# Decision Trees. Bagging. Random Forest

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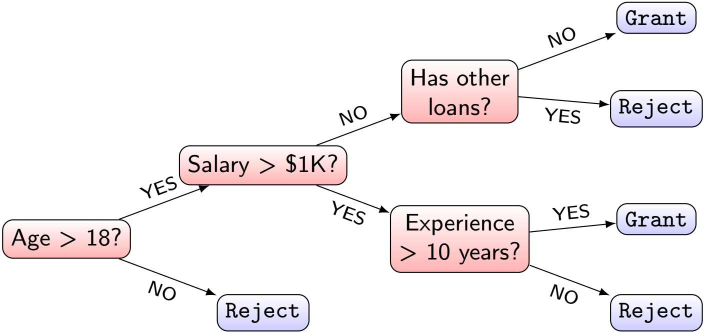
# Outline

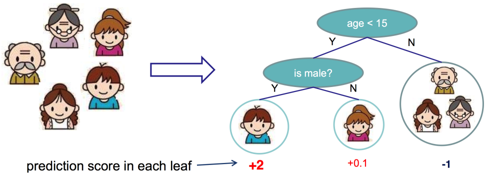
# Decision making at a bank



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?

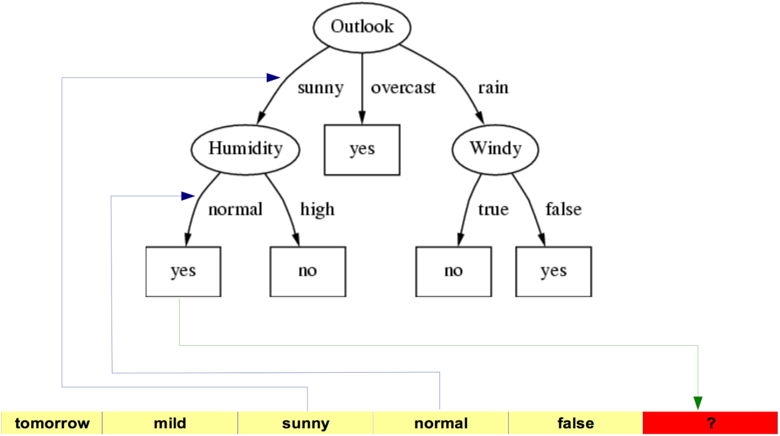


# Example: weather prediction

| 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 | ? |

# Decision Tree Learning



- 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

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- 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 $x_j$
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     c) Generate an edge that connects $DT$ and $DT_r$

# ID3 Algorithm

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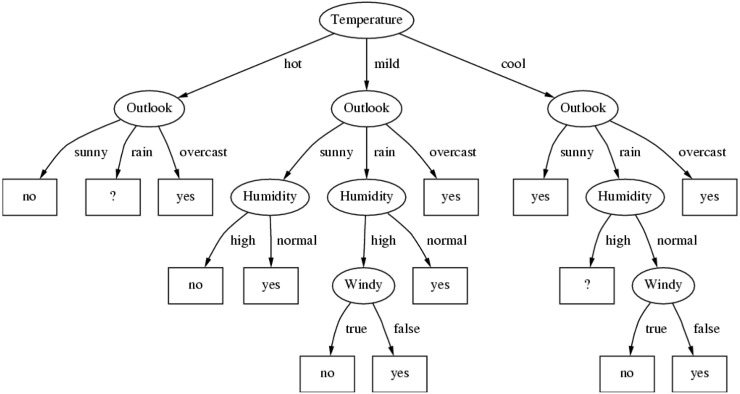
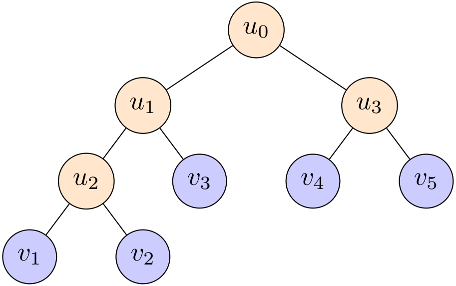



- also explains all of the training data
- will it generalize well to new data?

- 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* $y$



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  - Compute $b = \beta_u(\mathbf{x})$
  - If $b = 0$, $u \leftarrow \mathrm{LeftChild}(u)$
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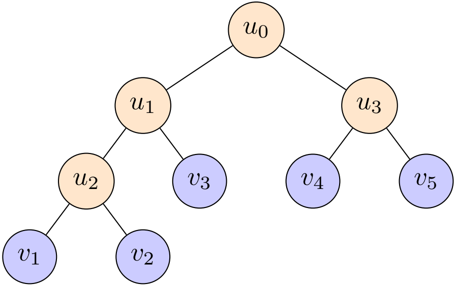
  - If $u$ is a leaf, return some $y$



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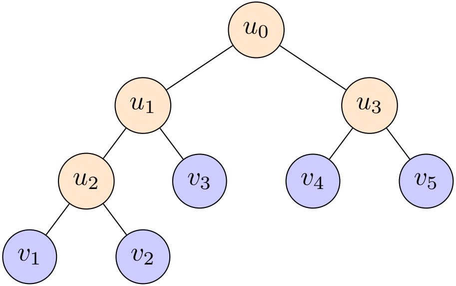
- In practice for a real variable: $\beta_u(\mathbf{x}; j, t) = 1[x_j < t]$



- Input: training set $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$
   1. Greedily split $S_m$ into $S_1$ and $S_2$:

      $$S_1(j,t) = \{(\mathbf{x}, y) \in S_m | x_j \leq t\}, \qquad S_2(j,t) = \{(\mathbf{x}, y) \in S_m | x_j > t\}$$

      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 $S_2(j,t)$
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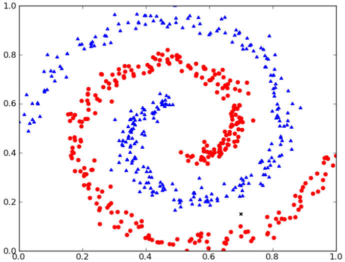
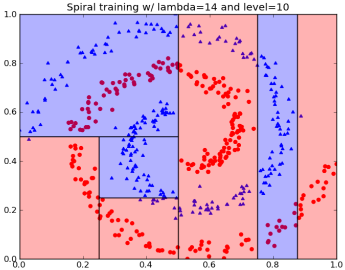
# Greedy tree learning for binary classification



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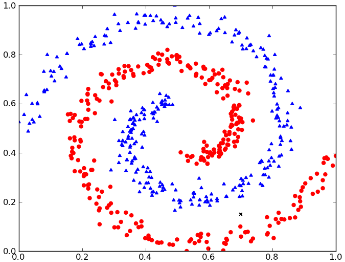


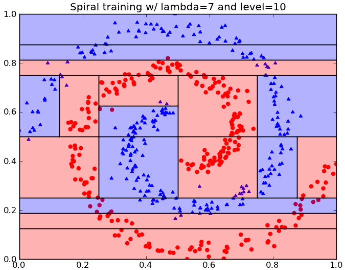

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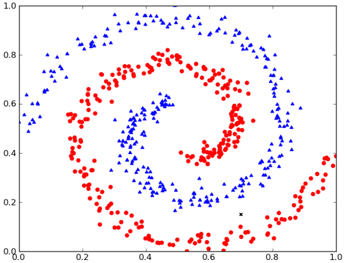
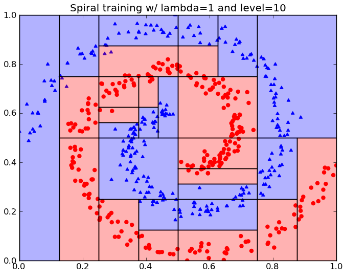
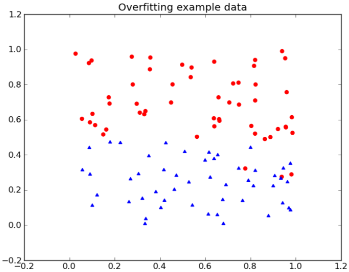
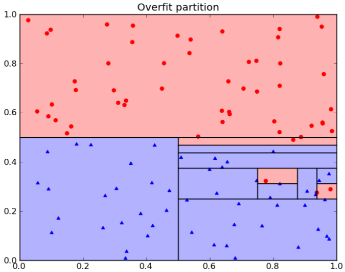


# With decision trees, overfitting is extra-easy!

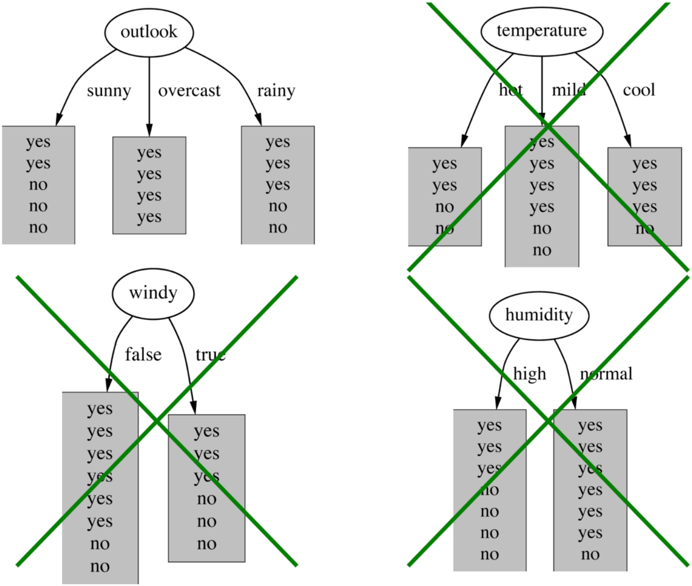


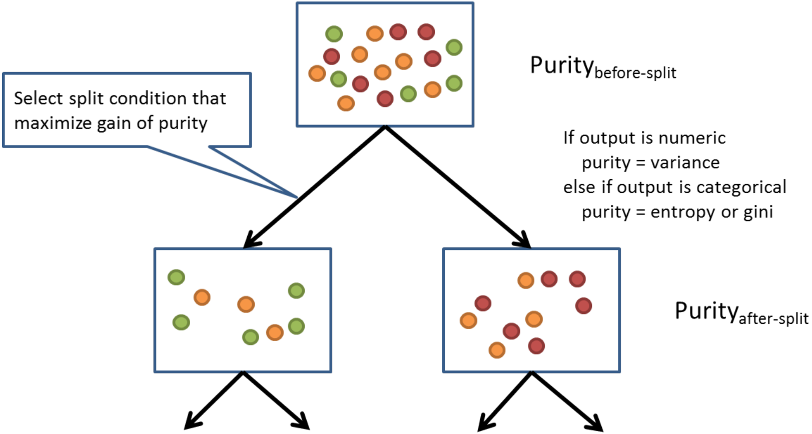
- Type of predicate in internal nodes
- The loss function $Q(S_m, j, t)$
- The stopping criterion
- Hacks: missing values, pruning, etc.

- CART, C4.5, ID3

# Which attribute to select as the root?



# The idea: maximize purity




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

- 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

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- $S$ 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

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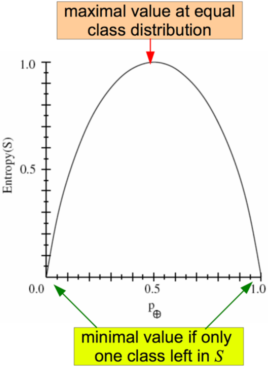

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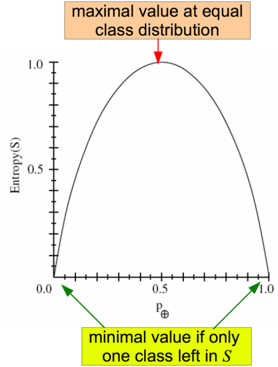

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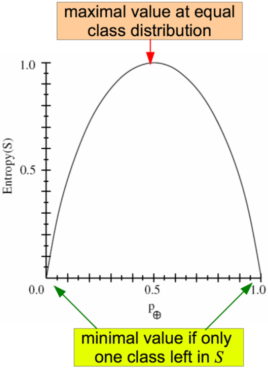

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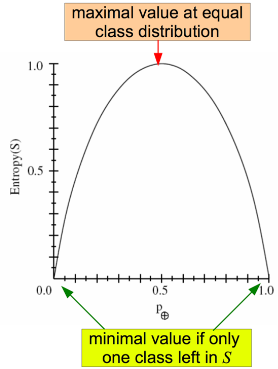


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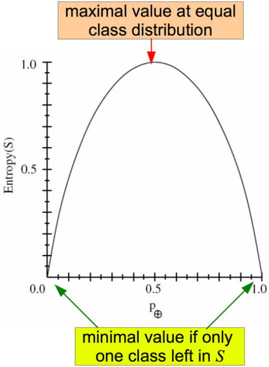
- $p_i$ is the proportion of examples in $S$ from the i-th class




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

- **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**

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

- **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

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

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

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- When an attribute $x_j$ splits the set $S$ into subsets $S_r$
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  - 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)** $= 0.246$; $Gain(S, Wind) = 0.048$; $Gain(S, Temperature) = 0.029$

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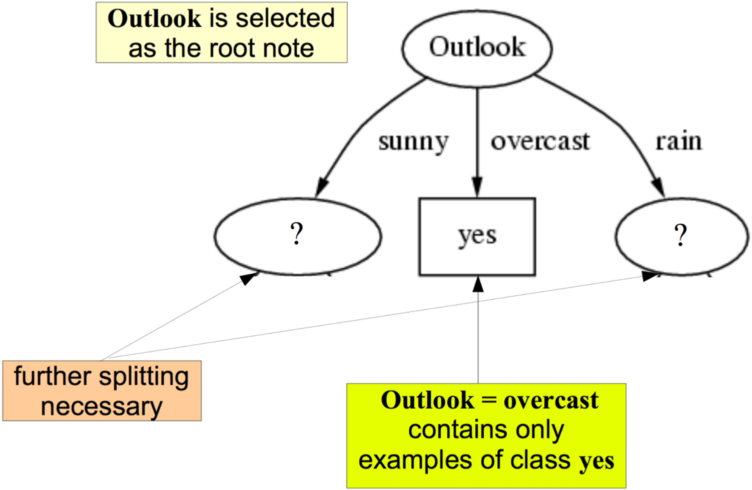
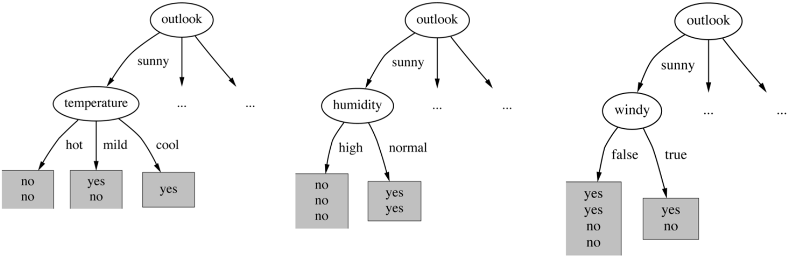

**Outlook** is selected as the root note
Outlook
sunny
overcast
rain
?
yes
?
further splitting necessary
**Outlook = overcast** contains only examples of class **yes**

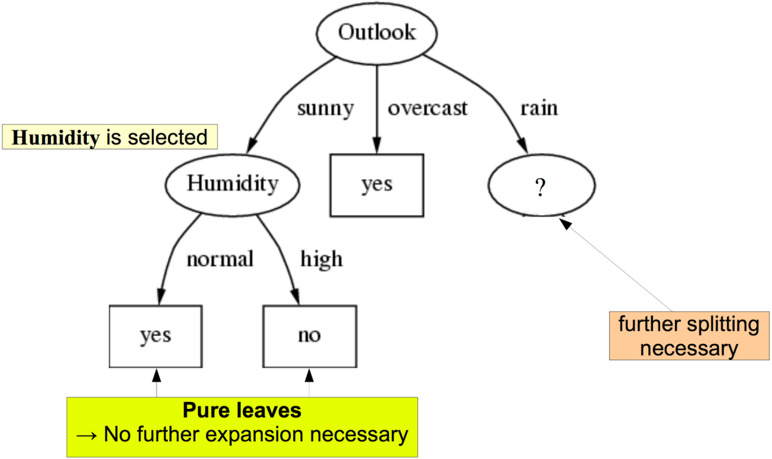
# Example



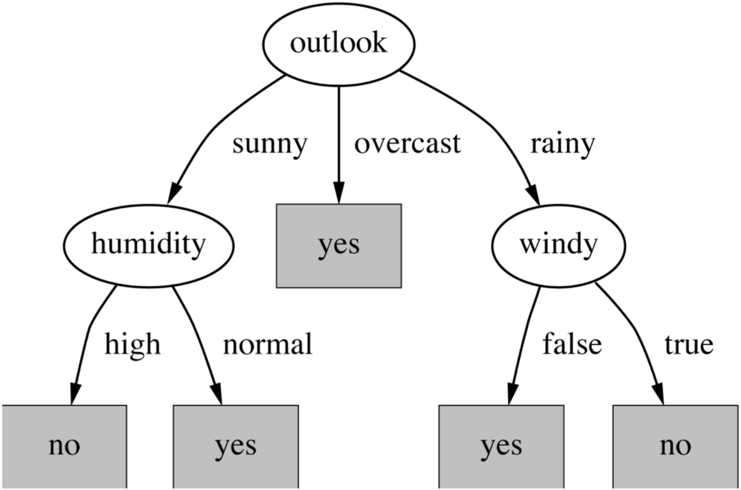

$$\left.\begin{aligned}\text{Gain}(\textit{Temperature}) &= 0.571 \text{ bits}\\ \text{Gain}(\textit{Humidity}) &= 0.971 \text{ bits}\\ \text{Gain}(\textit{Windy}) &= 0.020 \text{ bits}\end{aligned}\right\}$$

**Humidity is selected**

# Example


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

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

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  - 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
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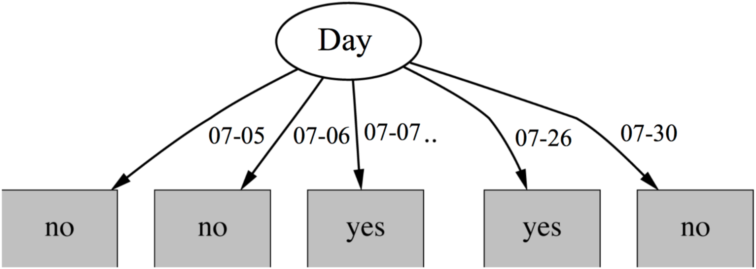
# Decision Tree for Day attribute




- 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

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

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- 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!!!

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- Most popular alternative: Gini index

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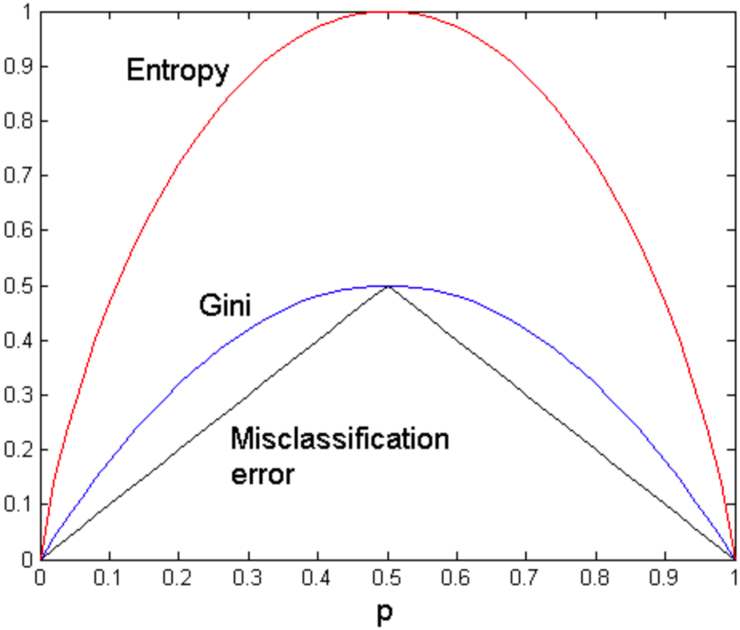
## Comparison among Splitting Criteria: binary case



- **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:
  $$E(S) = \min_{c \in \mathbb{Y}} \frac{1}{|S|} \sum_{(\mathbf{x}_i, y_i) \in S} [y_i \neq c]$$

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- 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
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  - First grow a full tree to capture all possible attributes interactions
  - Later remove those that are due to chance
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- Two subtree simplification operators
  - Subtree replacement
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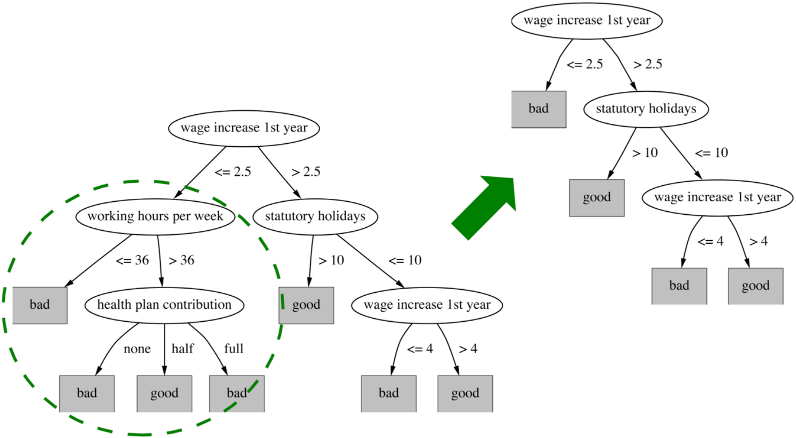
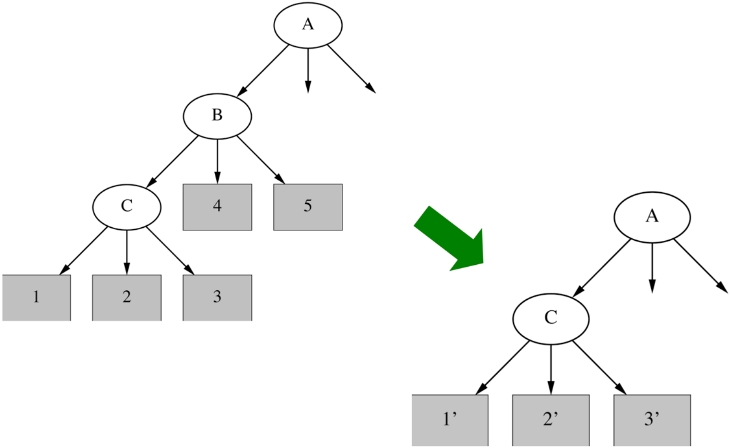
# Subtree replacement

- 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
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- Multiple choices available:
  - Maximum tree depth
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  - Maximum number of leafs in tree
  - Stop if all objects fall into same leaf
  - Constrain quality improvement
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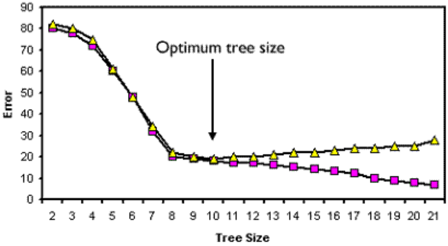


- Learn a large tree (effectively overfit the training set)
- Detect overfitting via $K$-fold cross-validation
- Optimize structure by removing least important nodes

- Assume
  - $d$ attributes
  - $m$ training instances
  - tree depth $O(\log m)$
- Building a tree $O(dm \log(m))$
- Subtree replacement $O(m)$
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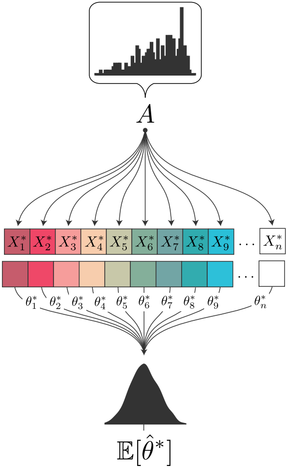
# The bootstrapping procedure

- Input: a sample $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$




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

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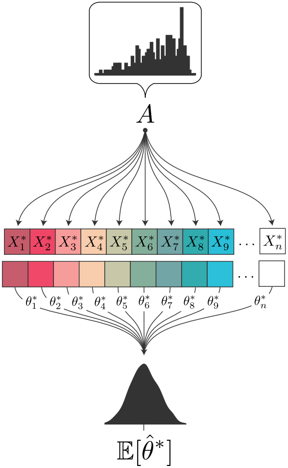


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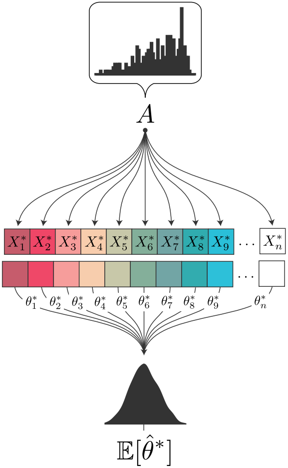
- **Ensemble learning idea:**
  1. Generate $N$ bootstrapped samples $S_m^1, \ldots, S_m^N$
  2. Learn $N$ hypotheses $h_1, \ldots, h_N$
  3. Average predictions to obtain $h(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N h_i(\mathbf{x})$
  4. Profit!

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# Bagging: bootstrap aggregation

- 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

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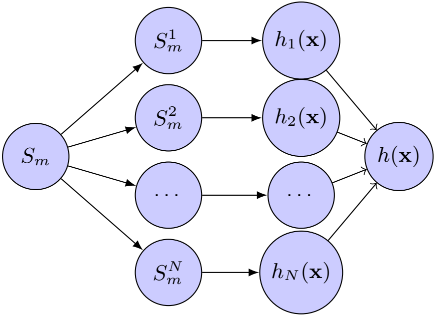

# The Random Forest algorithm

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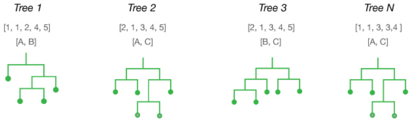
$\mathbf{x}_i \in \{\mathrm{A}, \mathrm{B}, \mathrm{C}\}$

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

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

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




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

# Random Forest: synthetic examples