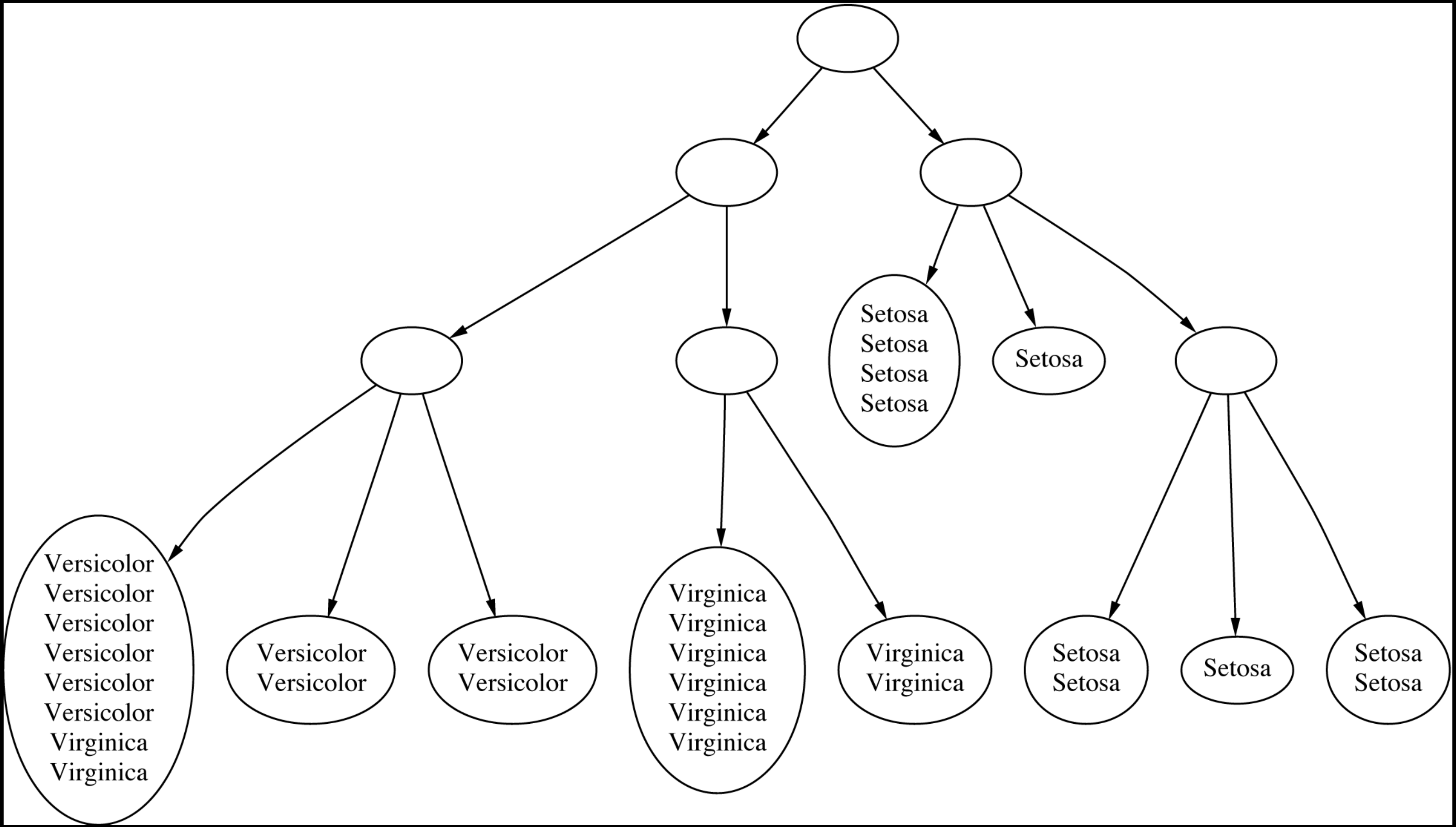
Final hierarchy



Example: the iris data (subset)



Clustering with cutoff



Category utility

- Category utility: quadratic loss function defined on conditional probabilities:

$$CU(C_1, C_2, \ldots, C_k) = \frac{\sum_l Pr[C_l] \sum_i \sum_j (Pr[a_i = v_{ij} | C_l]^2 - Pr[a_i = v_{ij}]^2)}{k}$$

- Every instance in different category ⇒ numerator becomes

$$\underset{\substack{\uparrow \\ \text{number of attributes}}}{n} - \sum_i \sum_j Pr[a_i = v_{ij}]^2 \longleftarrow \textit{maximum}$$

Numeric attributes

- Assume normal distribution:

$$f(a) = \frac{1}{\sqrt{(2\pi)}\sigma} \exp\left(-\frac{(a-\mu)^2}{2\sigma^2}\right)$$

- Then:

$$\sum_j Pr[a_i = v_{ij}]^2 \equiv \int f(a_i)^2 \, da_i = \frac{1}{2\sqrt{\pi}\sigma_i}$$

- Thus

$$CU(C_1, C_2, \ldots, C_k) = \frac{\sum_l Pr[C_l] \sum_i \sum_j (Pr[a_i = v_{ij} | C_l]^2 - Pr[a_i = v_{ij}]^2)}{k}$$

  becomes

$$CU(C_1, C_2, \ldots, C_k) = \frac{\sum_l Pr[C_l] \frac{1}{2\sqrt{\pi}} \sum_i \left(\frac{1}{\sigma_{il}} - \frac{1}{\sigma_i}\right)}{k}$$

- Prespecified minimum variance
  - *acuity* parameter

Probability-based clustering

- Problems with heuristic approach:
  - Division by *k?*
  - Order of examples?
  - Are restructuring operations sufficient?
  - Is result at least *local* minimum of category utility?
- Probabilistic perspective ⇒
  seek the *most likely* clusters given the data
- Also: instance belongs to a particular cluster *with a certain probability*

Finite mixtures

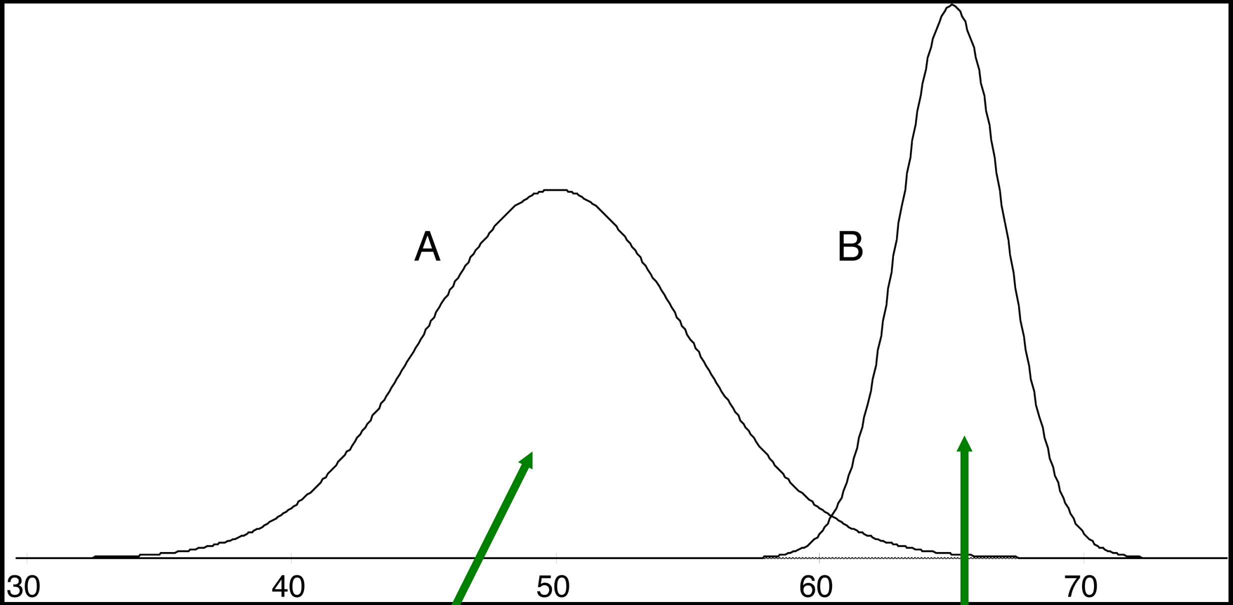
- Model data using a *mixture* of distributions
- One cluster, one distribution
  - governs probabilities of attribute values in that cluster
- *Finite mixtures* : finite number of clusters
- Individual distributions are normal (usually)
- Combine distributions using cluster weights

Two-class mixture model

data

A	51	B	62	B	64	A	48	A	39	A	51
A	43	A	47	A	51	B	64	B	62	A	48
B	62	A	52	A	52	A	51	B	64	B	64
B	64	B	64	B	62	B	63	A	52	A	42
A	45	A	51	A	49	A	43	B	63	A	48
A	42	B	65	A	48	B	65	B	64	A	41
A	46	A	48	B	62	B	66	A	48		
A	45	A	49	A	43	B	65	B	64		
A	45	A	46	A	40	A	46	A	48		

model



$\mu_A=50,\ \sigma_A=5,\ p_A=0.6$ $\mu_B=65,\ \sigma_B=2,\ p_B=0.4$

Using the mixture model

- Probability that instance x belongs to cluster A:

$$Pr[A|x] = \frac{Pr[x|A]Pr[A]}{Pr[x]} = \frac{f(x;\mu_A,\sigma_A)p_A}{Pr[x]}$$

  with

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{(2\pi)}\sigma}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- Probability of an instance given the clusters:

$$Pr[x|\text{the\_clusters}] = \sum_i Pr[x|\text{cluster}_i]Pr[cluster_i]$$

Learning the clusters

- Assume:
  - we know there are *k* clusters
- Learn the clusters ⇒
  - determine their parameters
  - I.e. means and standard deviations
- Performance criterion:
  - *probability of training data given the clusters*
- EM algorithm
  - finds a local maximum of the likelihood

EM algorithm

- EM = Expectation-Maximization
  - Generalize *k*-means to probabilistic setting
- Iterative procedure:
  - E "expectation" step:
    Calculate cluster probability for each instance
  - M "maximization" step:
    Estimate distribution parameters from cluster probabilities
- Store cluster probabilities as instance weights
- Stop when improvement is negligible

More on EM

- Estimate parameters from weighted instances

$$\mu_A = \frac{w_1 x_1 + w_2 x_2 + \ldots + w_n x_n}{w_1 + w_2 + \ldots + w_n}$$

$$\sigma_A = \frac{w_1 (x_1 - \mu)^2 + w_2 (x_2 - \mu)^2 + \ldots + w_n (x_n - \mu)^2}{w_1 + w_2 + \ldots + w_n}$$

- Stop when log-likelihood saturates

- Log-likelihood:

$$\sum_i \log(p_A Pr[x_i \mid A] + p_B Pr[x_i \mid B])$$

Extending the mixture model

- More then two distributions: easy
- Several attributes: easy—assuming independence!
- Correlated attributes: difficult
  - Joint model: bivariate normal distribution with a (symmetric) covariance matrix
  - n attributes: need to estimate $n + n\,(n+1)/2$ parameters

More mixture model extensions

- Nominal attributes: easy if independent
- Correlated nominal attributes: difficult
  - Two correlated attributes $\Rightarrow$ $v_1 v_2$ parameters
- Missing values: easy
- Can use other distributions than normal:
  - “log-normal” if predetermined minimum is given
  - “log-odds” if bounded from above and below
  - Poisson for attributes that are integer counts
- Use cross-validation to estimate *k* !

Bayesian clustering

- Problem: many parameters $\Rightarrow$ EM overfits
- *Bayesian approach* : give every parameter a prior probability distribution
  - Incorporate prior into overall likelihood figure
  - Penalizes introduction of parameters
- Eg: Laplace estimator for nominal attributes
- Can also have prior on number of clusters!
- Implementation: NASA's AUTOCLASS

Discussion

- Can interpret clusters by using supervised learning
  - post-processing step
- Decrease dependence between attributes?
  - pre-processing step
  - E.g. use *principal component analysis*
- Can be used to fill in missing values
- Key advantage of probabilistic clustering:
  - Can estimate likelihood of data
  - Use it to compare different models objectively

Semisupervised learning

- *Semisupervised learning*: attempts to use unlabeled data as well as labeled data
  - The aim is to improve classification performance
- Why try to do this? Unlabeled data is often plentiful and labeling data can be expensive
  - Web mining: classifying web pages
  - Text mining: identifying names in text
  - Video mining: classifying people in the news
- Leveraging the large pool of unlabeled examples would be very attractive

Clustering for classification

- Idea: use naïve Bayes on labeled examples and then apply EM
  - First, build naïve Bayes model on labeled data
  - Second, label unlabeled data based on class probabilities ("expectation" step)
  - Third, train new naïve Bayes model based on all the data ("maximization" step)
  - Fourth, repeat 2nd and 3rd step until convergence
- Essentially the same as EM for clustering with fixed cluster membership probabilities for labeled data and #clusters = #classes

Comments

- Has been applied successfully to document classification
  - Certain phrases are indicative of classes
  - Some of these phrases occur only in the unlabeled data, some in both sets
  - EM can generalize the model by taking advantage of co-occurrence of these phrases
- Refinement 1: reduce weight of unlabeled data
- Refinement 2: allow multiple clusters per class

Co-training

- Method for learning from *multiple views* (multiple sets of attributes), eg:
    - First set of attributes describes content of web page
    - Second set of attributes describes links that link to the web page
- Step 1: build model from each view
- Step 2: use models to assign labels to unlabeled data
- Step 3: select those unlabeled examples that were most confidently predicted (ideally, preserving ratio of classes)
- Step 4: add those examples to the training set
- Step 5: go to Step 1 until data exhausted
- Assumption: views are independent

EM and co-training

- Like EM for semisupervised learning, but view is switched in each iteration of EM
    - Uses all the unlabeled data (probabilistically labeled) for training
- Has also been used successfully with support vector machines
    - Using logistic models fit to output of SVMs
- Co-training also seems to work when views are chosen randomly!
    - Why? Possibly because co-trained classifier is more robust

Multi-instance learning

- Converting to single-instance learning
- Already seen aggregation of *input* or *output*
  - Simple and often work well in practice
- Will fail in some situations
  - Aggregating the input loses a lot of information because attributes are condensed to summary statistics individually and independently
- Can a bag be converted to a single instance without discarding so much info?

Converting to single-instance

- Can convert to single instance without losing so much info, but more attributes are needed in the "condensed" representation
- Basic idea: partition the instance space into *regions*
  - One attribute per region in the single-instance representation
- Simplest case → boolean attributes
  - Attribute corresponding to a region is set to true for a bag if it has at least one instance in that region

Converting to single-instance

- Could use numeric counts instead of boolean attributes to preserve more information
- Main problem: how to partition the instance space?
- Simple approach → partition into equal sized *hypercubes*
  - Only works for few dimensions
- More practical → use unsupervised learning
  - Take all instances from all bags (minus class labels) and cluster
  - Create one attribute per cluster (region)

Converting to single-instance

- Clustering ignores the class membership
- Use a decision tree to partition the space instead
  - Each leaf corresponds to one region of instance space
- How to learn tree when class labels apply to entire bags?
  - *Aggregating the output* can be used: take the bag's class label and attach it to each of its instances
  - Many labels will be incorrect, however, they are only used to obtain a partitioning of the space

Converting to single-instance

- Using decision trees yields "hard" partition boundaries
- So does k-means clustering into regions, where the cluster centers (reference points) define the regions
- Can make region membership "soft" by using distance – transformed into similarity – to compute attribute values in the condensed representation
    - Just need a way of aggregating similarity scores between each bag and reference point into a single value – e.g. max similarity between each instance in a bag and the reference point

Upgrading learning algorithms

- Converting to single-instance is appealing because many existing algorithms can then be applied without modification
  - May not be the most *efficient* approach
- Alternative: adapt single-instance algorithm to the multi-instance setting
  - Can be achieved elegantly for for distance/similarity-based methods (e.g. nearest neighbor or SVMs)
  - Compute distance/similarity between two bags of instances

Upgrading learning algorithms

- Kernel-based methods
  - Similarity must be a proper kernel function that satisfies certain mathematical properties
  - One example – so called *set kernel*
    - Given a kernel function for pairs of instances, the set kernel sums it over all pairs of instances from the two bags being compared
    - Is generic and can be applied with **any** single-instance kernel function

Upgrading learning algorithms

- Nearest neighbor learning
  - Apply variants of the Hausdorff distance, which is defined for sets of points
  - Given two bags and a distance function between pairs of instances, Hausdorff distance between the bags is

    Largest distance from any instance in one bag to its closest instance in the other bag
  - Can be made more robust to outliers by using the *n*th-largest distance

Dedicated multi-instance methods

- Some methods are not based directly on single-instance algorithms
- One basic approach $\rightarrow$ find a single hyperrectangle that contains at least one instance from each positive bag and no instances from any negative bags
    - Rectangle encloses an area of the instance space where all positive bags overlap
    - Originally designed for the drug activity problem mentioned in Chapter 2
- Can use other shapes – e.g hyperspheres (balls)
    - Can also use boosting to build an ensemble of balls

Dedicated multi-instance methods

- Previously described methods have hard decision boundaries – an instance either falls inside or outside a hyperectangle/ball
- Other methods use probabilistic soft concept descriptions
- Diverse-density
    - Learns a single reference point in instance space
    - Probability that an *instance* is positive decreases with increasing distance from the reference point

Dedicated multi-instance methods

- Diverse-density
  - Combine instance probabilities within a bag to obtain probability that *bag* is positive
  - "noisy-OR" (probabilistic version of logical OR)
  - All instance-level probabilities 0 → noisy-OR value and bag-level probability is 0
  - At least one instance-level probability is → 1 the value is 1
  - Diverse density, like the geometric methods, is maximized when the reference point is located in an area where positive bags overlap and no negative bags are present
    - Gradient descent can be used to maximize