# Decision Trees. Bagging. Random Forest
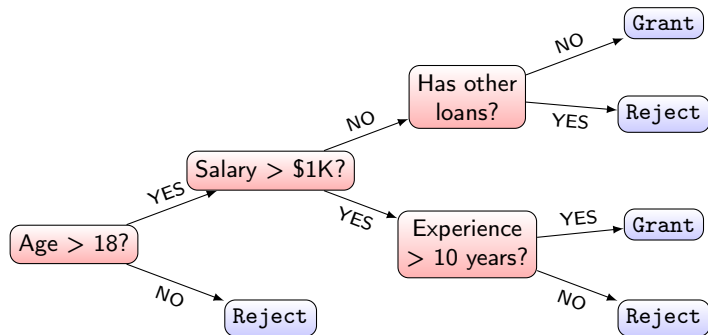
Evgeny Burnaev

Skoltech, Moscow, Russia

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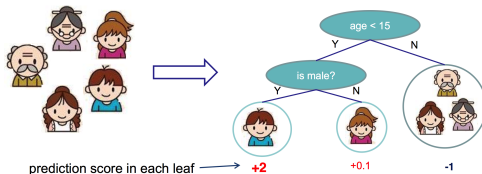
A decision tree consists of
- Nodes
  - — Test for the value of a certain attribute
- Edges
  - — Correspond to the outcome of a test
  - — Connect to the next node of leaf
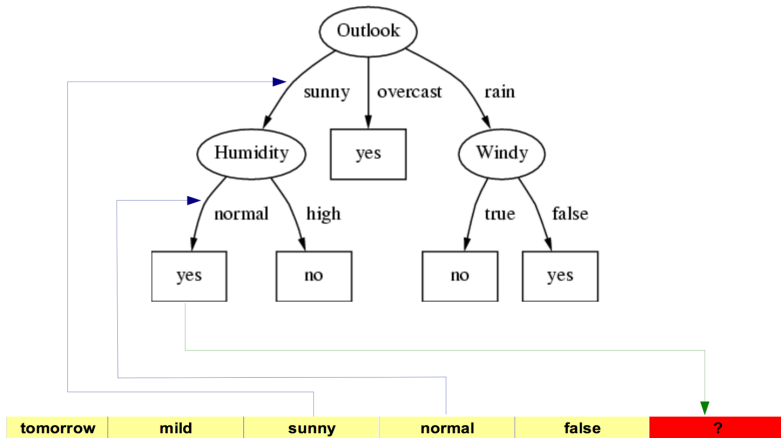- Leaves
  - — Terminal nodes that predict the outcome

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



prediction score in each leaf $\longrightarrow$ **+2**   +0.1   -1

# 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 | ? |

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| 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

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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 $c_r$ of $x_j$
     a) Let $S_r$ = all examples in $S_m$ with $x_j = c_r$
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     c) Generate an edge that connects $DT$ and $DT_r$

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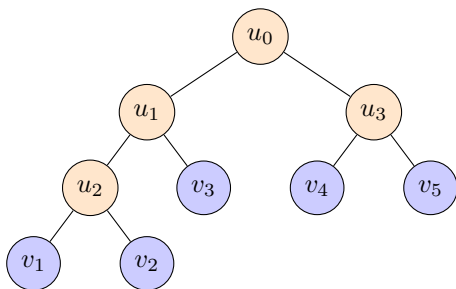     c) Generate an edge that connects $DT$ and $DT_r$

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Example: DT for weather prediction
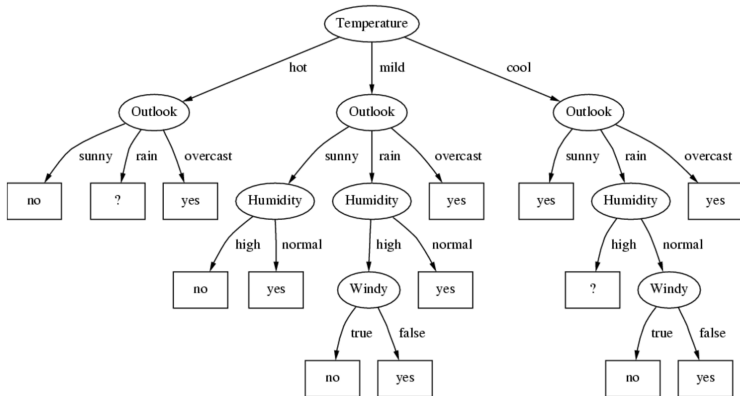


- also explains all of the training data
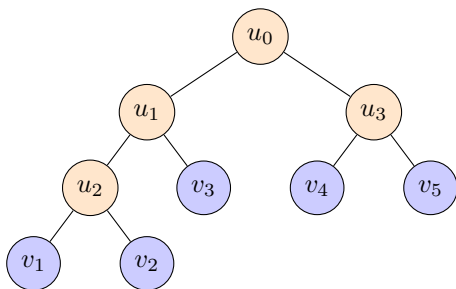- will it generalize well to new data?

- 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* $y$

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Binary Decision Tree

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- Internal nodes $u \in DT$: *predicates* $\beta_u : X \rightarrow \{0, 1\}$
- Leafs $v \in DT$: *predictions* $y$
- Algorithm $h(\mathbf{x})$ starts at $u = u_0$

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

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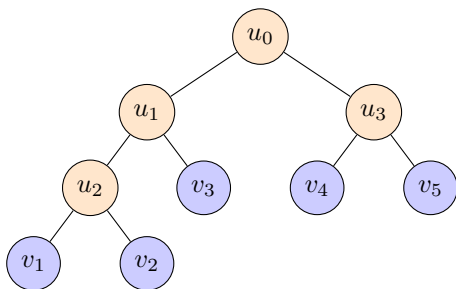
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- In practice for a real variable:
  $\beta_u(\mathbf{x}; j, t) = 1[x_j < t]$

# Greedy binary tree learning for classification

- Input: training set $S_m = \left\{ (\mathbf{x}_i, y_i) \right\}_{i=1}^m$

  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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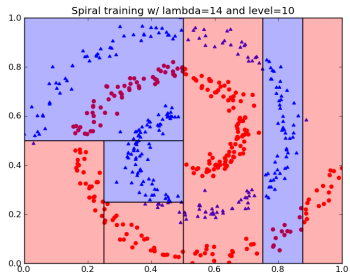  1. Greedily split $S_m$ into $S_1$ and $S_2$:
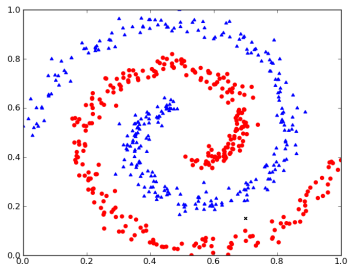     $$S_1(j,t) = \{(\mathbf{x}, y) \in S_m | x_j \le t\}, \qquad S_2(j,t) = \{(\mathbf{x}, y) \in S_m | x_j > t\}$$
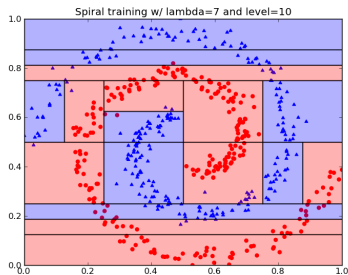     optimizing a given loss: $Q(S_m, j, t) \to \min_{(j,t)}$
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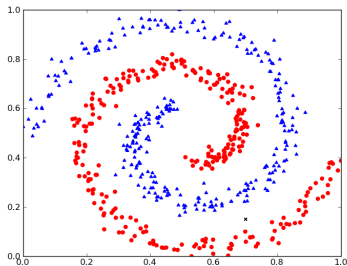     optimizing a given loss: $Q(S_m, j, t) \to \min_{(j, t)}$
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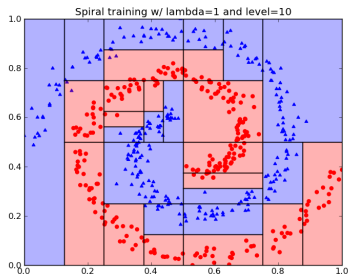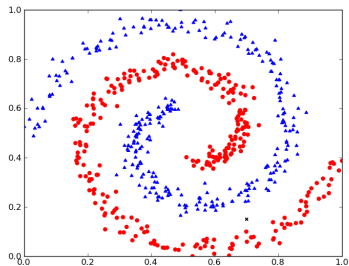- Output: a decision tree $DT$

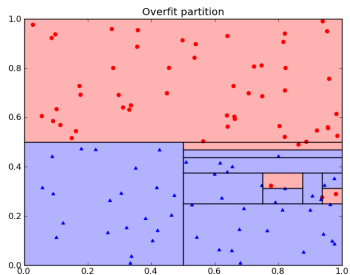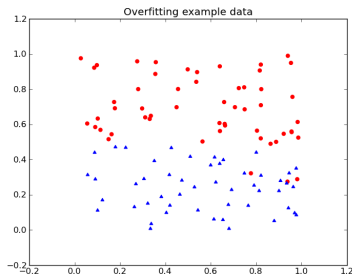# Greedy tree learning for binary classification



Spiral training w/ lambda=14 and level=10

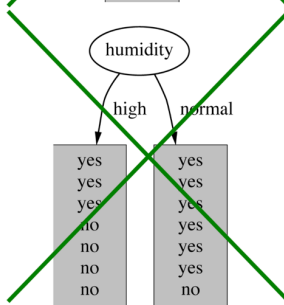Spiral training w/ lambda=7 and level=10

Spiral training w/ lambda=1 and level=10

# 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?
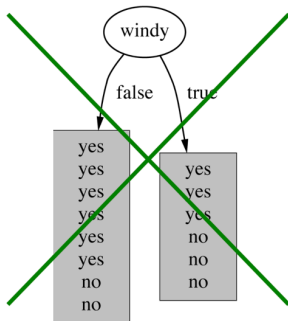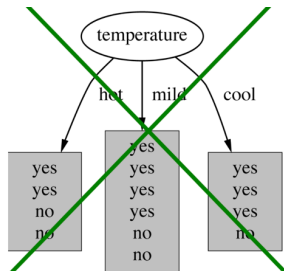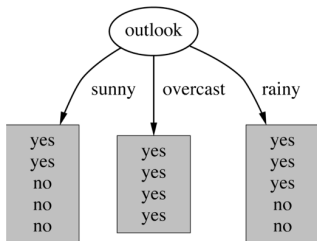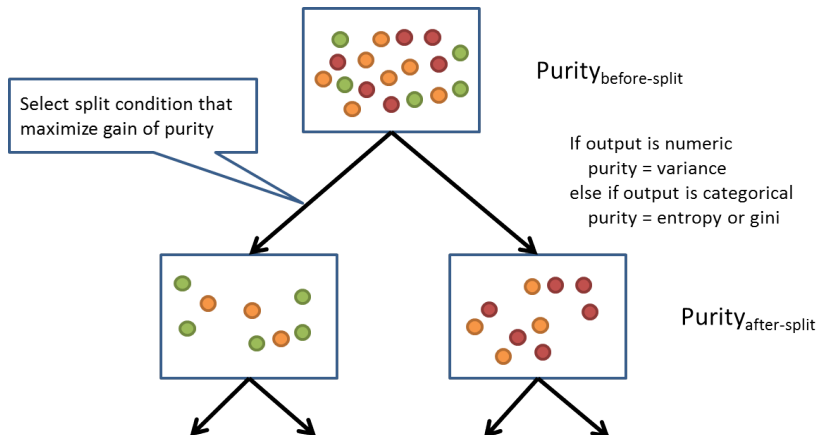
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Select split condition that maximize gain of purity

Purity$_{before-split}$

If output is numeric
    purity = variance
else if output is categorical
    purity = entropy or gini

Purity$_{after-split}$

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
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- 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



maximal value at equal class distribution

minimal value if only one class left in $S$

$$E(S) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 - \ldots - p_K \log_2 p_K = -\sum_{k=1}^{K} p_k \log_2 p_k$$
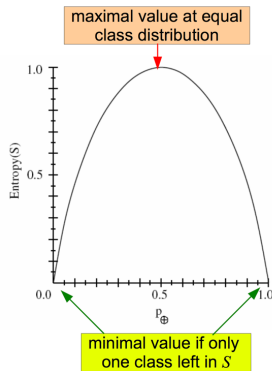
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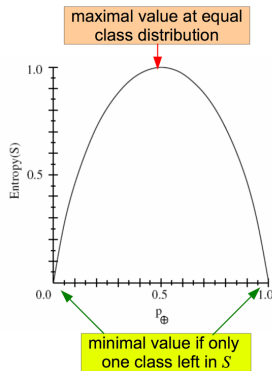minimal value if only one class left in $S$

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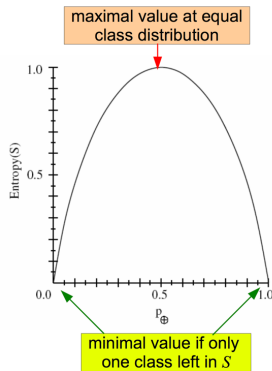- $p_i$ is the proportion of examples in $S$ from the i-th class

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

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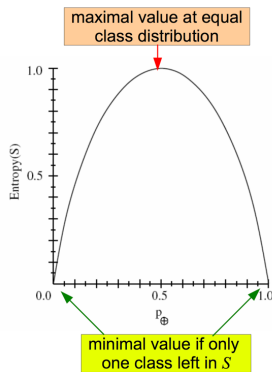- $p_i$ is the proportion of examples in $S$ from the i-th class



maximal value at equal class distribution

minimal value if only one class left in $S$

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

Example: Attribute "Outlook"

- **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**

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

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- 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)** $= 0.246$; $Gain(S, Wind) = 0.048$; $Gain(S, Temperature) = 0.029$

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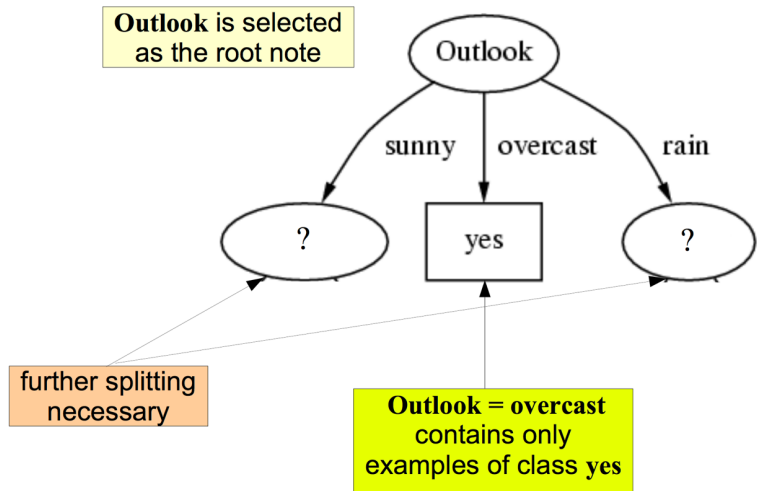- Information Gain for Attribute $x_j$

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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



$$\text{Gain}(Temperature) = 0.571 \text{ bits}$$
$$\text{Gain}(Humidity) = 0.971 \text{ bits}$$
$$\text{Gain}(Windy) = 0.020 \text{ bits}$$

**Humidity** is selected

Humidity is selected

Pure leaves
→ No further expansion necessary

further splitting
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
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- 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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- 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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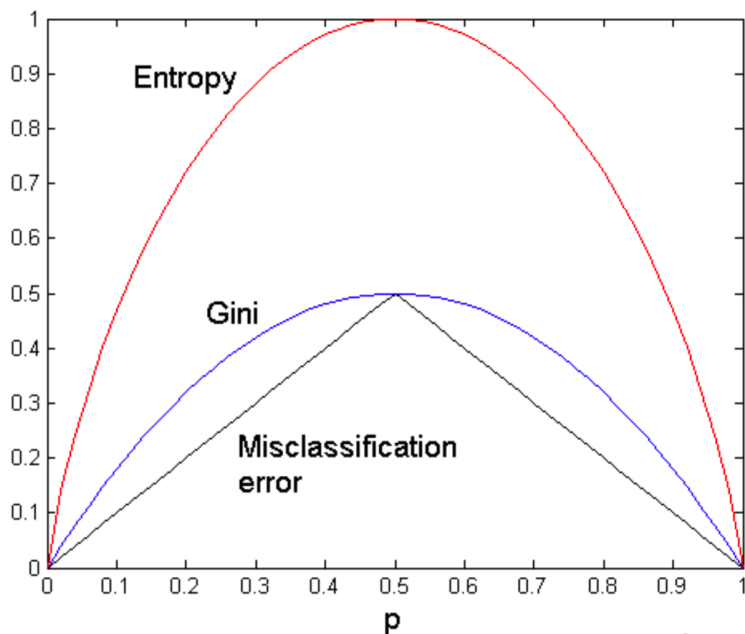- Most popular alternative: Gini index

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## 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

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  — Impurity ≡ 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
  - — use sums of weights instead of counts
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- 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"

Overfitting and Pruning

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  - First grow a full tree to capture all possible attributes interactions
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- Two subtree simplification operators
  - Subtree replacement
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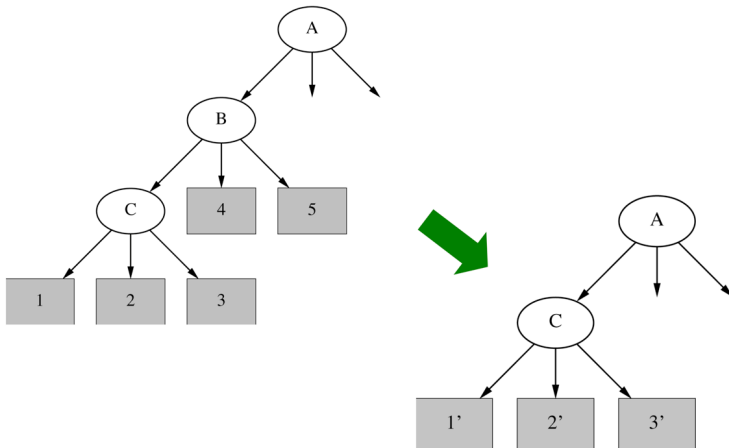  - Significance testing
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## Subtree replacement

- Bottom-up
- Consider replacing a tree only after all its subtrees
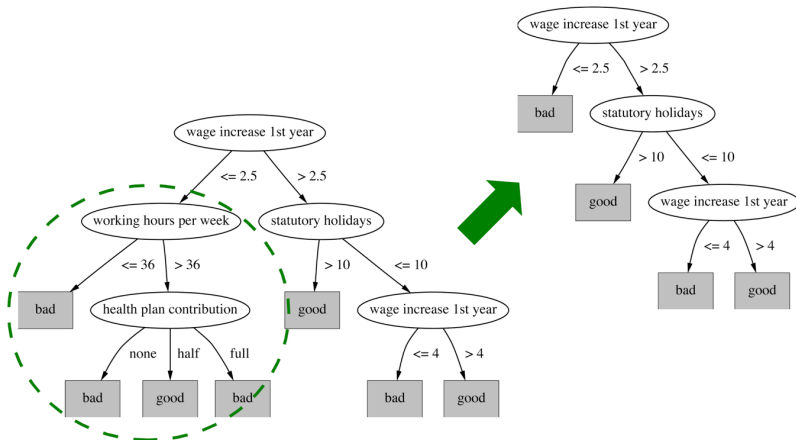
- Delete node B
- Redistribute instances of leaves 4 and 5 into C

**Skoltech**

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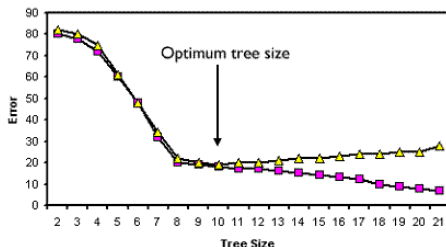
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- Learn a large tree (effectively overfit the training set)
- Detect overfitting via $K$-fold cross-validation
- Optimize structure by removing least important nodes

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

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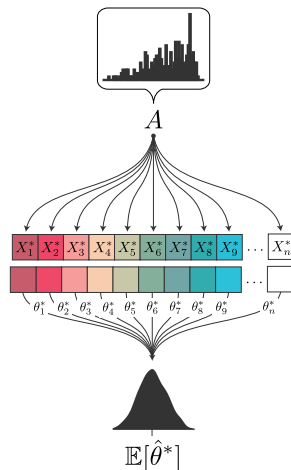- Total cost: $O(dm \log(m)) + O(m(\log(m))^2)$

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

# The bootstrapping procedure

- Input: a sample $S_m = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$
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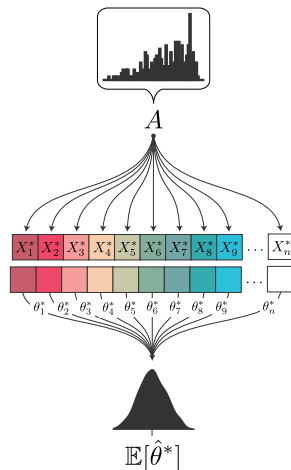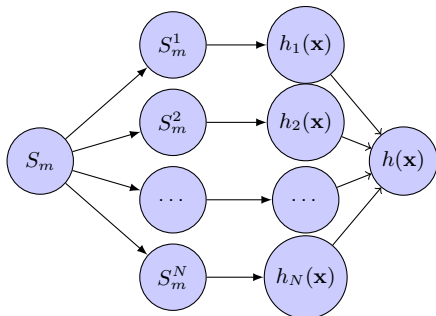Picture credit: http://www.drbunsen.org/bootstrap-in-picture

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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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- 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 $\mathbf{x}_i \in \mathbb{R}^p, y_i \in Y$
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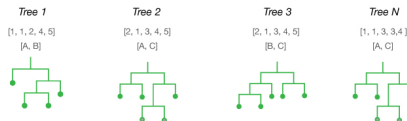
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$\mathbf{x}_i \in \{A, B, C\}$

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

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

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



Tree 1   [1, 1, 2, 4, 5]   [A, B]
Tree 2   [2, 1, 3, 4, 5]   [A, C]
Tree 3   [2, 1, 3, 4, 5]   [B, C]
Tree N   [1, 1, 3, 3, 4]   [A, C]

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

# Random Forest: synthetic examples