Ensemble Methods

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Content

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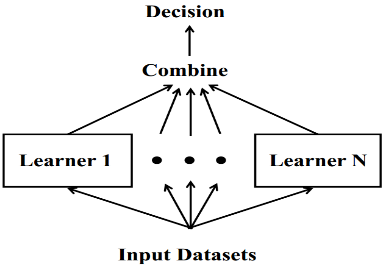
Ensemble Learning

- Ensemble learning: Combine numerous weak learners to a strong learner
- Main methods: Bagging , Boosting



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Decision Tree Example

Learning the Play Tennis Decision Tree

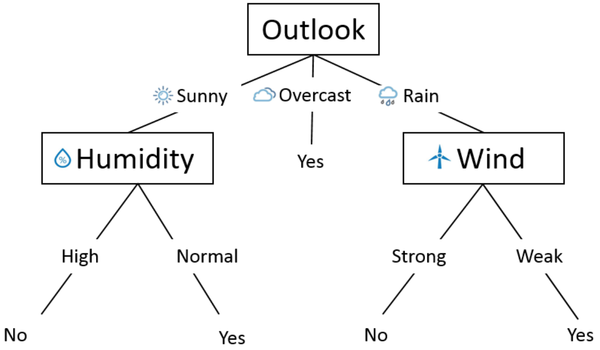
4 Attributes

Day	Outlook	Temp	Humidity	Wind	*PlayTennis*
D1	*Sunny*	*Hot*	*High*	*Weak*	*No*
D2	*Sunny*	*Hot*	*High*	*Strong*	*No*
D3	*Overcast*	*Hot*	*High*	*Weak*	*Yes*
D4	*Rain*	*Mild*	*High*	*Weak*	*Yes*
D5	*Rain*	*Cool*	*Normal*	*Weak*	*Yes*
D6	*Rain*	*Cool*	*Normal*	*Strong*	*No*
D7	*Overcast*	*Cool*	*Normal*	*Strong*	*Yes*
D8	*Sunny*	*Mild*	*High*	*Weak*	*No*
D9	*Sunny*	*Cool*	*Normal*	*Weak*	*Yes*
D10	*Rain*	*Mild*	*Normal*	*Weak*	*Yes*
D11	*Sunny*	*Mild*	*Normal*	*Strong*	*Yes*
D12	*Overcast*	*Mild*	*High*	*Strong*	*Yes*
D13	*Overcast*	*Hot*	*Normal*	*Weak*	*Yes*
D14	*Rain*	*Mild*	*High*	*Strong*	*No*

Decision Tree Example

Play Tennis: Yes or No?

- Learned function is a tree
- Classify instances by sorting them down from the root to the leaf node



Algorithm 1: Decision Tree

Input: Training set $D = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$; Attribute set $A = \{a_1, a_2, ..., a_d\}$.

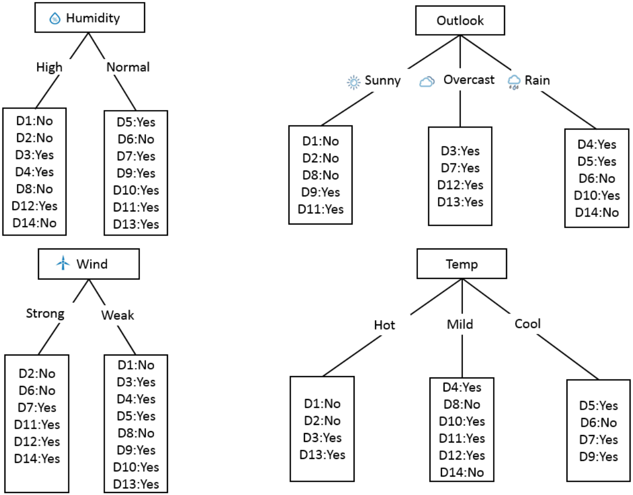
Procedure: Function TreeGenerate(D, A)

Generate node;
if all the samples in D belong to class C **then**
    mark this node as class C leaf node; **return**
end
if $A = \emptyset$ **OR** samples in D have the same value on A **then**
    mark this node as leaf node, and the class should be the most frequent occurrence class; **return**
end
Select the best partition attribute a_* from A;
for each value a_*^v of attribute a_* **do**
    D_v is the sample subset of D with $a_* = a_*^v$;
    if $D_v = \emptyset$ **then**
        mark this node as the leaf node, and the class should be the most frequent occurrence class; **return**
    else
        generate a branch for this node, TreeGenerate$(D_v, A \backslash \{a_*\})$
    end
end

Output: A decision tree

Decision Tree Example

Which Is The Best Partition Attribute?



Decision Tree Example

A Good Attribute

An attribute is good when:

- For one value we get all instances as positive
- For other value we get all instances as negative

Decision Tree Example

Poor Attribute

An attribute is poor when:

- It provides no discrimination
- Attribute is immaterial to the decision
- For each value we have same number of positive and negative instances

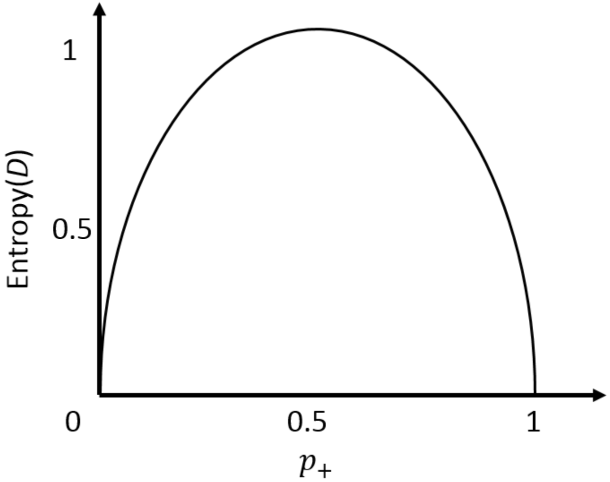
Measure of Homogeneity of Examples

- Entropy: Characterizes the (im)purity of an arbitrary collection of examples.
- Given a collection D of positive and negative examples, entropy of D relative to boolean classification is

$$Entropy(D) \equiv -p_+ log_2 p_+ - p_- log_2 p_-$$

Where p_+ is proportion of positive examples and p_- is proportion of negative examples.

Entropy Function Relative to A Boolean Classification



Entropy

- Illustration:
- D is a collection of 14 examples with 9 positive and 5 negative examples
- Entropy of D relative to the Boolean classification:

$$Entropy(9+,5-) = -\frac{9}{14}log_2\frac{9}{14} - \frac{5}{14}log_2\frac{5}{14} = 0.940$$

- Entropy is zero if all members of D belong to the same class

Entropy for Multi-Valued Target function

- If the target attribute can take on c different values, the entropy of D relative to this c-wise classification is

$$Entropy(D) \equiv \sum_{i=1}^{c} -p_i log_2 p_i$$

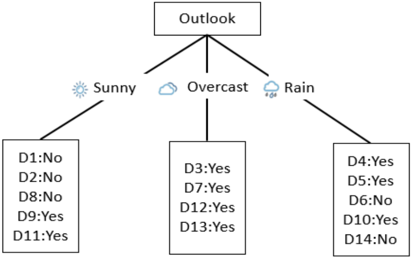
Information Gain Measures the Expected Reduction in Entropy

- Entropy measures the impurity of a collection
- Information gain of attribute A is the reduction in entropy caused by partitioning the set of examples D

$$Gain(D, A) \equiv Entropy(D) - \sum_{v \in Values(A)} \frac{|D_v|}{|D|} Entropy(D_v)$$

- Where $Values(A)$ is the set of all possible values for attribute A and D_v is the subset of D for which attribute A has value v

Measure of Purity: Information (bits)



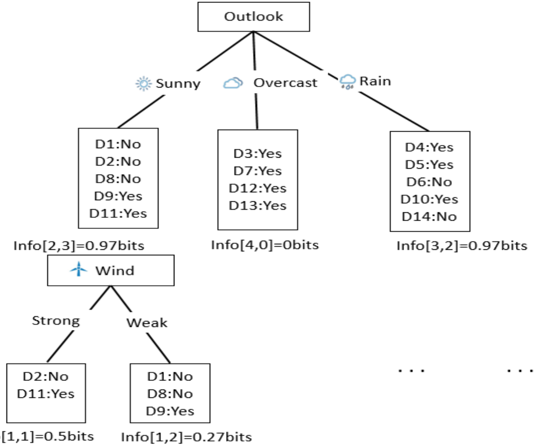
Info[2,3]=0.97bits Info[4,0]=0bits Info[3,2]=0.97bits

$$
\begin{aligned}
Info[2,3] &= entropy(2,3) \\
&= -\frac{2}{5}log_2\frac{2}{5} - \frac{3}{5}log_2\frac{3}{5} \\
&= 0.97bits
\end{aligned}
$$

Information Gain for Each Attribute

- Gain(outlook) = 0.94 - 0.693 = 0.247
- Gain(temperature)= 0.94 - 0.911 = 0.029
- Gain(humidity)= 0.94 - 0.788 = 0.152
- Gain(windy)= 0.94 - 0.892 = 0.048
- $\arg\max_A \{0.247, 0.029, 0.152, 0.048\}$ = outlook
- Select outlook as the splitting attribute of tree

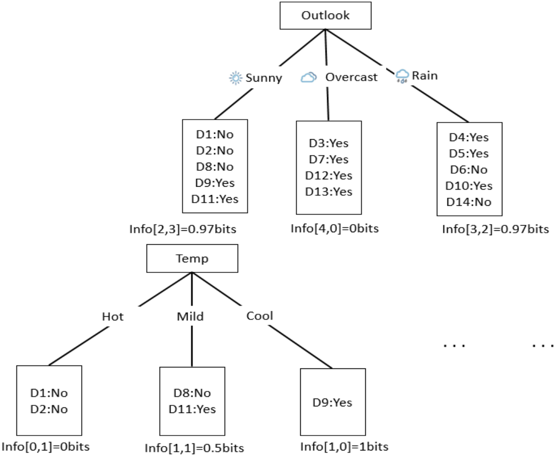
Expanded Tree Stumps for PlayTennis for Outlook=Sunny



Ave Info=$\frac{2}{5}\times 0.5+\frac{3}{5}\times 0.27$=0.36bits

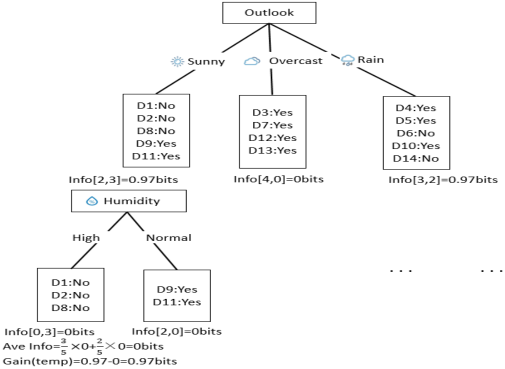
Gain(temp)=0.97-0.36=0.61bits

Expanded Tree Stumps for PlayTennis for Outlook=Sunny



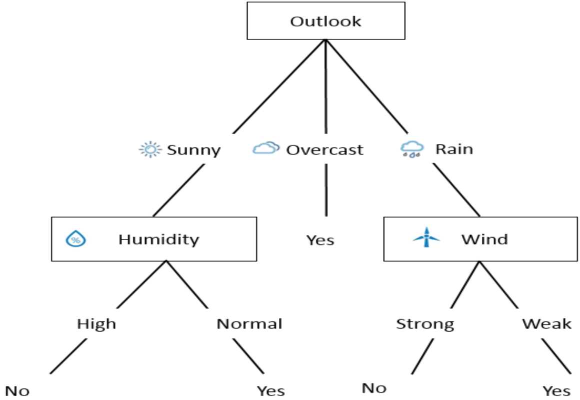
Ave Info=0+0+$\frac{1}{5}\times 1$=0.2bits
Gain(temp)=0.97-0.2=0.77bits

Expanded Tree Stumps for PlayTennis for Outlook=Sunny



- Since Gain(humidity) is highest, select humidity as splitting attribute
- No need to split further

Decision Tree for the Weather Data



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Bagging

Bootstrap Sampling

- Giveing a dataset D with m samples, we take samples to make dataset $D^{'}$
- Select a sample from D to $D^{'}$ and put it back to the data set D each time, so the sample has the probability to be selected next time
- Repeat the procedure m times to get $D^{'}$ with m samples

Bagging

Bootstrap Sampling

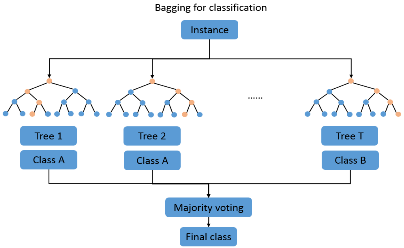
The probablility that a sample will not be selected:

$$\lim_{m \to +\infty} \left(1 - \frac{1}{m}\right)^m \to \frac{1}{e} \approx 0.368$$

- There are approximately $\frac{1}{3}$ samples used for testing which is called out-of-bag estimate
- Bootstrap sampling is useful in the case of small dataset and getting testing samples difficultly

Bagging

- Get T sampling sets through bootstrap sampling
- Train T base learners through the sampling sets respectively



- For classification:
  The class with the most votes becomes the final class
- For regression:
  The final output is the average output of every base learner

Random Forest

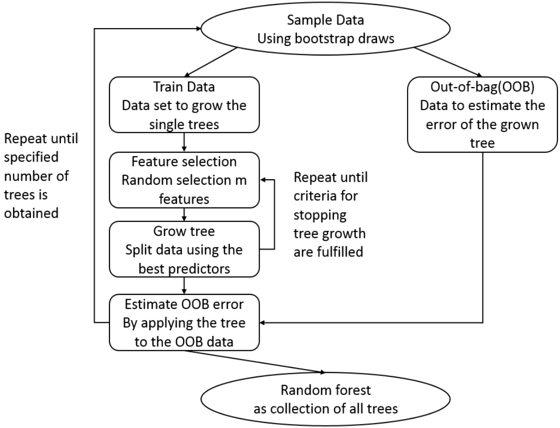
- Random forest is an extension of bagging using decision tree as base learner
- Randomly select m out of p features to get the optimal partition feature

Comparison between bagging and random forest

- The training efficiency of random forest is higher than bagging
- Bagging uses decision tree with definite structure
- Random forest uses decision tree with random structure

Random Forest

An example of the process flow is depicted below



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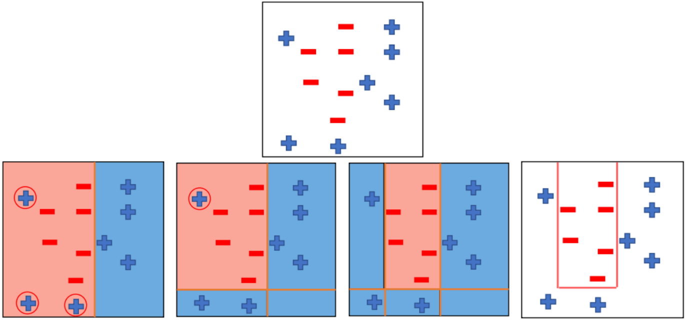
Adaboost

How to train the base leaner?

Make the wrong predictive samples more important, and handle it in next round:



Adaboost

Sample weight updating formula

$$w_{m+1}(i) = \frac{w_m(i)}{z_m} e^{-\alpha_m y_i h_m(\mathbf{x}_i)}$$

$z_m = \sum_{i=1}^{n} w_m(i) e^{-\alpha_m y_i h_m(\mathbf{x}_i)}$ is normalization term, makes $w_m(i)$ become probability distributions

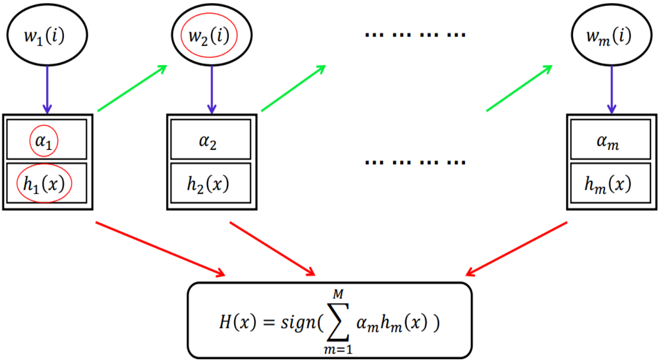
$$w_{m+1}(i) = \begin{cases} \dfrac{w_m(i)}{z_m} e^{-\alpha_m} & \text{for right predictive sample} \\ \dfrac{w_m(i)}{z_m} e^{\alpha_m} & \text{for wrong predictive sample} \end{cases}$$

so in next round, $\frac{w_{wrong}(i)}{w_{right}(i)} = e^{2\alpha_m} = \dfrac{1-\epsilon_m}{\epsilon_m}$ and $\epsilon_m < 0.5$, wrong samples will be more important

Adaboost

How to combine the base learner?

Every iteration generates a new base learner $h_m(\mathbf{x})$ and its importance score α_m



Adaboost

Evaluate the performance of the base learner

- Base learner

$$h_m(\mathbf{x}) : \mathbf{x} \mapsto \{-1, 1\}$$

- Error rate

$$\epsilon_m = p(h_m(\mathbf{x}_i) \neq y_i) = \sum_{i=1}^{n} w_m(i)\mathbb{I}(h_m(\mathbf{x}_i) \neq y_i)$$

$\epsilon_m < 0.5$, or the performance of Adaboost is weaker than random classfication.

Adaboost

Importance score of base learner

Make the base learner with lower ϵ_m more important

$$\alpha_m = \frac{1}{2} \log \frac{1 - \epsilon_m}{\epsilon_m}$$

Adaboost

Additive model

- Final learner

$$H(\mathbf{x}) = \mathrm{sign}(\sum_{m=1}^{M} \alpha_m h_m(\mathbf{x}))$$

Note: $h_m(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^\top \mathbf{x})$ is a nonlinear function, so the Adaboost can deal with nonlinear problem

Algorithm

Algorithm 2: Adaboost

Input: $D = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, **where** $\mathbf{x}_i \in X, y_i \in \{-1, 1\}$

Initialize: Sample distribution w_m

Base learner: $\mathcal{L}$

$w_1(i) = \frac{1}{n}$

for m=1,2,...,M **do**

$\quad h_m(x) = \mathcal{L}(D, w_m)$

$\quad \epsilon_m = \sum_{i=1}^{n} w_m(i)\mathbb{I}(h_m(\mathbf{x}_i) \neq y_i)$

$\quad$ **if** $\epsilon_m > 0.5$ **then**

$\quad\quad$ **break**

$\quad$ **end**

$\quad \alpha_m = \frac{1}{2} \log \frac{1-\epsilon_m}{\epsilon_m}$

$\quad w_{m+1}(i) = \frac{w_m(i)}{z_m} e^{-\alpha_m y_i h_m(\mathbf{x}_i)}$,**where** $i = 1, 2, ..., n$ **and**

$\quad z_m = \sum_{i=1}^{n} w_m(i) e^{-\alpha_m y_i h_m(\mathbf{x}_i)}$

end

Output: $H(\mathbf{x}) = \sum_{m=1}^{M} \alpha_m h_m(\mathbf{x})$

Contents

Gradient Boosting Decision Trees

GBDT is a decision tree algorithm with iteration

Example: What is the difference between regression tree and GBDT?

Suppose: There are 4 peoples A, B, C and D, whose age are 14, 16, 24, 26 respectively.

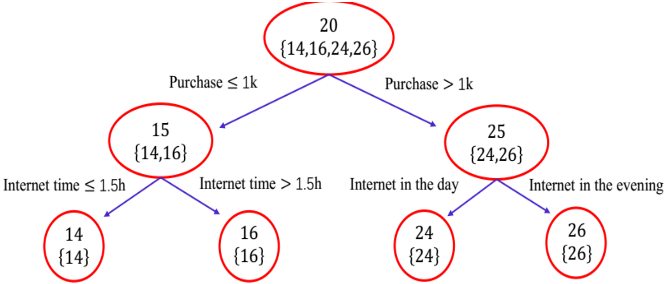
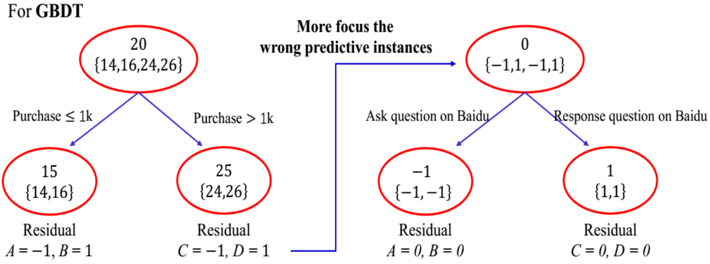


Figure: Single regression tree

Gradient Boosting Decision Trees

- The key of GBDT is that trees learn all the results and residuals of all trees before.
- The residual is the difference of predictive value and real value, so the predictive value is the sum of all results of trees.



- So,
  A=15+(-1)=14 B=15+1=16 C=25+(-1)=24 D=25+1=26

Gradient Boosting Decision Trees

Question

Q1:when results of these two algorithms are same, Why do we choose GBDT?

- The motivation of this algorithm is that every calculation of residual is to increase the weight of wrong predictive samples,and the residual of right predictive sample is zero.
- So in the next iteration, model can concentratively address these wrong predictive samples. Another function is to prevent over fitting.

Gradient Boosting Decision Trees

Question

Q2: Where does this algorithm reflect gradient boosting?

- In algorithm, residual is the gradient descent direction, which is the derivation of mean square error(MSE). Actually, MSE is the loss function of CART regression tree.

Setting	Loss Function	$-\partial L(y_i, f(x_i))/\partial f(x_i)$
Regression	$\frac{1}{2}[y_i - f(x_i)]^2$	$y_i - f(x_i)$
Regression	$\|y_i - f(x_i)\|$	$\text{sign}[y_i - f(x_i)]$
Regression	Huber	$y_i - f(x_i)$ for $\|y_i - f(x_i)\| \leq \delta_m$ $\delta_m \text{sign}[y_i - f(x_i)]$ for $\|y_i - f(x_i)\| > \delta_m$ where $\delta_m = \alpha$th-quantile$\{\|y_i - f(x_i)\|\}$
Classification	Deviance	kth component: $I(y_i = \mathcal{G}_k) - p_k(x_i)$

Algorithm

Algorithm 3: GBDT

Input: $D = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, **where** $\mathbf{x}_i \in X, y_i \in \{-1, 1\}$

Initialize: $f_0(x) = \arg\min_\mu \sum_{i=1}^n L(y_i, \mu)$

for m=1,2,...,M **do**

  for i=1,2,...,n **do**

    $r_{im} = -\left[\frac{\partial L(y_i, f_{m-1}(\mathbf{x}_i))}{\partial f_{m-1}(\mathbf{x}_i)}\right]$

    Fit a regression tree to targets r_{im} giving terminal regions $R_{jm}, j = 1, 2, ..., J_m$

  end

  for j=1,2,...,J_m **do**

    $\mu_{jm} = \arg\min_\mu \sum_{\mathbf{x}_i \in R_{jm}} L(y_i, f_{m-1}(\mathbf{x}_i) + \mu), j = 1, 2, ..., J_m$

    Update $f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \sum_{j=1}^{J_m} \mu_{jm} \mathbb{I}(\mathbf{x} \in R_{jm})$

  end

end

Output: $\hat{f}(\mathbf{x}) = f_M(\mathbf{x})$

THANK YOU!