Ensemble Methods

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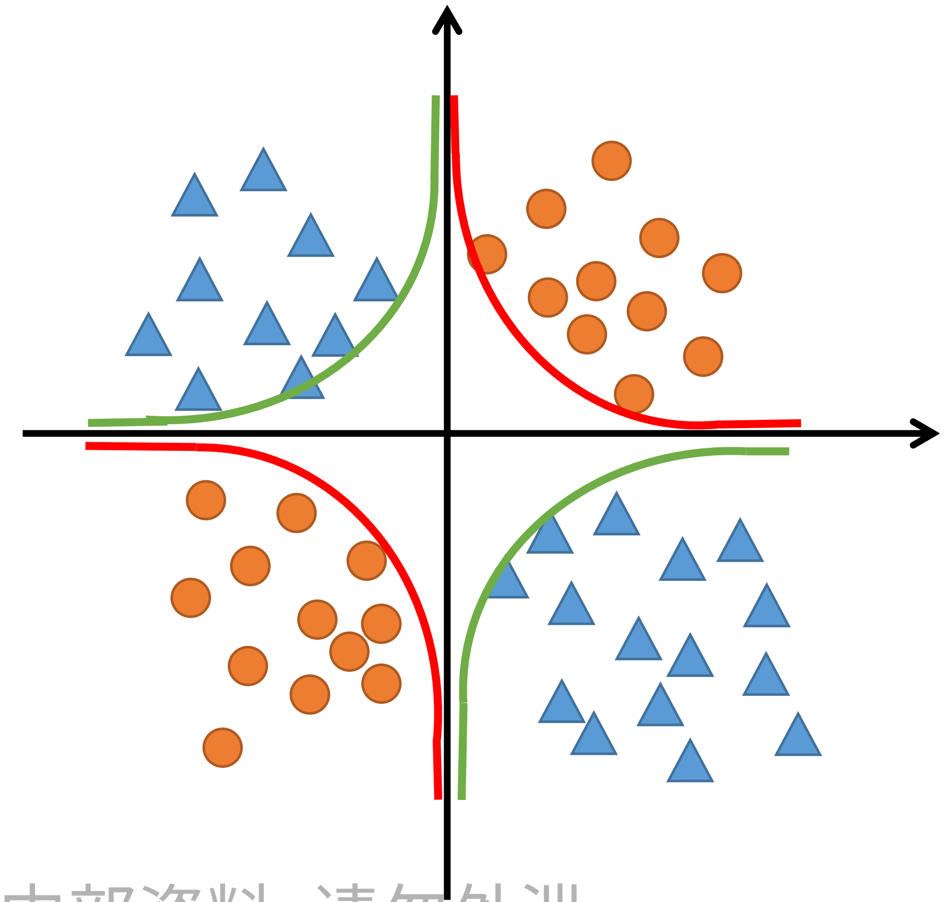
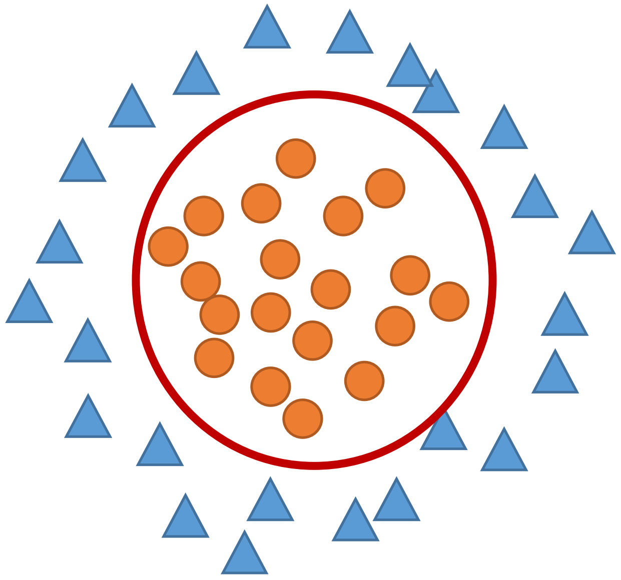
Classification Examples

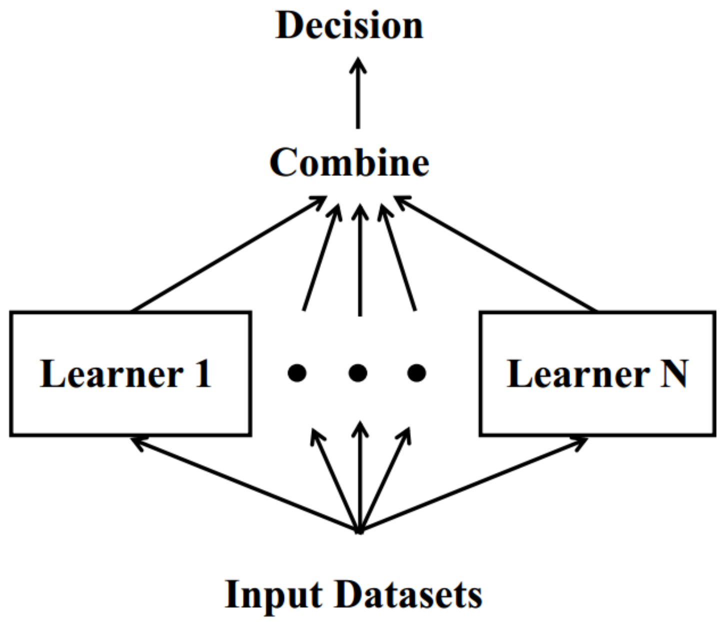
- How to classify?





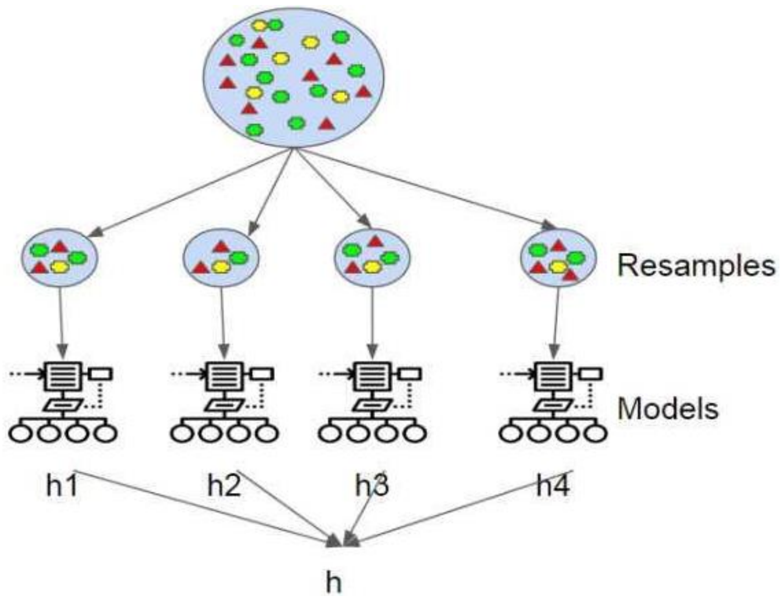
Ensemble Learning

- Ensemble learning: combine several base models to produce a better predictive model
- Main methods: Bagging, Boosting



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

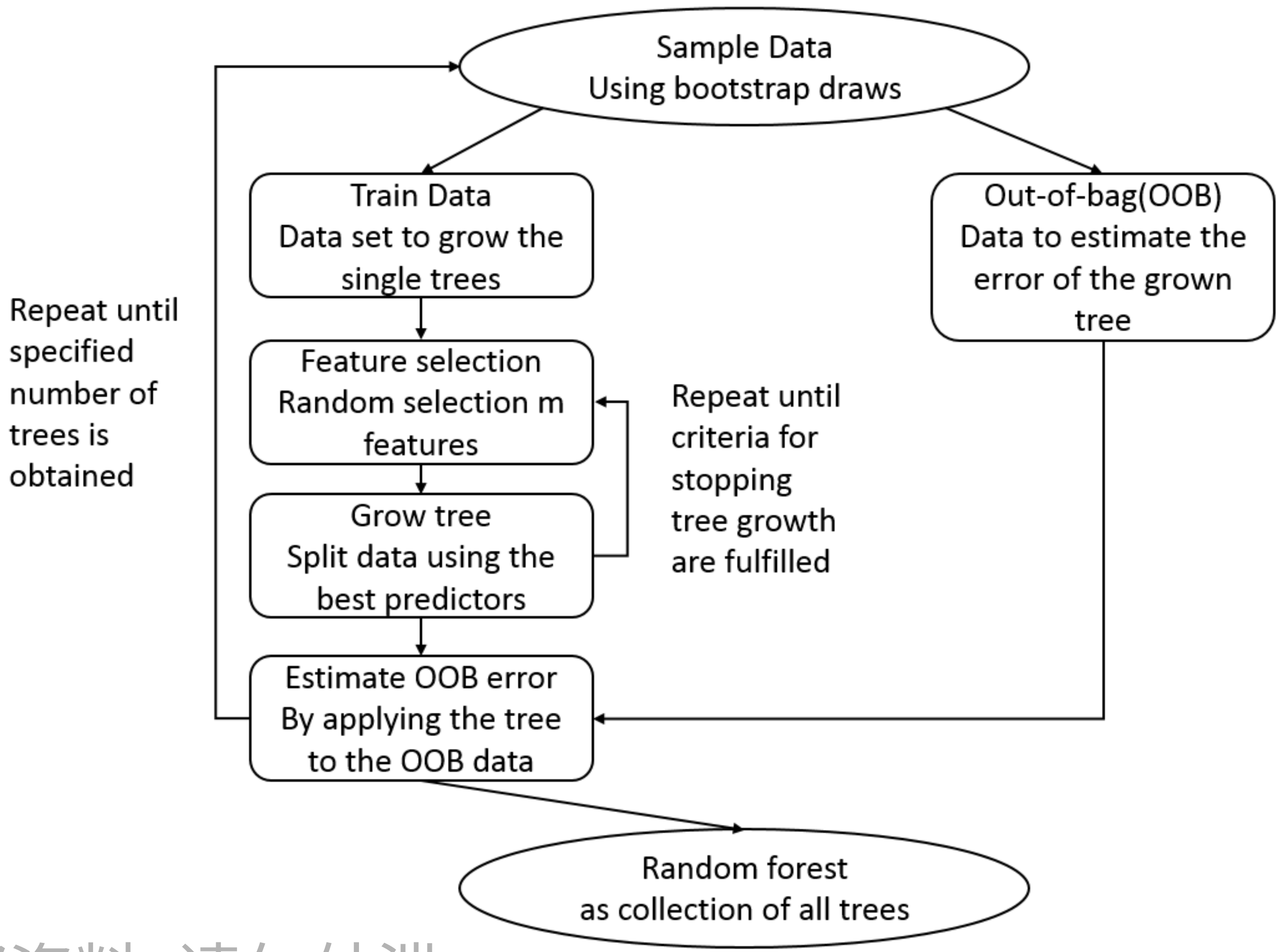
- Random forest is an extension of bagging using decision tree as base learner
- Randomly select *m* out of *p* features to get the optimal partition feature

Comparison between bagging and random forest

- The training efficiency of random forest is better 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:

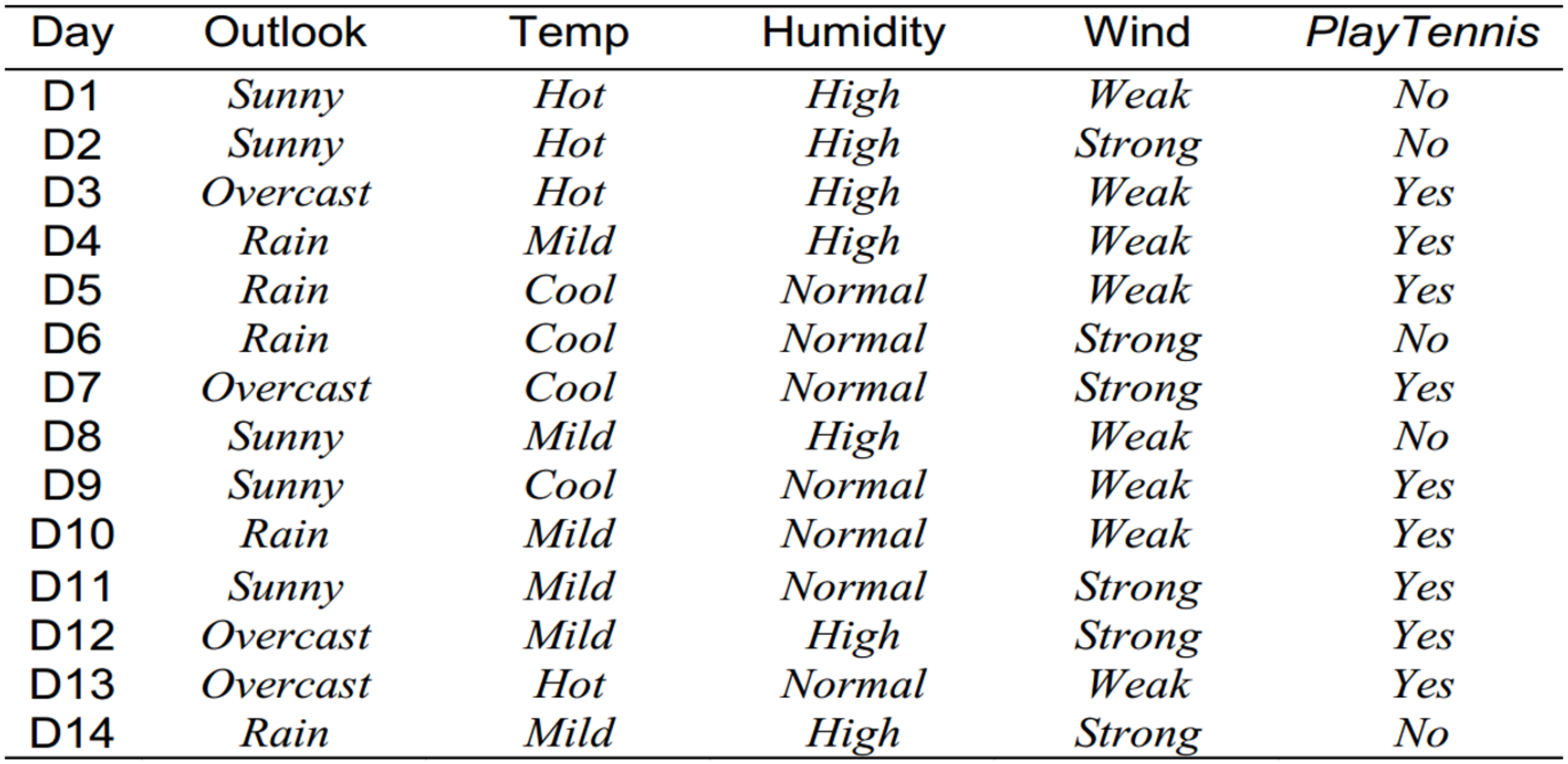

Sample Data
Using bootstrap draws
Train Data
Data set to grow the single trees
Out-of-bag(OOB)
Data to estimate the error of the grown tree
Repeat until specified number of trees is obtained
Feature selection
Random selection m features
Repeat until criteria for stopping tree growth are fulfilled
Grow tree
Split data using the best predictors
Estimate OOB error
By applying the tree to the OOB data
Random forest
as collection of all trees

Contents

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?

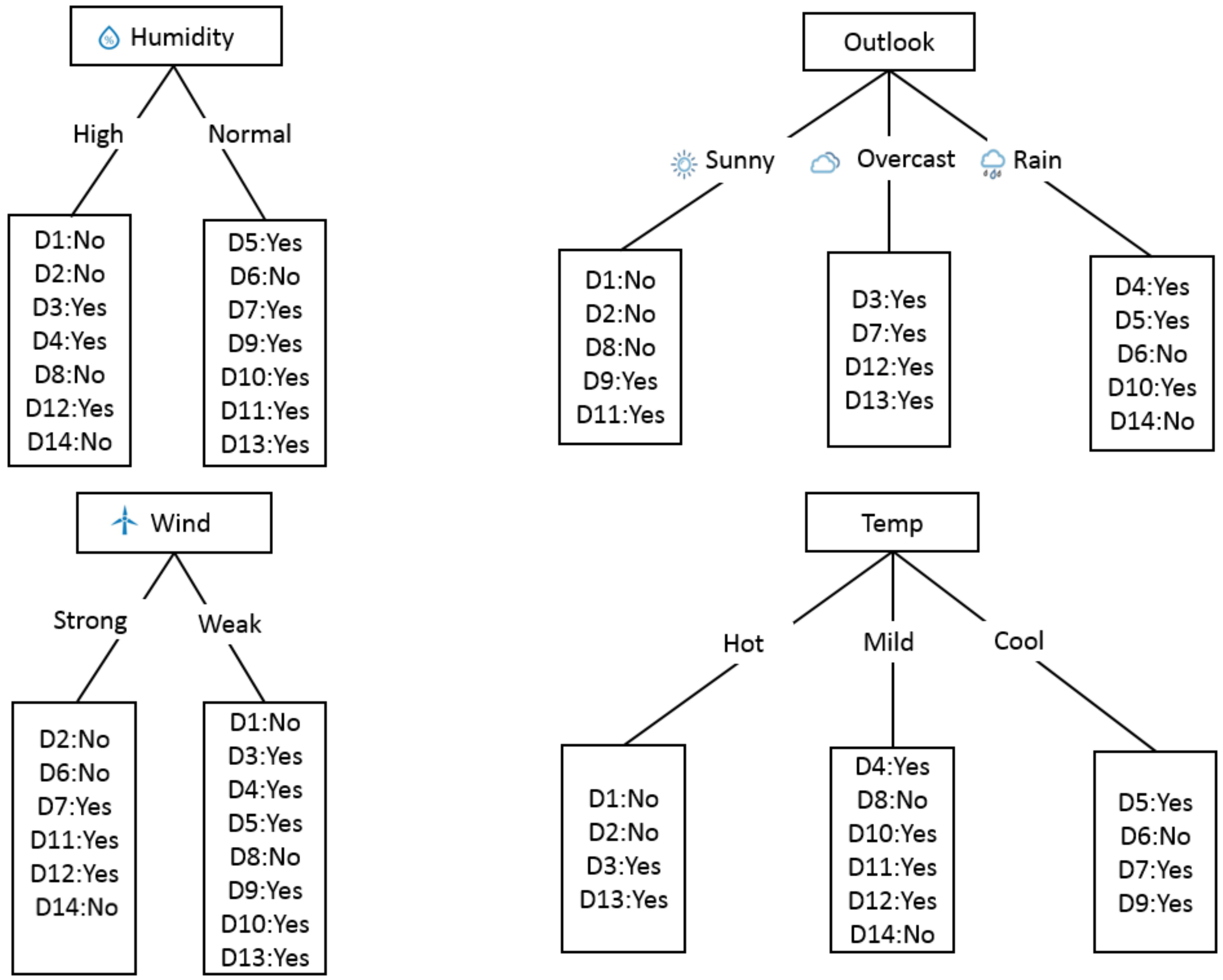
- Learned function is a tree
- Each branch of the tree represents a possible decision, outcome, or reaction
- The farthest branches (leaf nodes) on the tree represent the end results

Algorithm: Decision Tree

Input: Training set $D = \{(x_1, y_1), \ldots, (x_n, y_n)\}$; Attribute set $A = \{a_1, a_2, \ldots, a_d\}$.
Procedure: Function TreeGenerate(D, A). **Output**: A decision tree.

```
1  Generate node;
2  if all the samples in $D$ belong to class $C$ then
3      mark this node as class $C$ leaf node; return
4  end
5  if $A = \emptyset$ OR samples in $D$ have the same value on $A$ then
6      mark this node as leaf node, and the class should be the most frequent
       occurrence class; return
7  end
8  Select the best partition attribute $a_*$ from $A$;
9  for each value $a_*^v$ of attribute $a_*$ do
10     $D_v$ is the sample subset of $D$ with $a_* = a_*^v$;
11     if $D_v = \emptyset$ then
12         mark this node as the leaf node, and the class should be the most frequent
           occurrence class; return
13     else
14         generate a branch for this node, TreeGenerate($D_v$, $A \backslash \{a_*\}$)
15     end
16 end
```

Decision Tree Example


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

Which is the best partition attribute?

Decision Tree Example

An attribute is good when:

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

An attribute is poor when:

- It provides no discrimination
- Attribute is immaterial to the decision
- Same number of positive and negative instances for each value

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

$$\text{Entropy}(D) = -p_{+}\log_2 p_{+} - p_{-}\log_2 p_{-}$$

where p_{+} is proportion of positive examples

p_{-} is proportion of negative examples

Measure Homogeneity of Examples

Illustration:

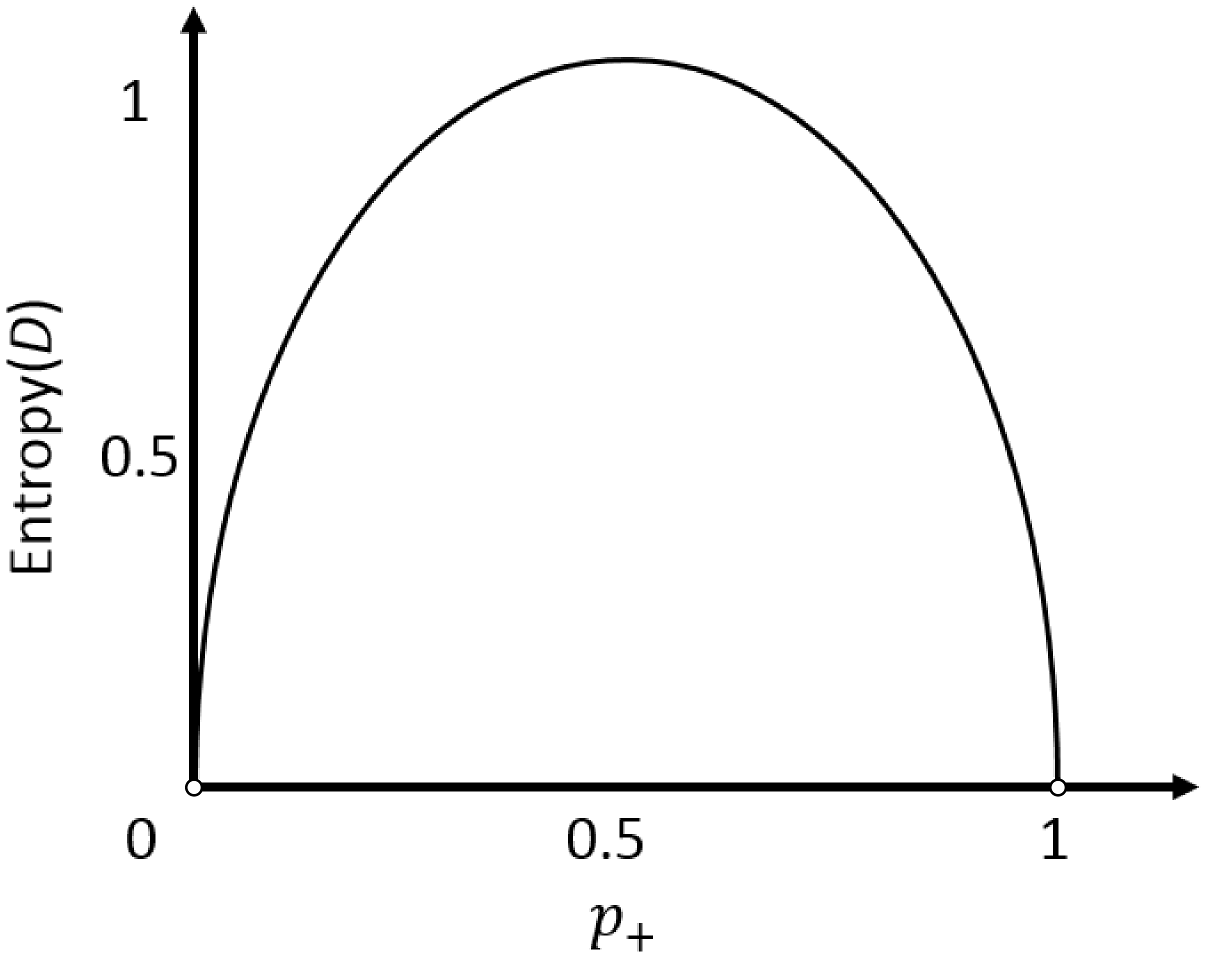
- *D* is a collection of 14 examples with 9 positive and 5 negative examples
- Entropy of *D* relative to the boolean classification:

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

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

Measure Homogeneity of Examples

Entropy Function Relative to a Boolean Classification



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:

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

Information Gain

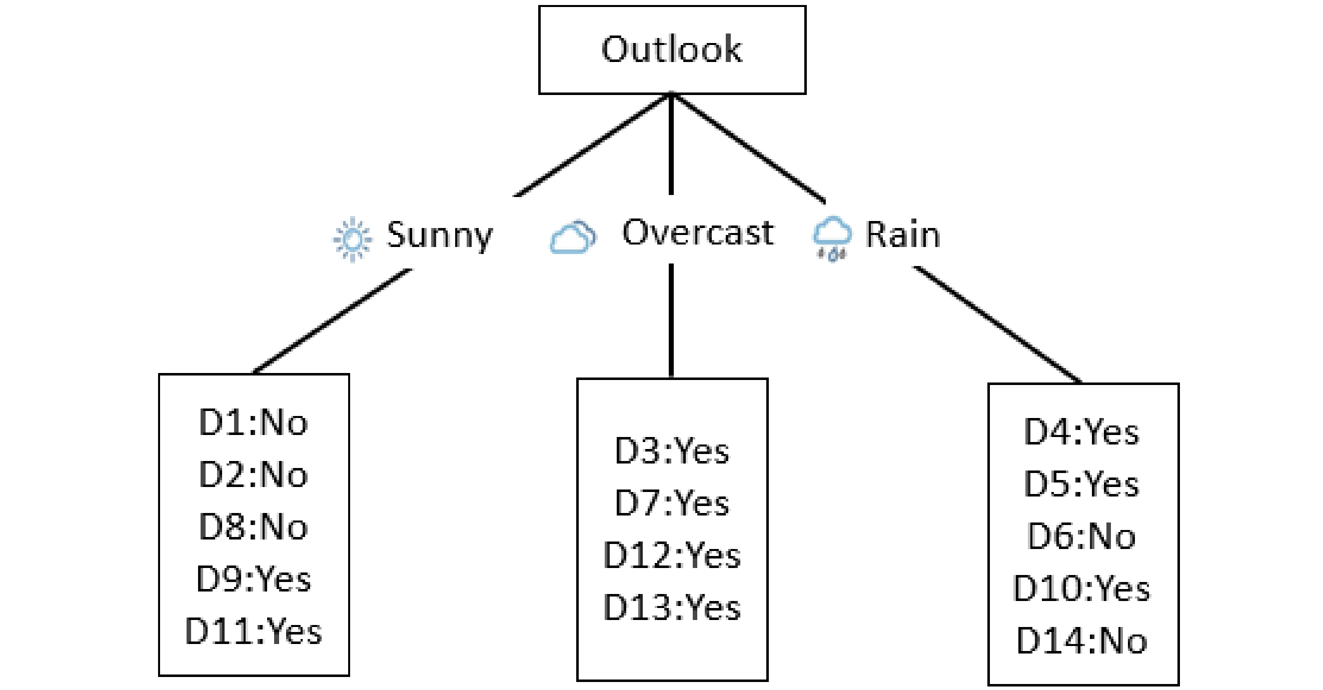
- Entropy measures the (im)purity of a collection
- Information gain of attribute *A* is the reduction in entropy caused by partitioning the set of examples *D*

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

where $\mathrm{Values}(A)$ is the set of all possible values for attribute A

D_v is the subset of D for which attribute A has value v

Measure of Purity: Information



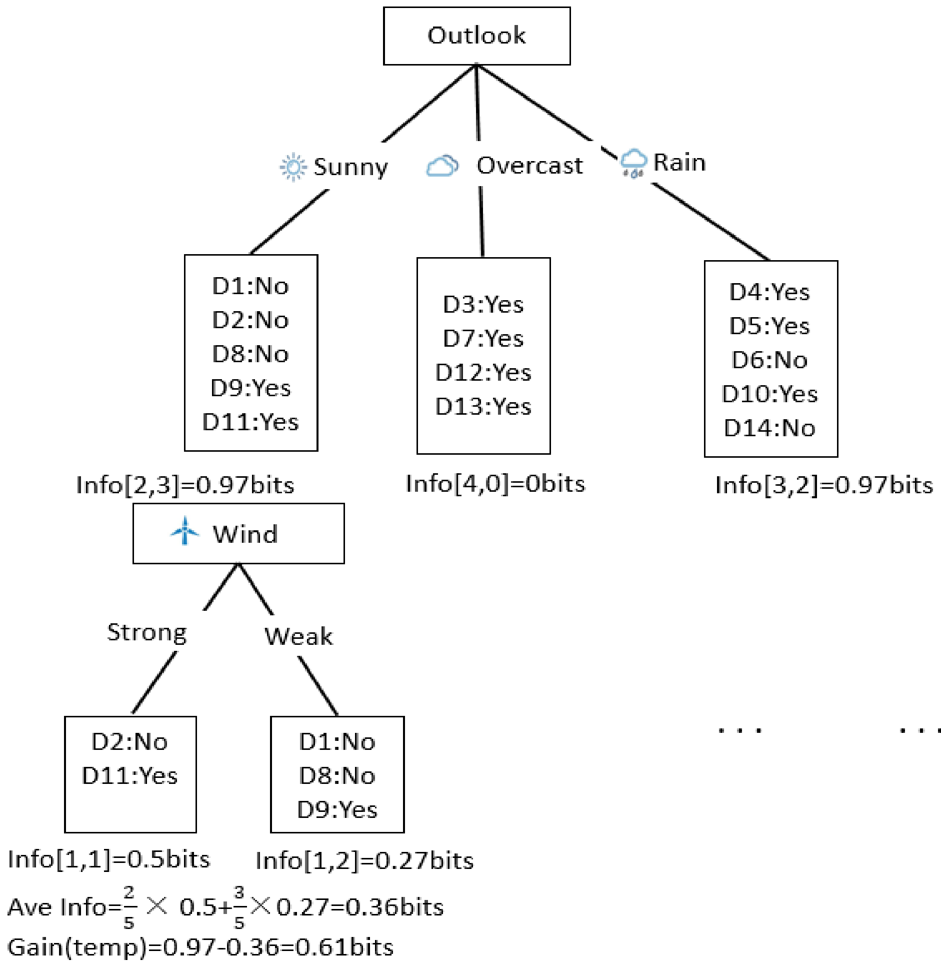
Info[2,3]=0.97bits Info[4,0]=0bits Info[3,2]=0.97bits

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

Information Gain for Each Attribute

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

Expanded Tree: Play Tennis for Outlook = Sunny

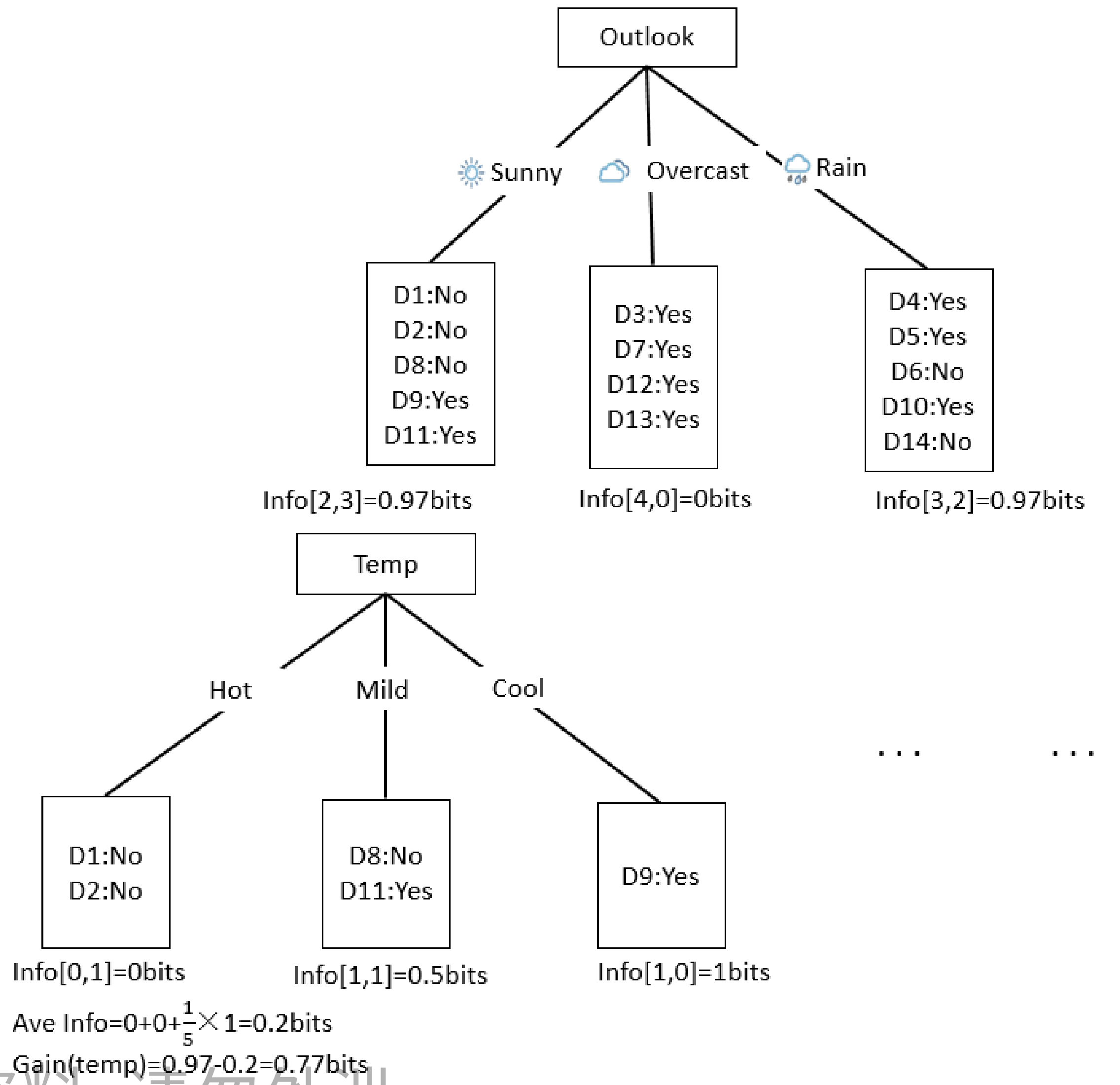


Ave Info=$\frac{2}{5}\times 0.5+\frac{3}{5}\times 0.27=0.36$bits

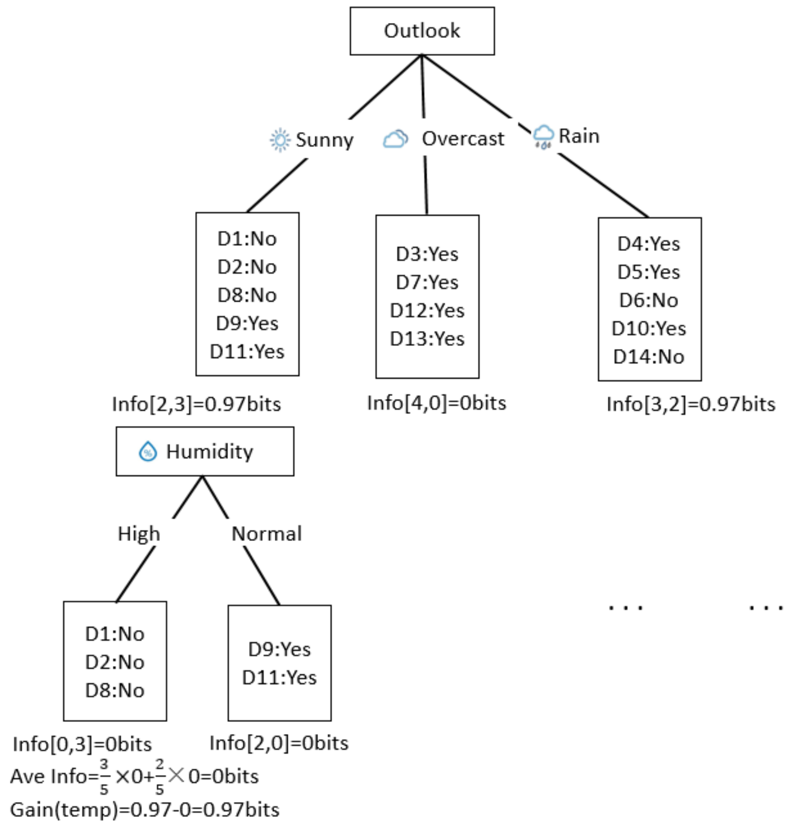
Gain(temp)=0.97-0.36=0.61bits

- Where *temp* contains wind, humidity and temperature

Expanded Tree: Play Tennis for Outlook = Sunny

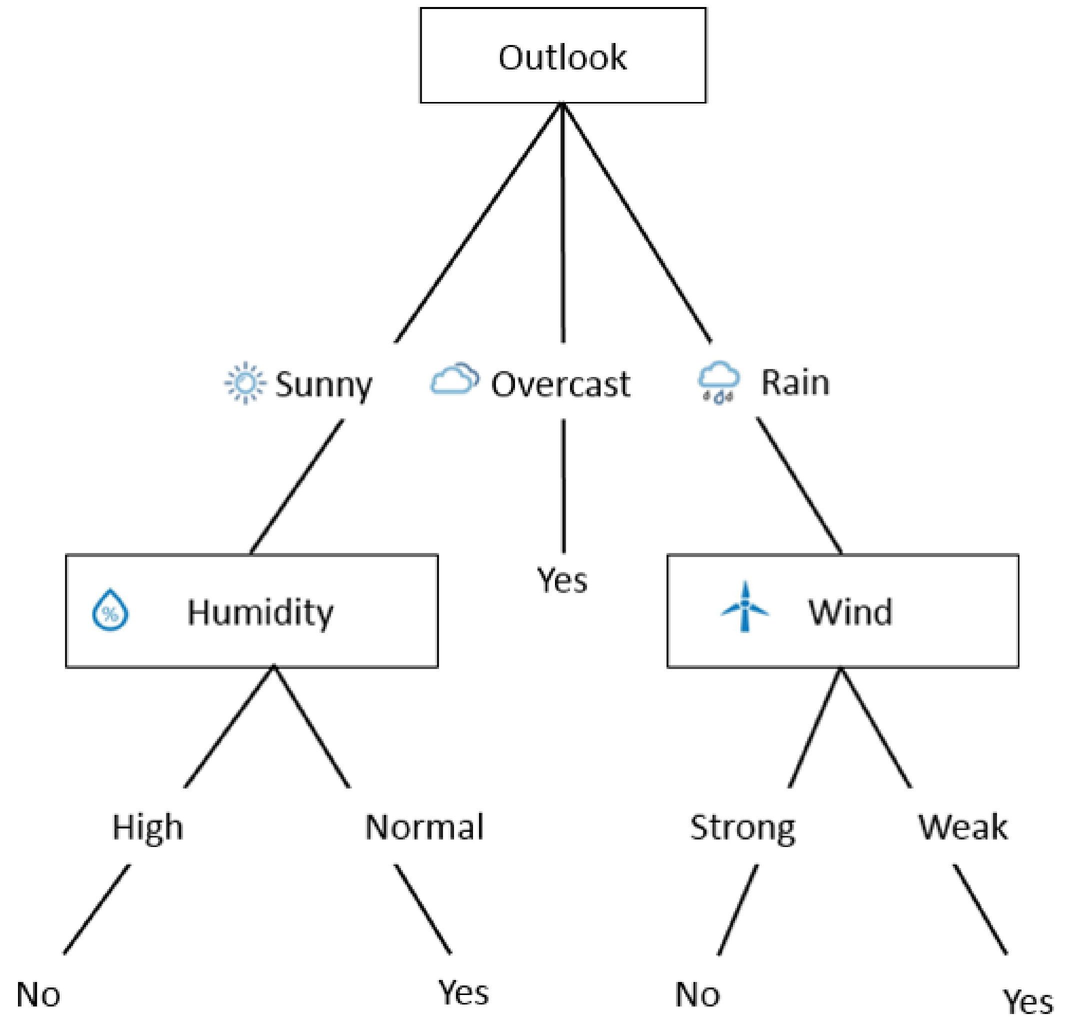


Expanded Tree: Play Tennis for Outlook = Sunny



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

Decision Tree for Weather Data



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AdaBoost: What is AdaBoost?

- Stands for Adaptive Boosting
- Combines base learners linearly
- Iteratively adapts to the errors made by base learners in previous iterations
- Re-weighting scheme:
  - Higher weight assigned to incorrectly classified data points
  - Lower weight assigned to correctly classified data points

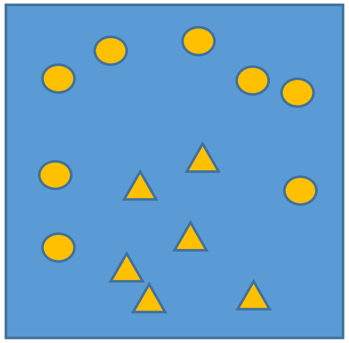
Algorithm: AdaBoost

Input: Training set $D = \{(x_1, y_1), \dots, (x_n, y_n)\}$; Weak learning algorithm.
Output: A strong classifier.

```
1  Initialize the weight vector: $w_1(i)=1/n, i=1,2,\dots,n$;
2  for $t = 1, \dots, T$ do
3      fit base learner $h_t(x) \in \{-1, +1\}$
4      Calculate the classification error rate $e_t$ of $h_t(x)$
           $$e_t = p(h_t(x) \neq y_i) = \sum_{i=1}^{N} w_t(i)\mathbb{I}(h_t(x_i) \neq y_i)$$
5      where $\mathbb{I}\{\cdot\}$ is the indicator function: $\mathbb{I}(X = x_i) = \begin{cases} 1, h_t(x_i) \neq y_i \\ 0, h_t(x_i) = y_i \end{cases}$
6      Calculate the weight $\alpha_t$ of $h_t(x)$
           $$\alpha_t = \frac{1}{2}\ln\frac{1-e_t}{e_t}$$
7      Update the weights of each data point
           $$w_{t+1}(i) = \frac{w_t(i)}{z_t} e^{-\alpha_t y_i h_t(x_i)}, \text{ where } z_t = \sum_{i=1}^{n} w_t(i) e^{-\alpha_t y_i h_t(x_i)}$$
8  end
9  Output the final hypothesis : $H(x) = sign(\sum_{t=1}^{T} \alpha_t h_t(x))$
```

AdaBoost: Initialization of the algorithm

Training data



- Assigning same weight $w_1(i)$ to all data points

$$w_1(i) = \frac{1}{n}, i = 1,2, \ldots, n$$

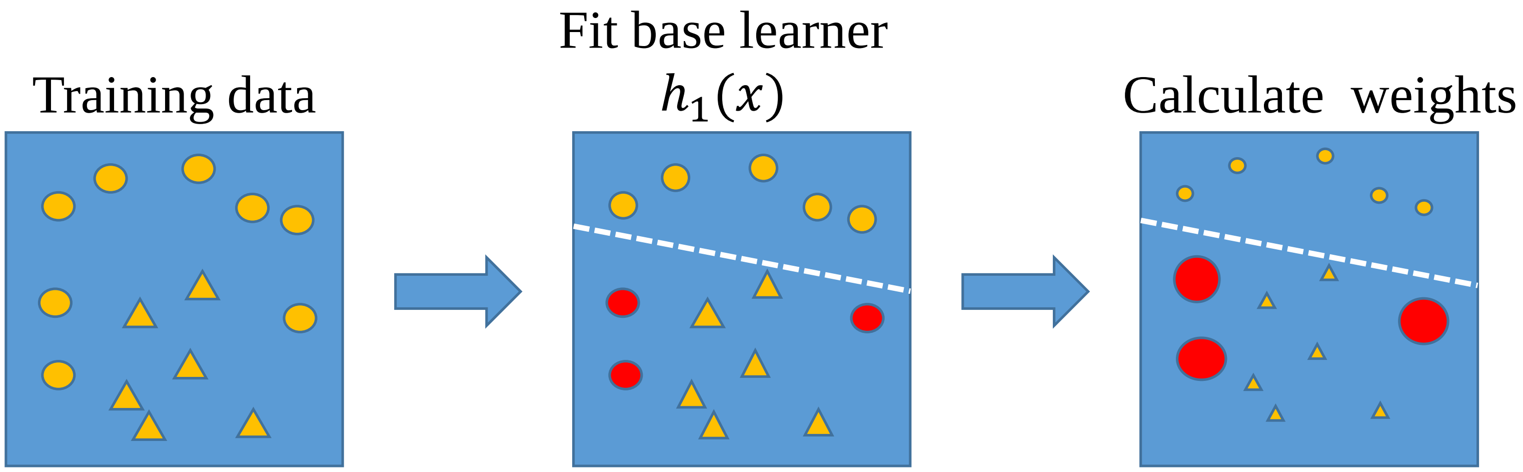
where n is the number of data points

AdaBoost: Iterations of Algorithm

For $t = 1, \ldots, T$ or until low enough error is achieved:

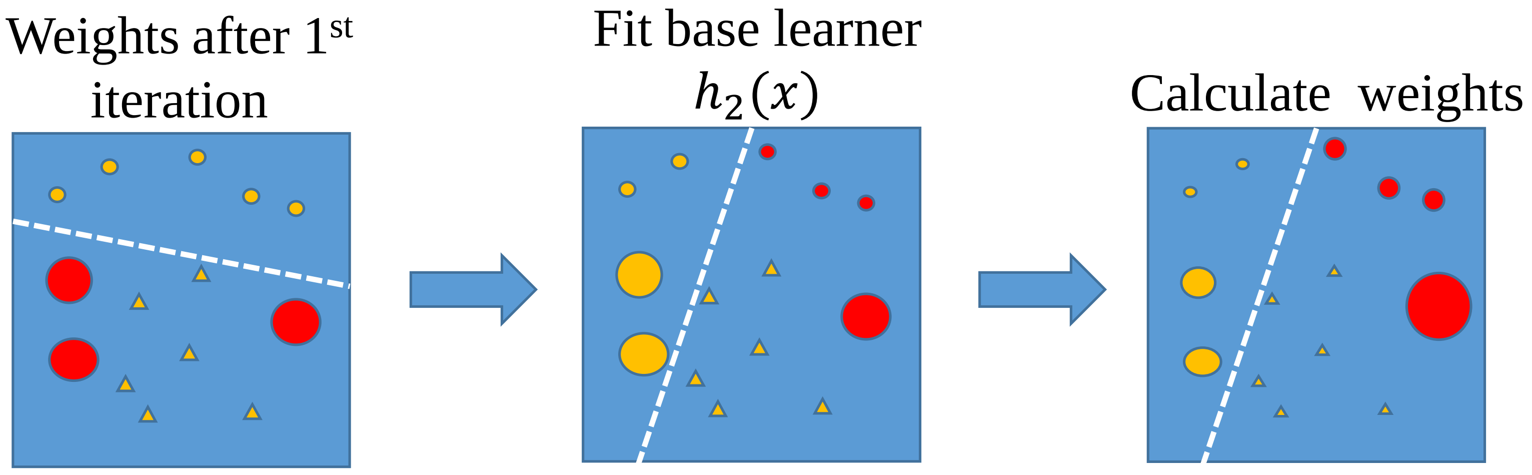
- Fit base learner $h_t(x)$ to data points
- Calculate the classification error rate e_t of $h_t(x)$
- Calculate the weight α_t of $h_t(x)$
- Update the weights of each data point

AdaBoost: Iteration 1



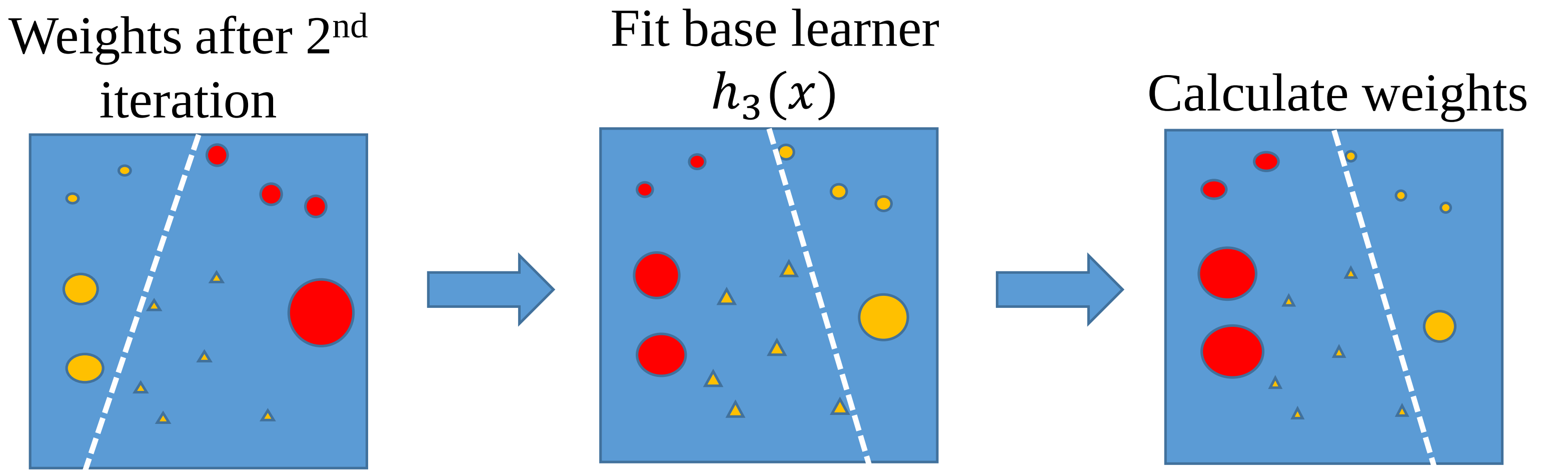
- Initially all data points have the same weight $1/n$
- The class correctly classified will be given less weights in the next iteration, and higher weights for misclassified class

AdaBoost: Iteration 2



- Base learner forms a decision boundary which classifies the data points better with higher weights

AdaBoost: Iteration 3

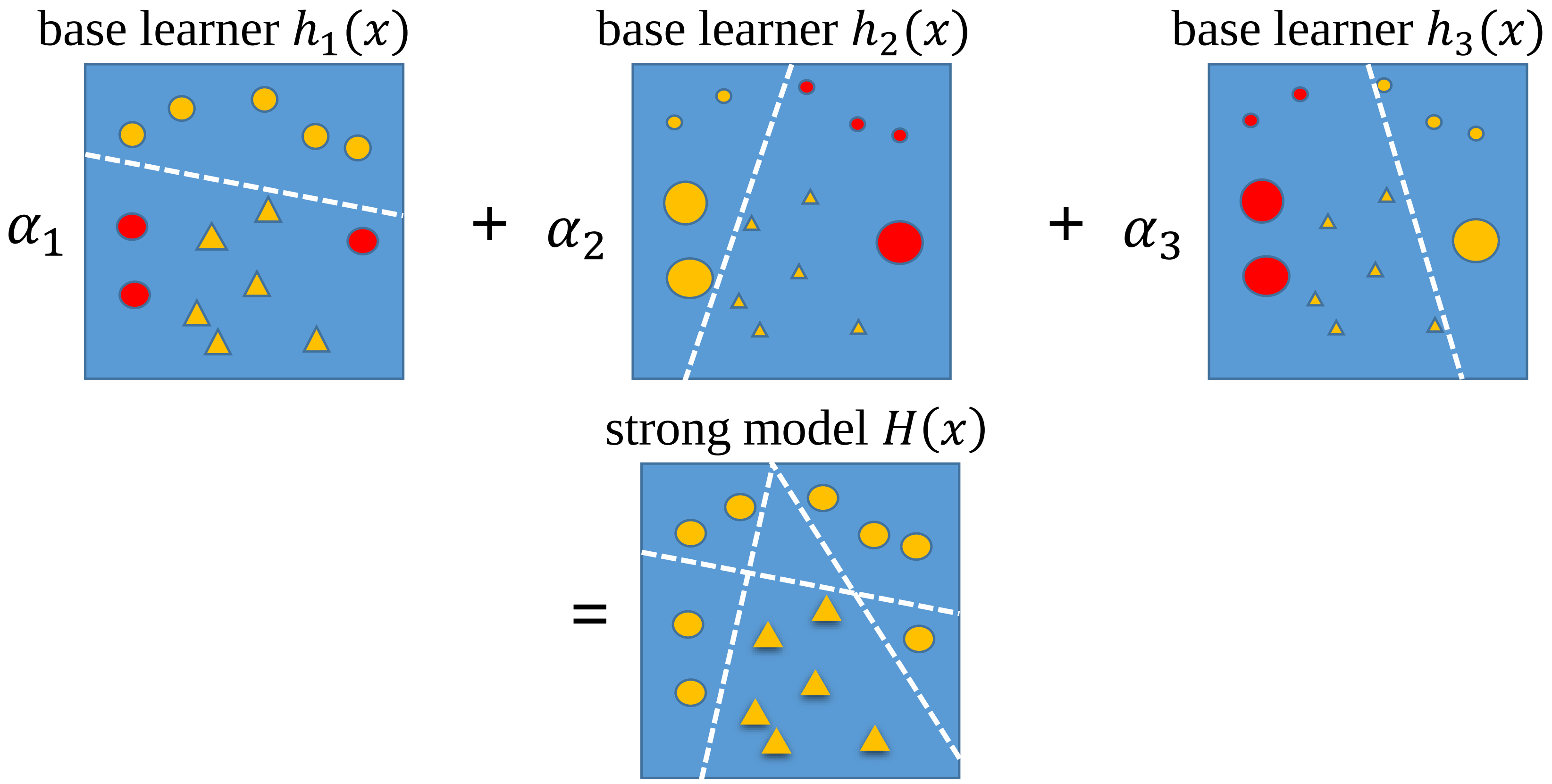


…continue iterating until either:

- Sufficiently low training error is achieved (with enough iterations, the algorithm can reach 100% accuracy)
- A pre-defined number of base learners was added

AdaBoost: Final Model

$$H(x) = sign(\sum_{t=1}^{T} \alpha_t h_t(x))$$



AdaBoost: More Details

- Fit base learner $h_t(x)$ to data points, we define base classifier $h_t(x)$ as

$$h_t(x) \in \{-1, +1\}$$

- Calculate the classification error rate e_t of $h_t(x)$ on the training data set

$$e_t = p(h_t(x) \neq y_i) = \sum_{i=1}^{n} w_t(i)\mathbb{I}(h_t(x_i) \neq y_i)$$

For binary classification case, $\mathbb{I}(X = x_i) = \begin{cases} 1, h_t(x_i) \neq y_i \\ 0, h_t(x_i) = y_i \end{cases}$

AdaBoost: More Details

- Calculate the weight α_t of $h_t(x)$ in the final classifier

$$\alpha_t = \frac{1}{2}\ln\frac{1-e_t}{e_t}$$

Here, when $e_t \leq 0.5$, $\alpha_t \geq 0$, with the decreasing of e_t, α_t will be larger

Note: classifier with smaller error rate would be more important

AdaBoost: More Details

- Update the weights

$$w_{t+1}(i) = \frac{w_t(i)}{z_t} e^{-\alpha_t y_i h_t(x_i)}$$

Here, $z_t = \sum_{i=1}^{n} w_t(i) e^{-\alpha_t y_i h_t(x_i)}$ is normalization term,

and makes $w_t(i)$ a probability distribution

To simplify, $w_{t+1}(i) = \begin{cases} \frac{w_t(i)}{z_t} e^{-\alpha_t}, & \text{for right predictive sample} \\ \frac{w_t(i)}{z_t} e^{\alpha_t}, & \text{for wrong predictive sample} \end{cases}$

AdaBoost: More Details

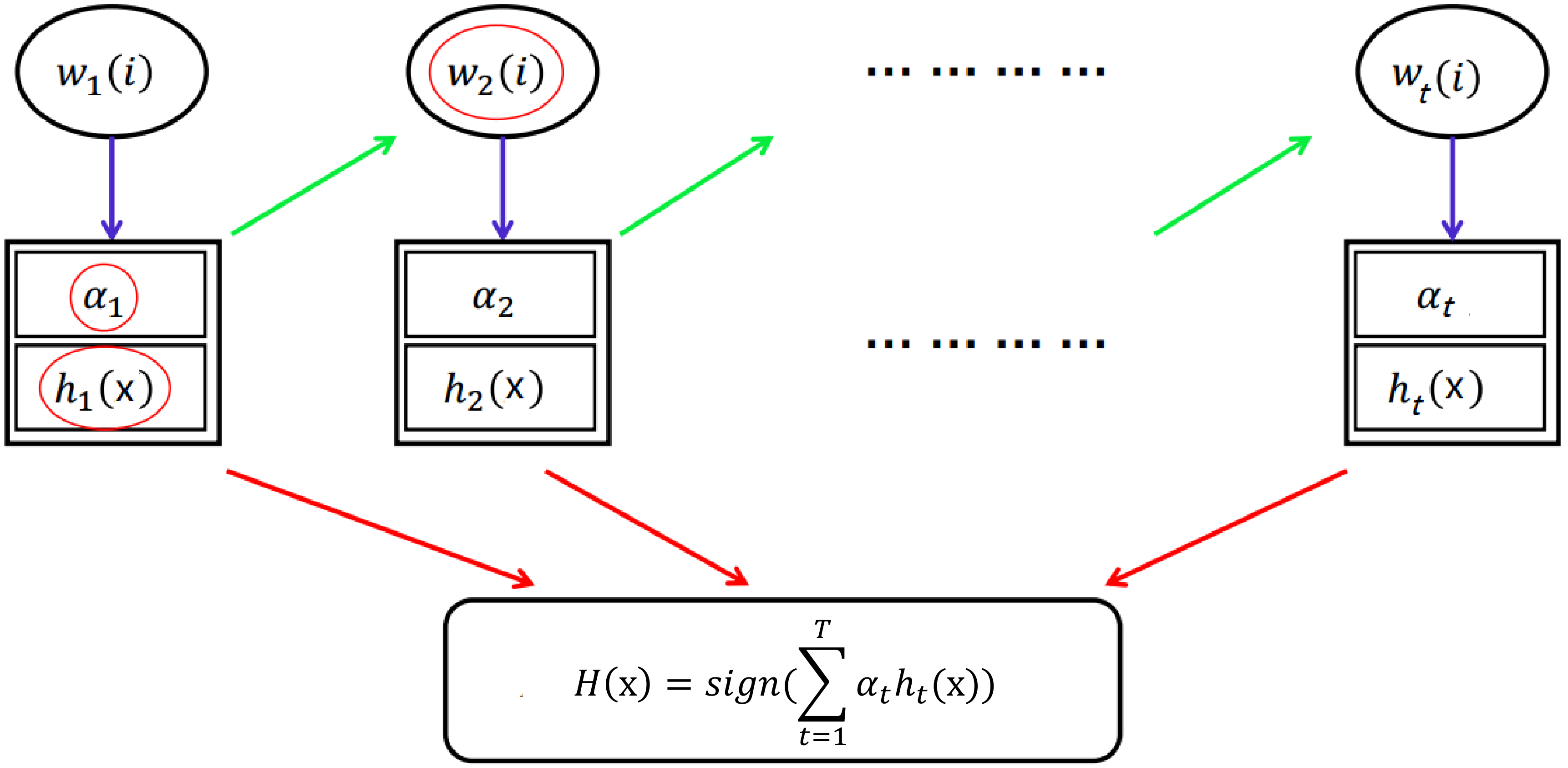
- Ensemble learner

$$H(\mathrm{x}) = sign\left(\sum_{t=1}^{T} \alpha_t h_t(\mathrm{x})\right)$$

Note: $h_t(\mathrm{x}) = sign(\mathrm{w}^{\mathrm{T}}\mathrm{x})$ is a nonlinear function, so AdaBoost can deal with nonlinear problem

AdaBoost: More Details

Every iteration generates a new base learner $h_t(x)$ with weight α_t



AdaBoost: Example

Given the following training samples:

Index	1	2	3	4	5	6	7	8	9	10
x	0	1	2	3	4	5	6	7	8	9
y	-1	-1	-1	1	1	1	-1	-1	-1	1

- Initialize the same weights for data points at the beginning, $w_1(1),\ w_1(2), \ldots, w_1(10) = 0.1$
- Assume the threshold of x is 2.5, when $x \leq 2.5$, $h_1(x) = -1$, when $x > 2.5$, $h_1(x) = 1$
- So the right samples are Index 1, 2, 3, 4, 5, 6, 10, and the wrong samples are Index 7, 8, 9 (three data points)
- The error rate $e_1 = 3 * 0.1 = 0.3$
- For all samples, the threshold is chosen to be 2.5, which has the lowest error rate e_1

AdaBoost: Example

- Now, the first base classifier is

$$h_1(\mathrm{x}) = \begin{cases} 1, x \le 2.5 \\ -1, x > 2.5 \end{cases}$$

- Then, for $h_1(\mathrm{x}), \alpha_1$ is

$$\alpha_1 = \frac{1}{2} \ln \frac{1 - e_1}{e_1} = 0.424$$

- For the first round, the weight of $h_1(\mathrm{x})$ is 0.424, it is used to update the weights of data points of the next round

$$w_{t+1}(i) = \frac{w_t(i)}{z_t} e^{-\alpha_t y_i h_t(x_i)}$$

- $w_2(i), i = 1, \dots, 10$ are as shown in the table below:

index	1	2	3	4	5	6	7	8	9	10
x	0	1	2	3	4	5	6	7	8	9
y	-1	-1	-1	1	1	1	-1	-1	-1	1
w_2	0.0714	0.0714	0.0714	0.0714	0.0714	0.0714	0.1667	0.1667	0.1667	0.0714

AdaBoost: Why Use AdaBoost?

- Needs only a simple classifier as a base learner
- Can achieve prediction similar to powerful classifiers
- Can combine with any learning algorithms
- Requires little parameter tuning
- Extended to problems beyond binary classification

AdaBoost: Summary

- AdaBoost (i.e. Adaptive boosting) is one of the most popular and powerful ensemble methods
- AdaBoost focuses on the data points that are erroneous
- Simple to implement and depend on the base learner
- However, vulnerable to noisy data

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Gradient Boosting Decision Trees

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 people A, B, C and D, whose age are 14, 16, 24, 26 respectively

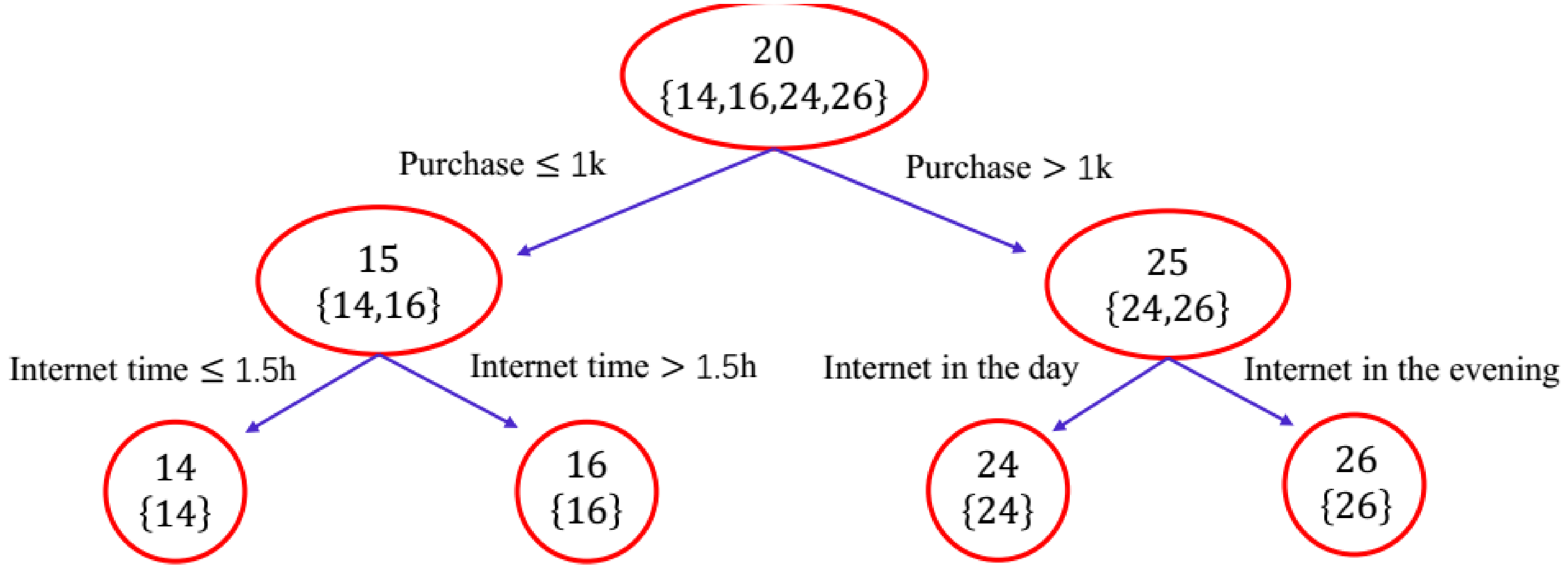
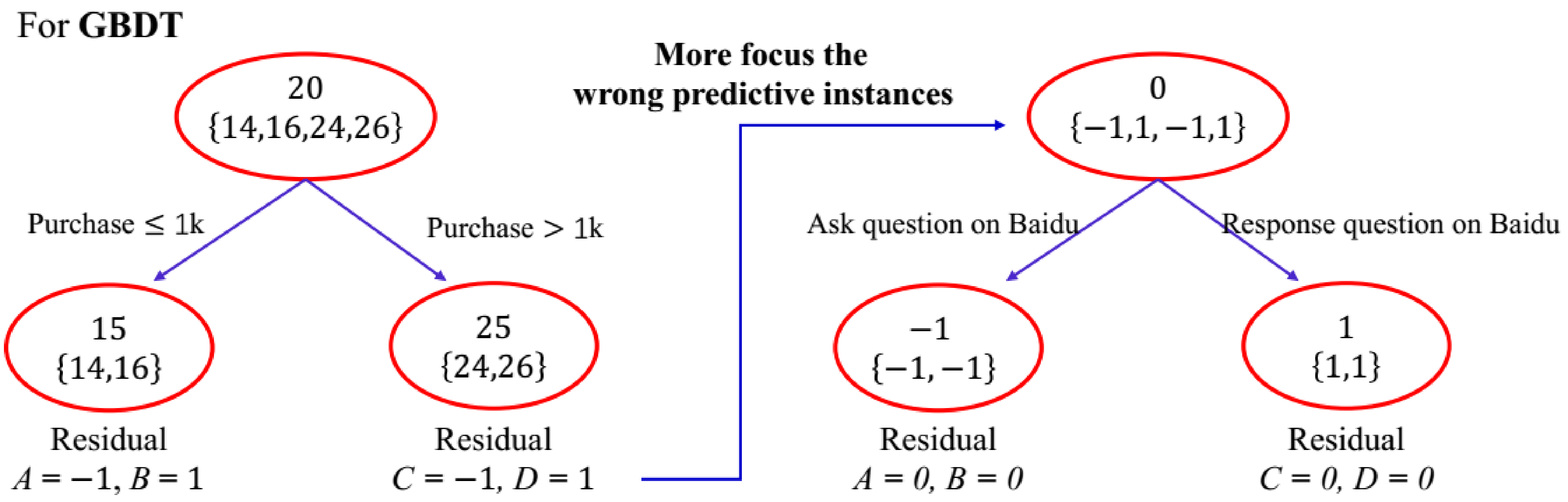


Figure: Single regression tree

GBDT

- 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: Questions

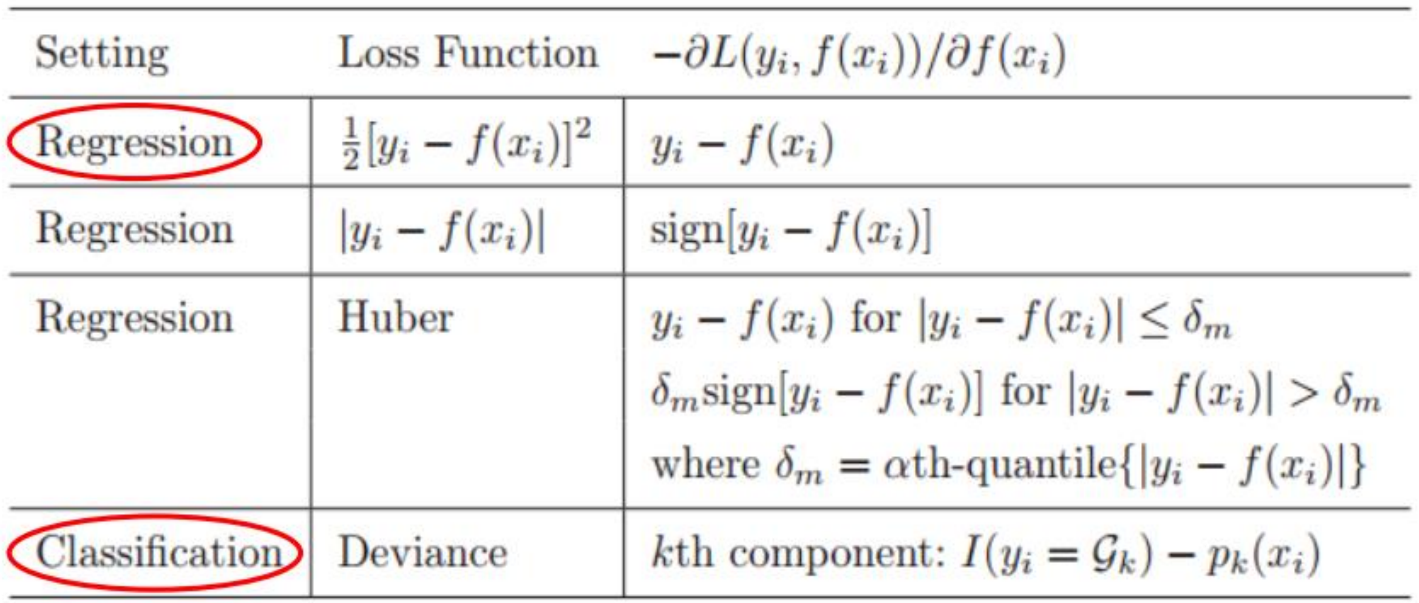
Q1:Why do we need GBDT?

- The motivation of this algorithm
  - Every calculation of residual is to increase the weight of wrong predictive samples
  - The residual of right predictive sample is zero
- In the next iteration, the model can concentratively address these wrong predictive samples
- Another function is to prevent overfitting

Gradient Boosting Decision Trees: Questions

Q2:Where does this algorithm reflect gradient boosting?

- Residual is the gradient descent direction, which is the derivation of mean square error (MSE)
- 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	$\lvert y_i - f(x_i)\rvert$	$\text{sign}[y_i - f(x_i)]$
Regression	Huber	$y_i - f(x_i)$ for $\lvert y_i - f(x_i)\rvert \leq \delta_m$ $\delta_m \text{sign}[y_i - f(x_i)]$ for $\lvert y_i - f(x_i)\rvert > \delta_m$ where $\delta_m = \alpha$th-quantile$\{\lvert y_i - f(x_i)\rvert\}$
Classification	Deviance	kth component: $I(y_i = \mathcal{G}_k) - p_k(x_i)$

Algorithm: GBDT

Input: $D = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, **where** $x_i \in X, y_i \in \{-1, 1\}$

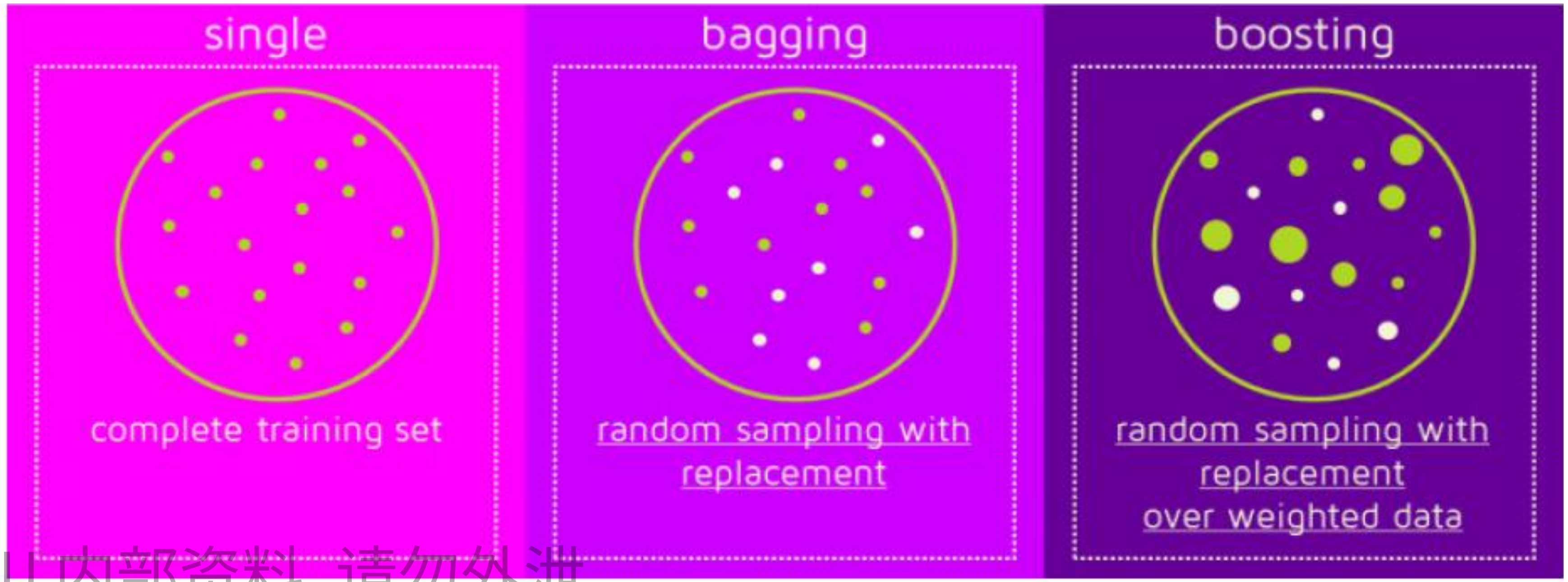
Initialize: $f_o(x) = \text{argmin}_\mu \sum_{i=1}^{n} L(y_1, \mu)$

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

```
1  for $m = 1,2, \ldots, M$ do
2      for $i = 1,2, \ldots, n$ do
3          $r_{im} = -[\frac{\partial L(y_i, f_{m-1}(x_i))}{\partial f_{m-1}(x_i)}]$
4          Fit a regression tree to targets $r_{im}$ giving terminal regions
5          $R_{jm},\ j = 1,2, \ldots, J_m$
6      end
7      for $j = 1,2, \ldots, J_m$ do
8          $\mu_{jm} = \text{argmin}_\mu \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \mu), j = 1,2, \ldots, J_m$
9          Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \mu j_m (x \in R_{jm})$
10     end
11 end
```

Summary

- Instead of training different models on same data, training same model will
  - multiple times on different data sets
  - combine different models
- We can use some simple/weak model as the base model
- How do we get multiple training data sets (in practice, we only have one data set at training time)?


single
complete training set
bagging
random sampling with replacement
boosting
random sampling with replacement over weighted data

Thank You