Data Mining

Practical Machine Learning Tools and Techniques

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

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, ...)
- Extending linear models
  - Support vector machines and neural networks
- Instance-based learning
  - Pruning examples, generalized exemplars, distance functions
- Numeric prediction
  - Regression/model trees, locally weighted regression
- Clustering: hierarchical, incremental, probabilistic
  - Hierarchical, incremental, probabilistic
- Bayesian networks
  - Learning and prediction, fast data structures for learning

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 dealing 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	Normal	False	Yes
...	...	...	...	...

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

Weather data (again!)

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

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

```
If outlook = s
If outlook = r
If outlook = o
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 = yes
If none of the above then play = yes
```


Example

- Split on temperature attribute:

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

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

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

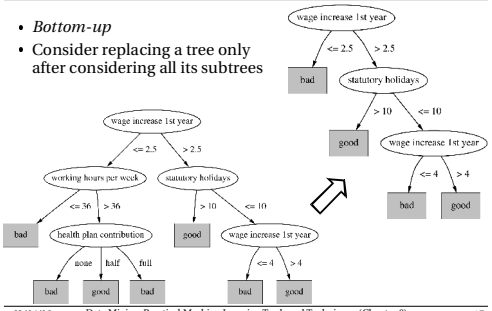
- Pre-pruning may stop the growth process prematurely: *early stopping*
- Classic example: XOR/Parity-problem
  - No *individual* attribute exhibits any significant association to the class
  - Structure is only visible in fully expanded tree
  - Prepruning won't expand the root node
- But: XOR-type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

Postpruning

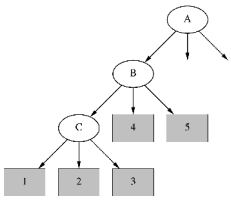
- First, build full tree
- Then, prune it
  - Fully-grown tree shows all attribute interactions
- Problem: some subtrees might be due to chance effects
- Two pruning operations:
  - *Subtree replacement*
  - *Subtree raising*
- Possible strategies:
  - error estimation
  - significance testing
  - MDL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

Subtree replacement

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

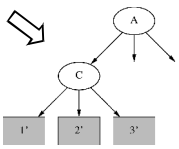


Subtree raising



- 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)

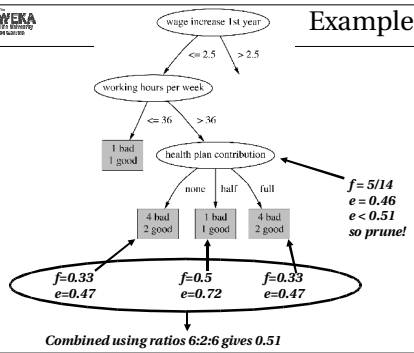
C4.5's method

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

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

- 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



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)

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 Reduce 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

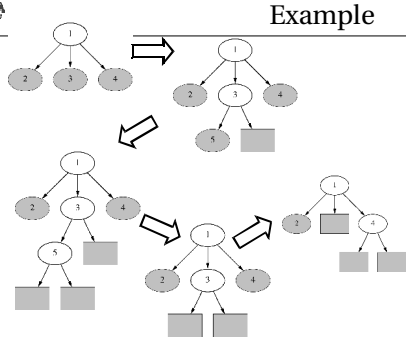
PART

- 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



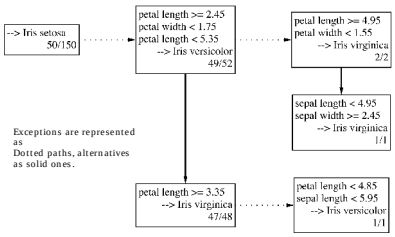
Notes on PART

- 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



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 $n = 3$:

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

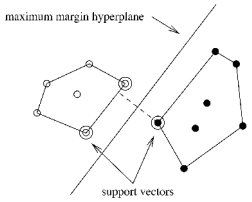
Problems with this approach

- 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

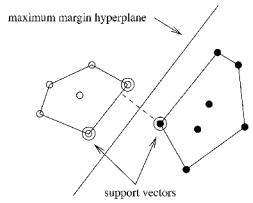
The maximum margin hyperplane



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

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

Finding support vectors

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

- 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:
  $$x = b + \sum_{i \text{ is supp. vector}} \alpha_i y_i (\vec{a}(i) \cdot \vec{a})^n$$
- 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 $x = b + \sum_{i \text{ is supp. vector}} \alpha_i y_i (\vec{a}(i) \cdot \vec{a})^n$
- We can use others: $x = b + \sum_{i \text{ is supp. vector}} \alpha_i y_i K(\vec{a}(i) \cdot \vec{a})$
- Only requirement: $K(\vec{x}_i, \vec{x}_j) = \phi(\vec{x}_i) \cdot \phi(\vec{x}_j)$
- Examples:

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

$$K(\vec{x}_i, \vec{x}_j) = \exp\left(\frac{-(\vec{x}_i - \vec{x}_j + 1)^2}{2\sigma^2}\right)$$

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

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 ⇒ 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

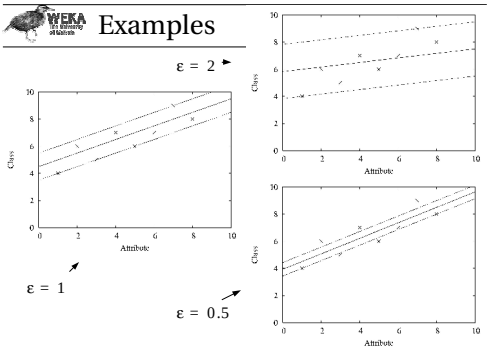
Support vector regression

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



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 class value 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:

$$\sum_j y(j) K(\vec{a}'(j), \vec{a})$$

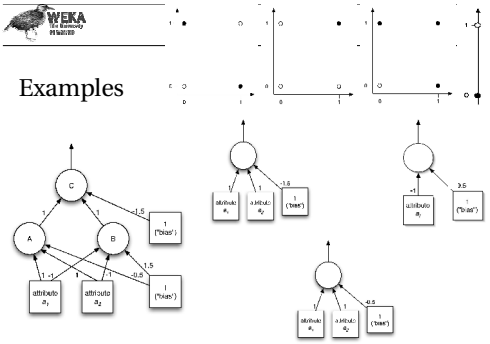
Comments on kernel perceptron

- 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 of
- Structure of MLP is usually found by experimentation
- Parameters can be found using *backpropagation*

Examples



Backpropagation

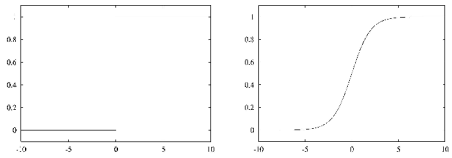
- Hot to learn weights given network structure?
  - Cannot simply use perceptron learning rule because we have hidden layer(s)
  - Function we are trying to minimize: error
  - Can use a general function minimization technique called *gradient descent*
    - Need differentiable *activation function*: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

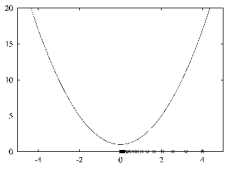
$$E = \frac{1}{2}(y - f(x))^2$$

The two activation functions



Gradient descent example

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

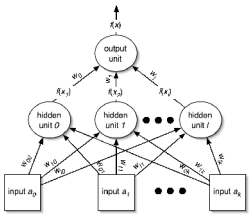


Can only find a local minimum!

Minimizing the error I

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

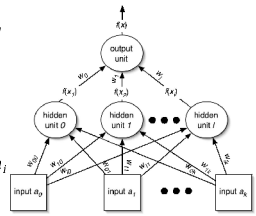
$$\frac{dE}{dw_i} = (y - f(\mathbf{x}))\frac{df(x)}{dw_i}$$
$$\frac{df(x)}{dx} = f(\mathbf{x})(1 - f(\mathbf{x}))$$
$$\mathbf{x} = \sum_i w_i f(\mathbf{x}_i)$$
$$\frac{df(x)}{dw_i} = f'(\mathbf{x}) f(\mathbf{x}_i)$$
$$\frac{dE}{dw_i} = (y - f(\mathbf{x}))\, f'(\mathbf{x})\, f(\mathbf{x}_i)$$



Minimizing the error II

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

$$\frac{dE}{dw_{ij}} = \frac{dE}{dx}\frac{dx}{dw_{ij}} = (y - f(\mathbf{x}))\, f'(\mathbf{x})\frac{dx}{dw_{ij}}$$
$$\mathbf{x} = \sum_i w_i f(\mathbf{x}_i)$$
$$\frac{dx}{dw_{ij}} = w_i \frac{df(x_i)}{dw_{ij}}$$
$$\frac{df(x_i)}{dw_{ij}} = f'(\mathbf{x}_i)\frac{dx_i}{dw_{ij}} = f'(\mathbf{x}_i)\, a_j$$
$$\frac{dE}{dw_{ij}} = (y - f(\mathbf{x}))\, f'(\mathbf{x})\, w_i f'(\mathbf{x}_i)\, a_j$$



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

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 $|x_i - y_i|$

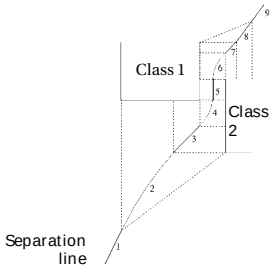
Rectangular generalizations

- 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



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 ⇒ 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:

$$\frac{n+v}{n+v} \times \texttt{average\_absolute\_error}$$

  - 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:

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

- 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)
}
```

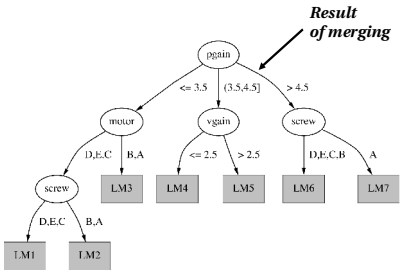

prune

```
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 kth 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

Clustering: how many clusters?

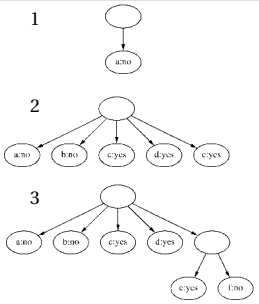
- How to choose k in k-means? Possibilities:
  - Choose k that minimizes cross-validated squared distance to cluster centers
  - Use penalized squared distance on the training data (eg. using an MDL criterion)
  - Apply k-means recursively with $k = 2$ and use stopping criterion (eg. based on MDL)
    - 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)

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



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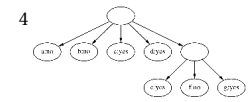
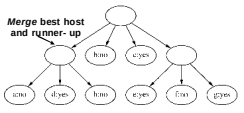


5

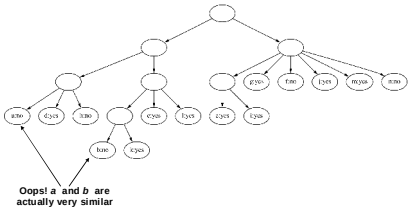
Merge best host and runner- up



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

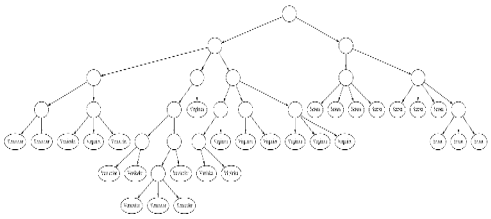
Final hierarchy

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

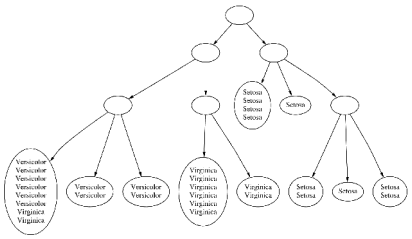


Oops! *a* and *b* are actually very similar

Example: the iris data (subset)



Clustering with cutoff



Category utility

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

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

- Every instance in different category ⇒ numerator becomes

$$n - \sum_i \sum_j Pr[a_j = v_{ij}]^2 \quad \longleftarrow \textit{maximum}$$

number of attributes

Numeric attributes

- Assume normal distribution:

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

- Then:

$$\sum_j Pr[a_j = v_{ij}]^2 \equiv \int f(a_j)^2 \, da_j = \frac{1}{2\sqrt{\pi}\sigma_j}$$

- Thus

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

becomes

$$CU(C_1, C_2, \ldots, C_k) = \frac{\sum_i Pr[C_i] \frac{1}{2\sqrt{\pi}} \sum_j (\frac{1}{\sigma_{ij}} - \frac{1}{\sigma_j})}{k}$$

- 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

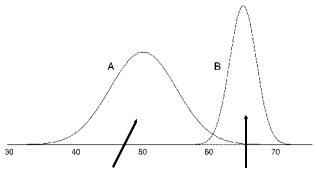
- Model data using a *mixture* of distributions
- One cluster, one distribution
  - governs probabilities of attribute values in that cluster
- *Finite mixtures*: finite number of clusters
- Individual distributions are normal (usually)
- Combine distributions using cluster weights

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:

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

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:

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

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:

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

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

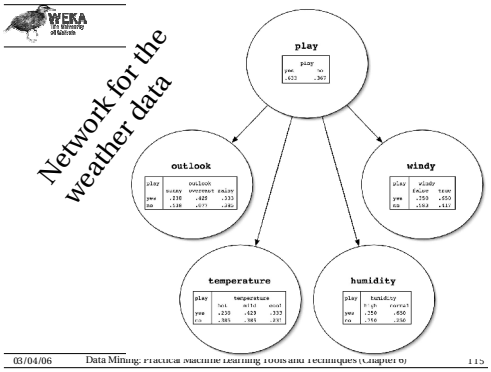
- Can interpret clusters by using supervised learning
  - post-processing step
- Decrease dependence between attributes?
  - pre-processing step
  - E.g. use *principal component analysis*
- Can be used to fill in missing values
- Key advantage of probabilistic clustering:
  - Can estimate likelihood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

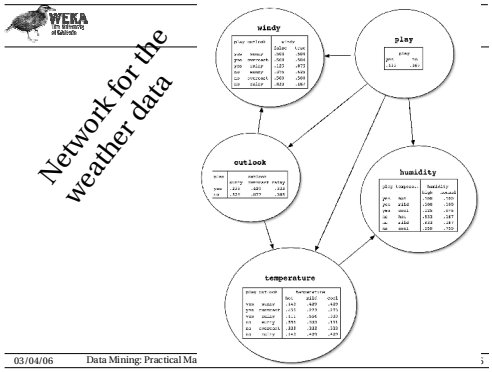
From naïve Bayes to Bayesian Networks

- 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)





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:

$$Pr[a_1, a_2, \ldots, a_n] = \prod_{i=1}^{n} Pr[a_i | a_{i-1}, \ldots, a_1] = \prod_{i=1}^{n} Pr[a_i | a_i \text{'s parents}]$$

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: $AICscore = -\text{LL} + K$
  - MDL measure: $MDLscore = -\text{LL} + \frac{K}{2}\log N$
  - *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 likelihoo

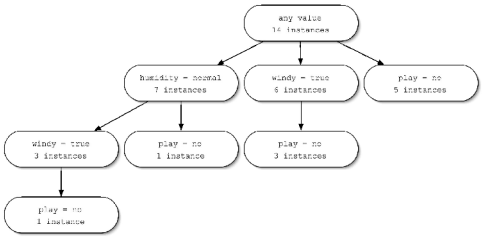
- In classification what we really want is to maximize probability of class given other attributes
  - *Not* probability of the instances
- But: no closed-form solution for probabilities in nodes' tables that maximize this
- However: can easily compute conditional probability of data based on given network
- 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	7
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