Decision Trees. Bagging. Random Forest

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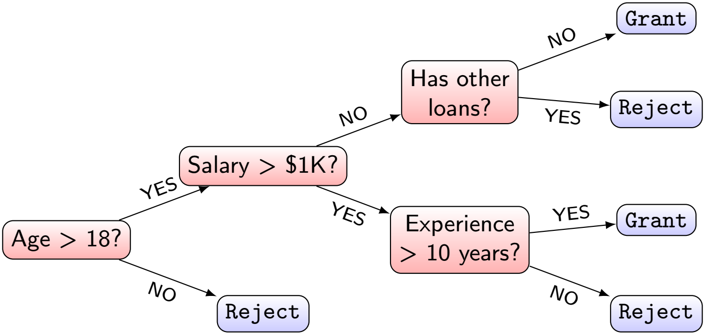
Outline

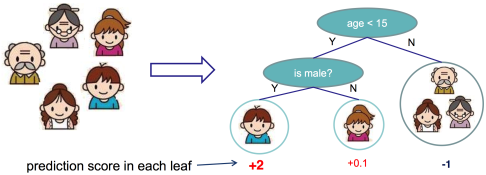
Decision making at a bank



A decision tree consists of

- Nodes
  - Test for the value of a certain attribute
- Edges
  - Correspond to the outcome of a test
  - Connect to the next node of leaf
- Leaves
  - Terminal nodes that predict the outcome

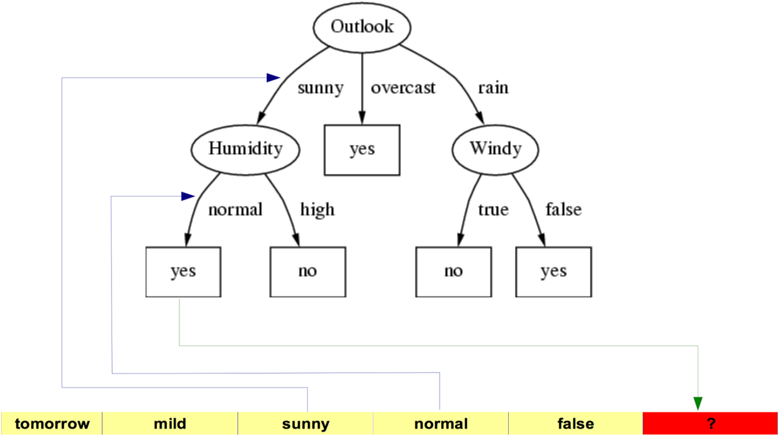
Input: age, gender, occupation,... $\Rightarrow$ Does the person like computer games?



Example: weather prediction

Day	Temperature	Outlook	Humidity	Windy	Play Golf?
07-05	hot	sunny	high	false	no
07-06	hot	sunny	high	true	no
07-07	hot	overcast	high	false	yes
07-09	cool	rain	normal	false	yes
07-10	cool	overcast	normal	true	yes
07-12	mild	sunny	high	false	no
07-14	cool	sunny	normal	false	yes
07-15	mild	rain	normal	false	yes
07-20	mild	sunny	normal	true	yes
07-21	mild	overcast	high	true	yes
07-22	hot	overcast	normal	false	yes
07-23	mild	rain	high	true	no
07-26	cool	rain	normal	true	no
07-30	mild	rain	high	false	yes

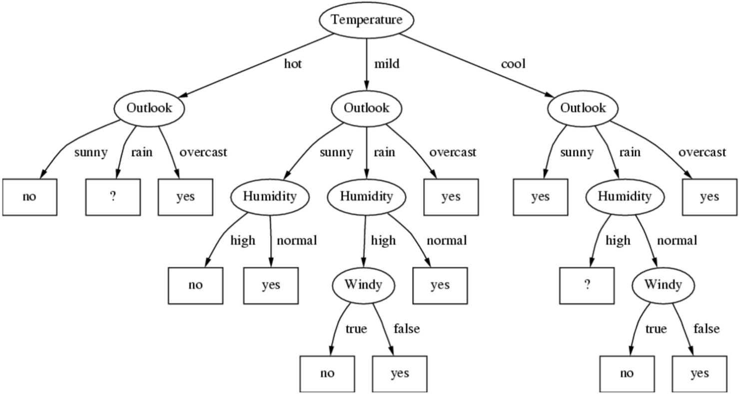
today	cool	sunny	normal	false	?
tomorrow	mild	sunny	normal	false	?


Outlook
sunny
overcast
rain
Humidity
yes
Windy
normal
high
true
false
yes
no
no
yes
tomorrow
mild
sunny
normal
false
?

- Typical decision tree learning algorithms
  — Top-Down Induction of Decision Trees
- Learn trees in a Top-Down fashion
  — Divide the problem in subproblems
  — Solve each subproblem
- Basic Divide-And-Conquer algorithm
  1. Select a test for root node
     Create branch for each possible outcome of the test
  2. Split instances into subsets
     One for each branch extending from the node
  3. Repeat recursively for each branch, using only instances that reach the branch
  4. Stop recursion for a branch if all its instances have the same class

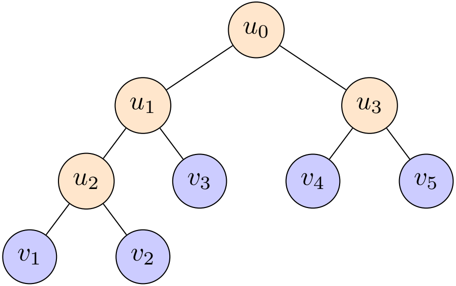
- Function ID3
  - **Input**: example set S_m
  - **Output**: Decision Tree DT
- If all examples in S_m belong to the same class c
  - Return a new leaf and label it with c
- Else
  1. Select an attribute x_j according to some heuristic approach
  2. Generate a new node in DT with x_j as test
  3. For each possible value e_r of x_j
     a) Let $S_r =$ all examples in S_m with $x_j = e_r$
     b) Use ID3 to construct a decision tree DT_r for examples in S_r
     c) Generate an edge that connects DT and DT_r

Example: DT for weather prediction



- also explains all of the training data
- will it generalize well to new data?

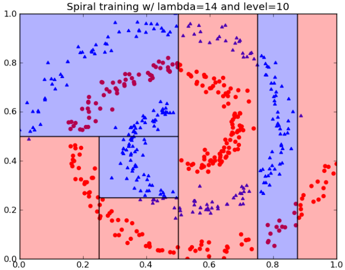
- Decision tree is often a binary tree DT
- Internal nodes $u \in DT$: *predicates* $\beta_u : X \to \{0, 1\}$
- Leafs $v \in DT$: *predictions* y
- Algorithm $h(\mathbf{x})$ starts at $u = u_0$
  - Compute $b = \beta_u(\mathbf{x})$
  - If $b = 0$, $u \leftarrow \mathrm{LeftChild}(u)$
  - If $b = 1$, $u \leftarrow \mathrm{RightChild}(u)$
  - If u is a leaf, return some y
- In practice for a real variable: $\beta_u(\mathbf{x}; j, t) = 1[x_j < t]$

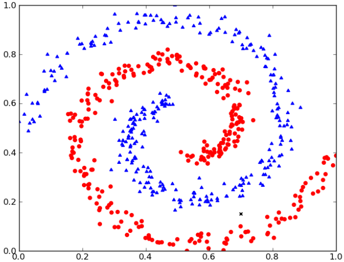


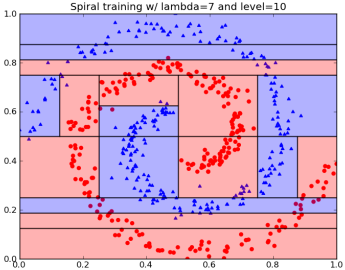
Greedy binary tree learning for classification

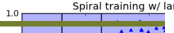
- Input: training set $S_m = \big\{(\mathbf{x}_i, y_i)\big\}_{i=1}^{m}$
  1. Greedily split S_m into S_1 and S_2:
     $$S_1(j,t) = \{(\mathbf{x}, y) \in S_m | x_j \le t\}, \qquad S_2(j,t) = \{(\mathbf{x}, y) \in S_m | x_j > t\}$$
     optimizing a given loss: $Q(S_m, j, t) \to \min\limits_{(j,t)}$
  2. Create internal node u corresponding to the predicate $1[x_j < t]$
  3. If a stopping criterion is satisfied for u,
     declare it a leaf, setting some $c_u \in Y$ as leaf prediction
  4. If not, repeat 1–2 for $S_1(j,t)$ and $S_2(j,t)$
- Output: a decision tree DT

Greedy tree learning for binary classification

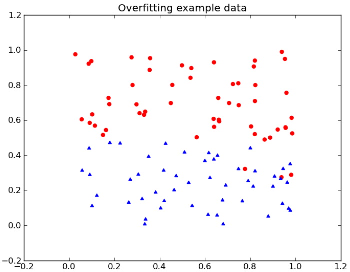


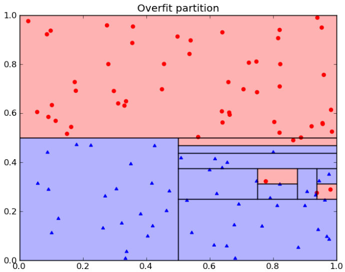






With decision trees, overfitting is extra-easy!



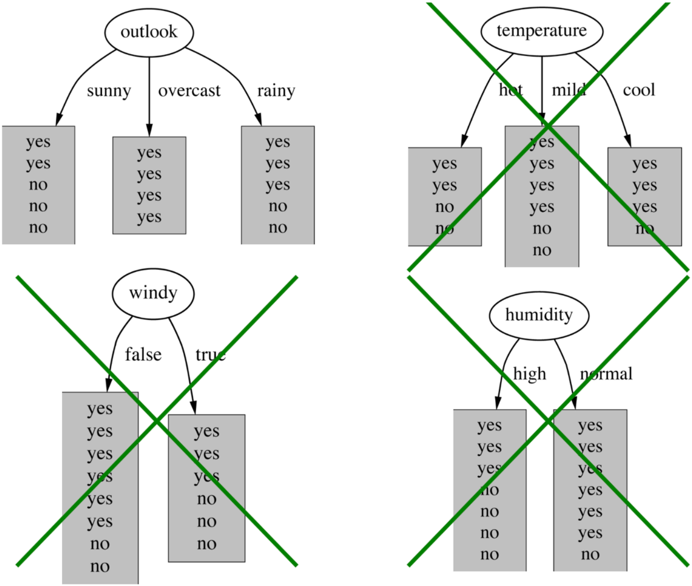


Design choices for learning a decision tree classifier

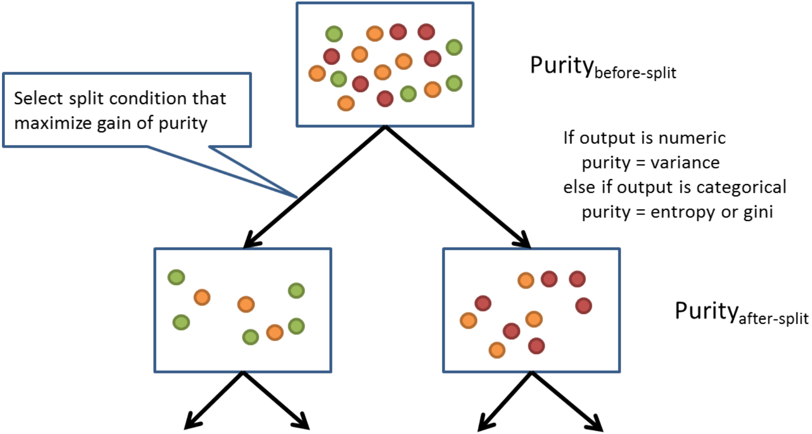
- Type of predicate in internal nodes
- The loss function $Q(S_m, j, t)$
- The stopping criterion
- Hacks: missing values, pruning, etc.

- CART, C4.5, ID3

Which attribute to select as the root?



The idea: maximize purity



Picture credit: https://dzone.com/refcardz/machine-learning-predictive

What is a good Attribute?

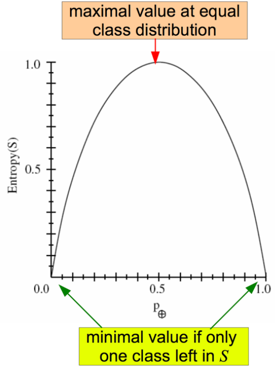
- We want to grow a simple tree
  - A good attribute split the data so that each successor node is as pure as possible, e.g. it contains mostly a singlel class
- We want a measure that prefers attributes with high degree of order:
  - Maximum order: all examples are of the same class
  - Minimum order: all classes are equally likely
- Entropy is a measure for (un)-orderliness

Entropy (binary classification)

- S is a set of examples
- p_+ is the proportion of examples in positive class
- $p_- = 1 - p_+$ is the proportion of examples in negative class
- Entropy

$$E(S) = -p_+ \cdot \log_2 p_+ - p_- \cdot \log_2 p_-$$

- Amount of un-orderliness in the class distribution of S
- p_i is the proportion of examples in S from the i-th class



$$E(S) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 - \ldots - p_K \log_2 p_K = -\sum_{k=1}^{K} p_k \log_2 p_k$$

- **Outlook** = **sunny**: 3 examples **yes**, 2 examples **no**

$$E(Outlook = sunny) = -\frac{2}{5}\log\left(\frac{2}{5}\right) - \frac{3}{5}\log\left(\frac{3}{5}\right) = 0.971$$

- **Outlook** = **overcast**: 4 examples **yes**, 0 examples **no**

$$E(Outlook = overcast) = -1\log(1) - 0\log(0) = 0$$

- **Outlook** = **rainy**: 2 examples **yes**, 3 examples **no**

$$E(Outlook = rainy) = -\frac{3}{5}\log\left(\frac{3}{5}\right) - \frac{2}{5}\log\left(\frac{2}{5}\right) = 0.971$$

Average Entropy/Information

- **Problem**:
  - Entropy can be applied only to a single (sub-)set of examples
  - Quality of an entire split, corresponding to the attribute x_j?
- **Solution**:
  - Average over all sets resulting from the split, weighted by their size

$$I(S, j) = \sum_r \frac{|S_r|}{|S|} \cdot E(S_r)$$

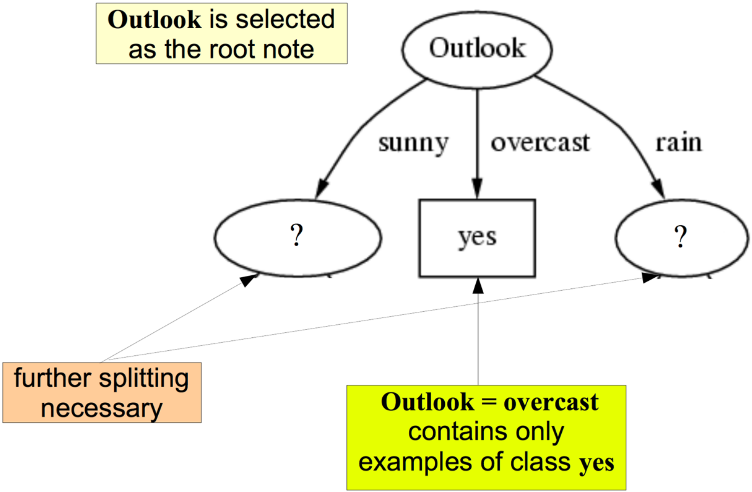
  - **Example**: average entropy for attribute **Outlook**

$$I(Outlook) = \frac{5}{14} \cdot 0.971 + \frac{4}{14} \cdot 0 + \frac{5}{14} \cdot 0.971 = 0.693$$

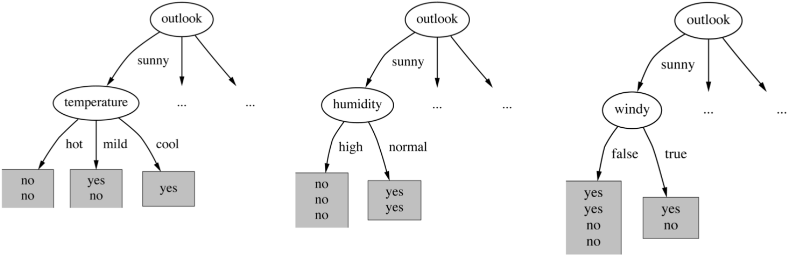
- When an attribute x_j splits the set S into subsets S_r
  - we compute the average entropy
  - and compare the sum to the entropy of the original set S
- Information Gain for Attribute x_j

$$Q(S, j) = E(S) - I(S, j) = E(S) - \sum_r \frac{|S_r|}{|S|} \cdot E(S_r)$$

  - We select an attribute maximizing the difference, i.e. attribute that reduces the un-orderliness most
  - Maximizing IG $\Leftrightarrow$ minimizing average entropy
- $Gain(S, Humidity) = 0.151$; **Gain(S, Outlook)** $= 0.246$; $Gain(S, Wind) = 0.048$; $Gain(S, Temperature) = 0.029$

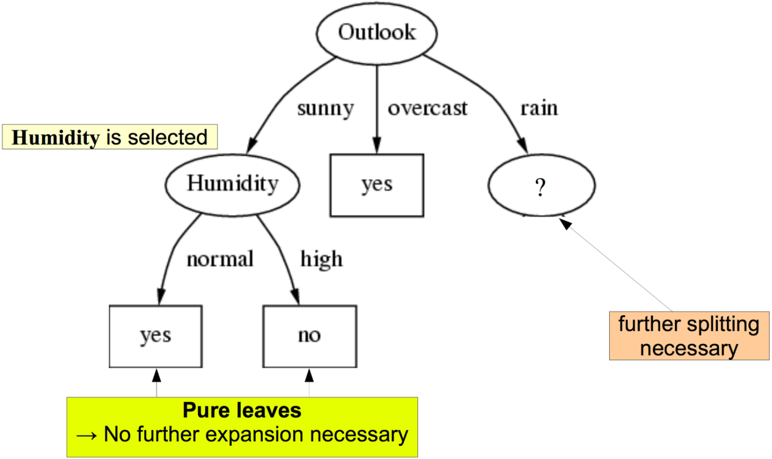

Outlook is selected as the root note
Outlook
sunny
overcast
rain
?
yes
?
further splitting necessary
Outlook = overcast contains only examples of class **yes**

Example

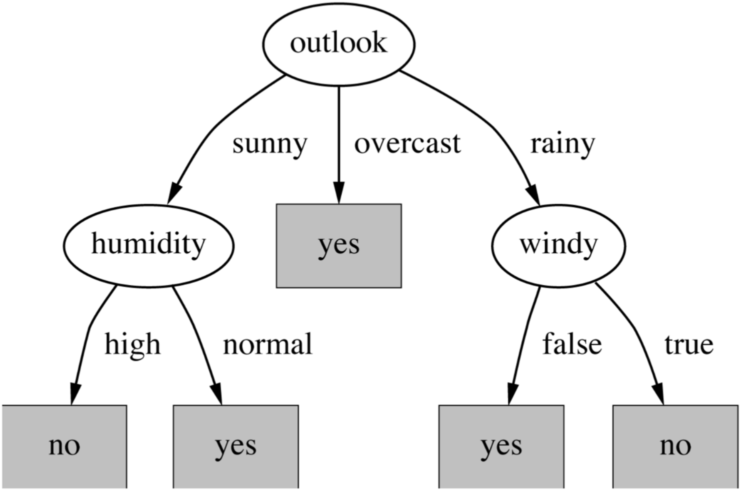


$$\begin{aligned}\text{Gain}(\textit{Temperature}) &= 0.571 \text{ bits}\\ \text{Gain}(\textit{Humidity}) &= 0.971 \text{ bits}\\ \text{Gain}(\textit{Windy}) &= 0.020 \text{ bits}\end{aligned}$$

Humidity is selected


Outlook
sunny
overcast
rain
Humidity is selected
Humidity
yes
?
normal
high
yes
no
further splitting necessary
Pure leaves
→ No further expansion necessary

Example: final decision tree



Formal definition: Loss function $Q(S, j)$ for a binary tree

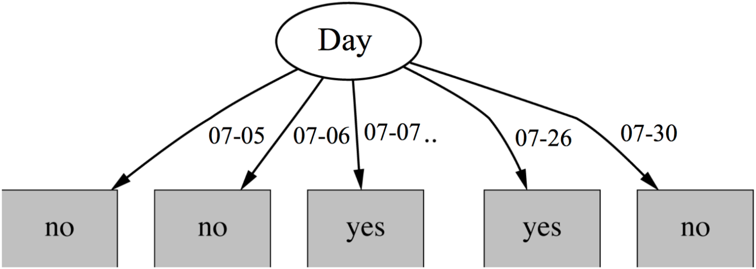
- S_t: the subset of S at step t
- With the current split, let $S_l \subseteq S_t$ go left and $S_r \subseteq S_t$ go right
- Choose predicate to optimize

$$Q(S_t, j) = E(S_t) - \frac{|S_l|}{|S_t|} E(S_l) - \frac{|S_r|}{|S_t|} E(S_r) \to \max$$

- $E(S)$: impurity criterion
- Generally

$$E(S) = \min_{c \in Y} \frac{1}{|S|} \sum_{(\mathbf{x}_i, y_i) \in S} L(y_i, c)$$

- Problematic: attributes with a large number of values
  - Extreme case: each example has its own value
  - E.g. ID; Day attribute in weather data
- Subsets are more likely to be pure if there is a large number of different attribute values
  - Information gain is biased towards choosing attributes with a large number of values
- Problems:
  - Overfitting
  - Data is fragmented into too many small sets



- Entropy of split

$$I(Day) = \frac{1}{14}\left(E([0,1]) + E([0,1]) + \ldots + E([0,1])\right) = 0$$

- Information gain is maximal for **Day** (0.940 bits)

- Intrinsic information of a split, done w.r.t.
- Entropy of distribution of instances into branches
- i.e. how much information do we need to tell which branch as instance belongs to

$$IntI(S, j) = -\sum_{r} \frac{|S_r|}{|S|} \log_2 \frac{|S_r|}{|S|}$$

- Empirical Observation: attributes with higher intrinsic information are less useful
- Intrinsic information of **Day** attribute

$$IntI(Day) = 14 \times \left(-\frac{1}{14} \cdot \log \left(\frac{1}{14} \right) \right) = 3.807$$

- Modification of the information gain that reduces its bias towards multi-values attributes
- Takes number and size of branches into account when choosing an attribute
- Gain Ratio

$$GR(S, j) = \frac{Q(S, j)}{IntI(S, j)}$$

- **Example**: GR of **Day** attribute

$$GR(Day) = \frac{0.940}{3.807} = 0.246$$

- $GR(Outlook) = 0.157$; $GR(Humidity) = 0.152$; $GR(Temperature) = 0.019$; $GR(Windy) = 0.049$
- **Day** attribute would still win... $\Rightarrow$ careful analysis!!!
- Anyway, GR is more reliable than IG!!!

- Many alternatives measures to Information Gain
- Most popular alternative: Gini index

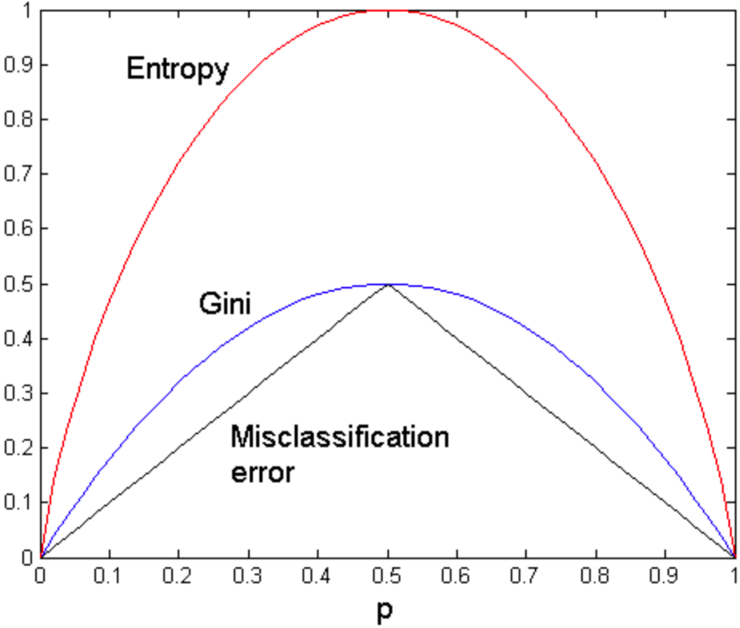
$$Gini(S) = \sum_k p_k(1 - p_k) = 1 - \sum_k p_k^2$$

- Average Gini index (instead of average entropy/information)

$$Gini(S, j) = \sum_r \frac{|S_r|}{|S|} \cdot Gini(S_r)$$

- Gini Gain:
  - Can be defined analogously to information gain
  - Typically avg. Gini is minimized instead of maximizing Gini gain

Comparison among Splitting Criteria: binary case



Other information criteria

- **Regression:**
  - Impurity
$$E(S) = \min_{c \in Y} \frac{1}{|S|} \sum_{(\mathbf{x}_i, y_i) \in S} (y_i - c)^2$$
  - Sum of squared residuals minimized by
$$c = \frac{1}{|S|} \sum_{(\mathbf{x}_i, y_i) \in S} y_i$$
  - Impurity $\equiv$ variance of the target
- **Classification:**
  - Let (share of y_i's equal to k)
$$p_k = \frac{1}{|S|} \sum_{(\mathbf{x}_i, y_i) \in S} [y_i = k]$$
  - Miss rate:
$$E(S) = \min_{c \in \mathbb{Y}} \frac{1}{|S|} \sum_{(\mathbf{x}_i, y_i) \in S} [y_i \neq c]$$

    Impurity criterion is defined as

    Minimizing miss rate $\quad 1 - E(S)$

- Permit numeric attributes
- Allow missing values
- Be robust in the presence of noise
- Be able to approximate arbitrary concept description
- Computationally efficient

As a result C4.5 has been developed!

- Standard method: binary splits: E.g. temperature < 20
- Unlike nominal attributes, there are many possible split points
- Selection of “best” split points computationally is more demanding
- Split points can be placed between values or directly at values
- Sort values before performing scan!

- Splitting (multi-way) on a nominal attribute exhausts all information in that attributed
  - 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 attributed, or
  - Multi-way splits instead of binary ones

- If an attribute with a missing value needs to be tested:
  - split the instance into fractional instances (pieces)
  - one piece for each outgoing branch of the node
  - a piece going down a branch receives a weight proportional to the popularity of the branch
  - weights sum to 1
- Info gain or gain ratio work with fractional instances
  - use sums of weights instead of counts
- During classification split the instance in the same way
  - Merge probability distribution using weights of fractional instances

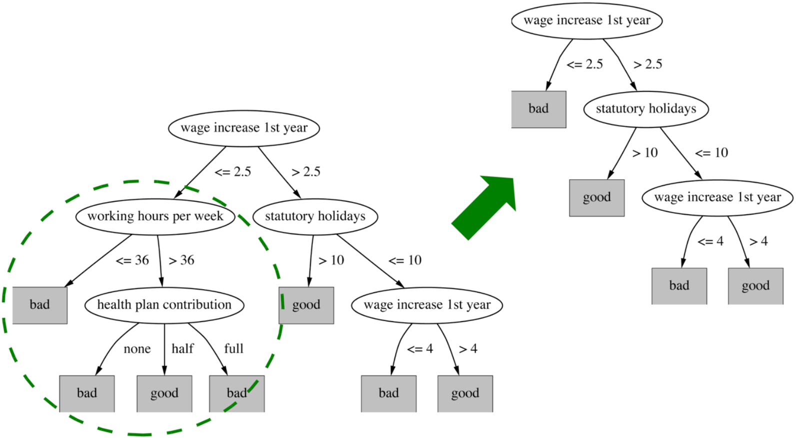
- The smaller the complexity of a concept, usually the better its generalization ability is
- We need to try to keep the learned concepts simple
- **Pre-pruning**:
  - Stop growing a branch when information becomes unreliable
- **Post-pruning**
  - Grow a decision tree that correctly classifies all training data
  - Simplify it later by replacing some nodes with leafs
- Post-pruning is preferred in practice, pre-pruning can “stop early”

- Based on statistical significant 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-square test
- ID3 uses chi-square test in addition to information gain
  - Only statistically significant attributes are allowed to be selected by information gain procedure
- Pre-pruning is faster than post-pruning. However, the process may stop too early

Post-pruning

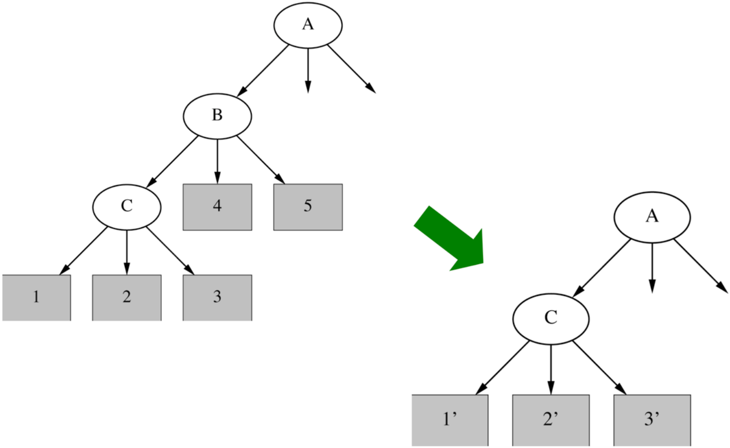
- Basic idea
  - First grow a full tree to capture all possible attributes interactions
  - Later remove those that are due to chance
  - As long as the performance not decreases try simplification operators
- Two subtree simplification operators
  - Subtree replacement
  - Subtree raising
- Possible performance evaluation strategies
  - Error estimation e.g. on a separate pruning set
  - Significance testing
  - MDL principle

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



Subtree raising

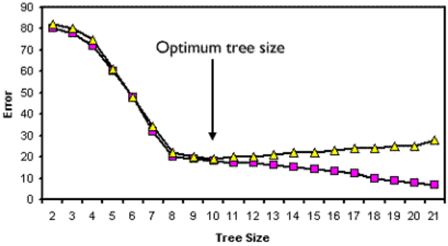
- Delete node B
- Redistribute instances of leaves 4 and 5 into C



- Prune only if it does not increase the estimated error
  - Error on the training data is NOT a useful estimator
- Reduced Error Pruning
  - Use hold-out set for pruning
- C4.5 method
  - Derive confidence interval from training data
  - Assume that the true error is on the upper bound of this confidence interval
- Optimize the accuracy of a decision tree on a separate pruning (validation) set. Prune as long as the error on the validation set does not increase

Stopping rules for decision tree learning

- Significantly impacts learning performance
- Multiple choices available:
  - Maximum tree depth
  - Minimum number of objects in leaf
  - Maximum number of leafs in tree
  - Stop if all objects fall into same leaf
  - Constrain quality improvement
    (stop when improvement gains drop below $s\%$)
- Typically selected via exhaustive search and cross-validation

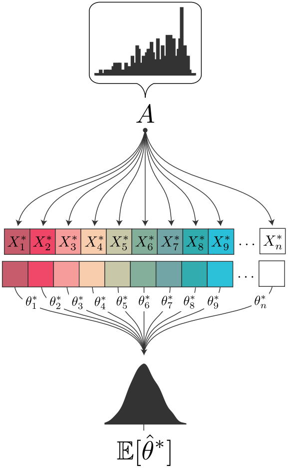


- Learn a large tree (effectively overfit the training set)
- Detect overfitting via K-fold cross-validation
- Optimize structure by removing least important nodes

Complexity of tree induction

- Assume
  - d attributes
  - m training instances
  - tree depth $O(\log m)$
- Building a tree $O(dm \log(m))$
- Subtree replacement $O(m)$
- Subtree raising $O(m(\log(m))^2)$
- Total cost: $O(dm \log(m)) + O(m(\log(m))^2)$

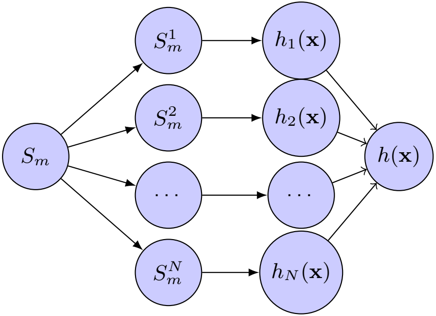
- Input: a sample $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$
- Bootstrapping: generate new samples S_m^* of $(\mathbf{x}_i, y_i)$ drawn from S_m uniformly at random with replacement (replicated $(\mathbf{x}_i, y_i)$ possible!)
- **Ensemble learning idea:**
  1. Generate N bootstrapped samples $S_m^1, \dots, S_m^N$
  2. Learn N hypotheses $h_1, \dots, h_N$
  3. Average predictions to obtain $h(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N h_i(\mathbf{x})$
  4. Profit!



Picture credit: http://www.drbunsen.org/bootstrap-in-picture

- Input: a sample $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$
- Weak learners via bootstrapping $h_i(\mathbf{x}) = h_i(\mathbf{x}|S_m^i)$
- Ensemble average

$$h(\mathbf{x}) = \frac{1}{N}\sum_{i=1}^{N} h_i(\mathbf{x}) = \\ = \frac{1}{N}\sum_{i=1}^{N} h_i(\mathbf{x}|S_m^i)$$



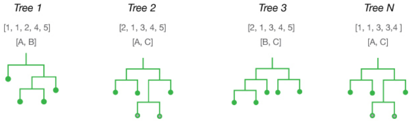
- Bagging over (weak) decision trees
- Reduce error via averaging over instances and features
- Input: a sample $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$, where $\mathbf{x}_i \in \mathbb{R}^d, y_i \in Y$
- The algorithm iterates for $i = 1, \ldots, N$:
  1. Pick p random features out of d
  2. Bootstrap a sample $S_m^i = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$, where $\mathbf{x}_i \in \mathbb{R}^p, y_i \in Y$
  3. Learn a decision tree $h_i(\mathbf{x})$ using bootstrapped S_m^i
  4. Stop when leafs in h_i contain less that $n_{\min}$ instances

$\mathbf{x}_i \in \{\mathrm{A}, \mathrm{B}, \mathrm{C}\}$

$S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^5$

Bootstrap $S_m^i, i \in \{1, 2, 3, 4\}$

Learn $\mathrm{Tree}_i(\mathbf{x})$ using S_m^i



Picture credit: http://www.thefactmachine.com/random-forests

Random Forest: synthetic examples