Nonlinear Machine Learning and Ensemble Methods

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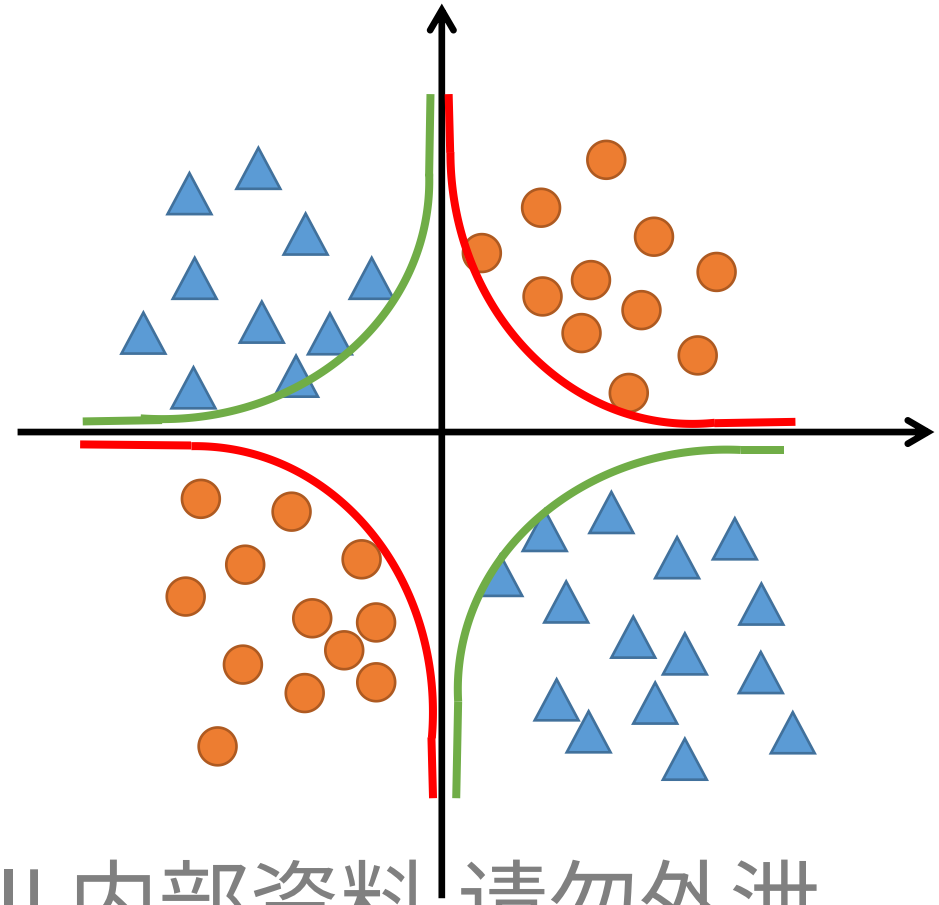
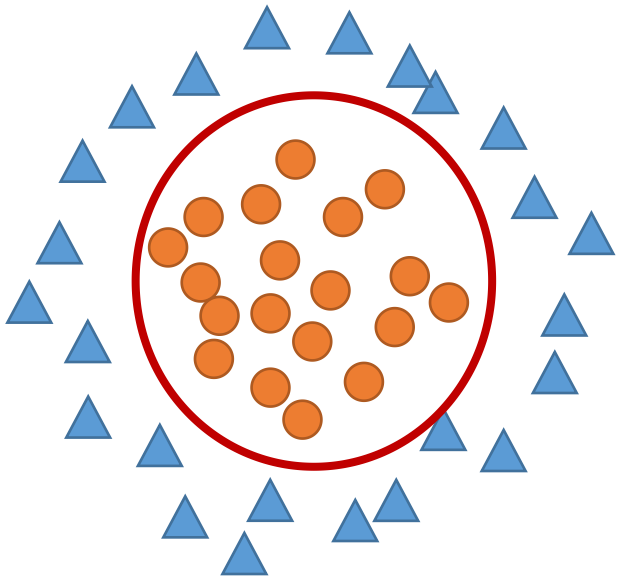
Classification Examples

- How to classify?





Contents

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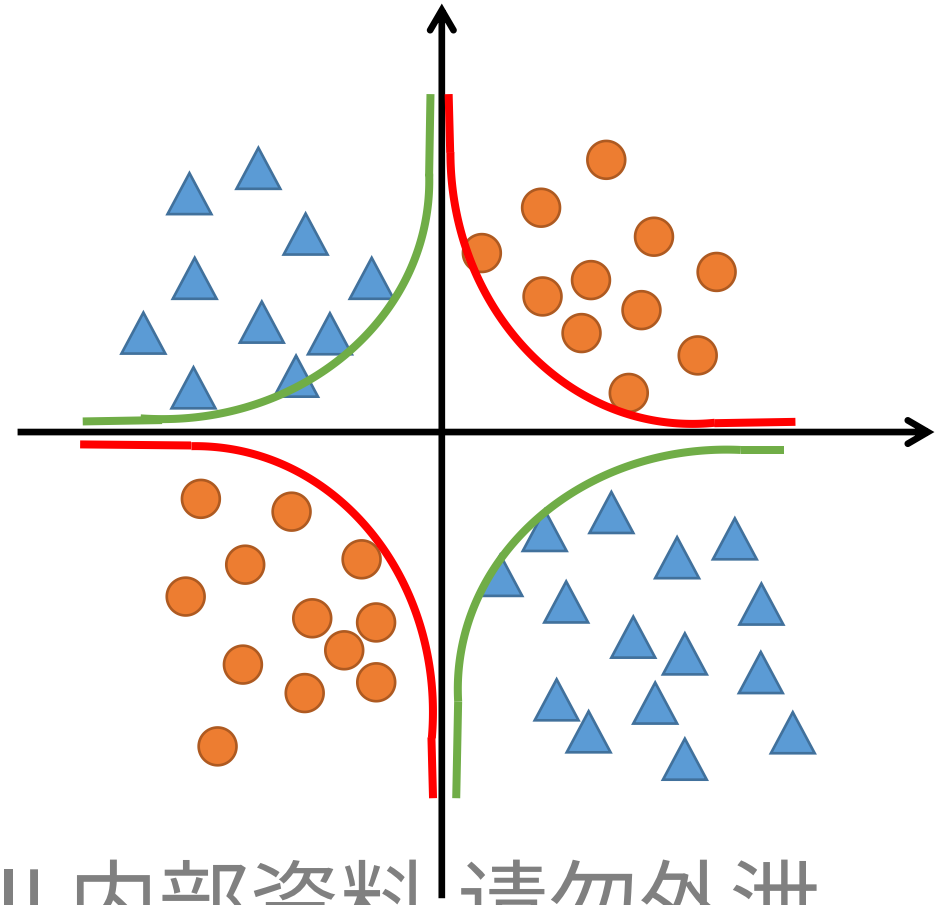
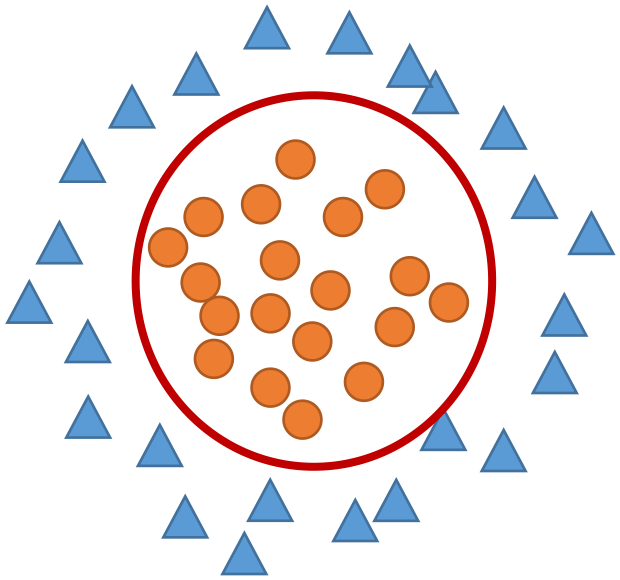
Classification Examples

- How to classify?





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?

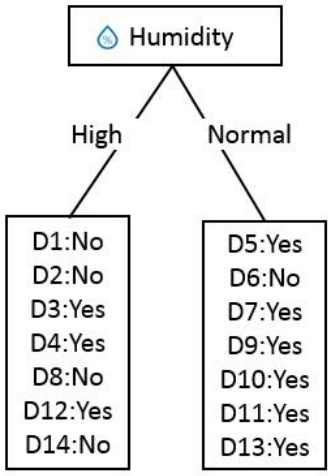
- Learned function is a tree
- Each branch of the tree represents a possible decision, outcome, or reaction
- The farthest branches (leaf nodes) on the tree represent the end results

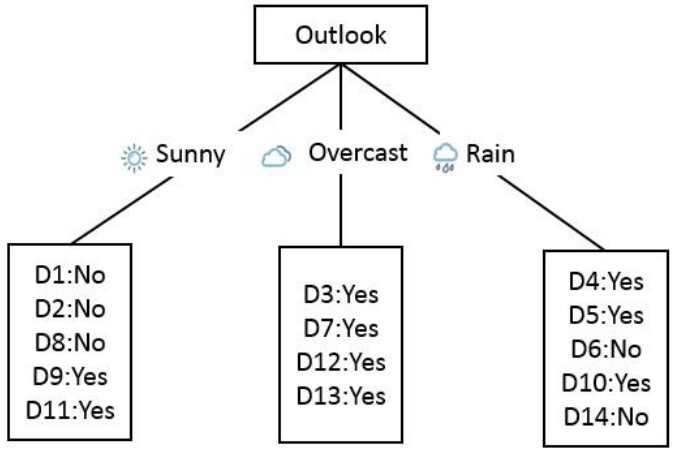
Algorithm: Decision Tree

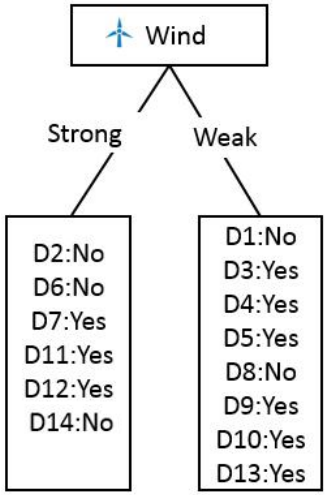
Input: Training set $D = \{(x_1, y_1), ..., (x_n, y_n)\}$; Attribute set $A = \{a_1, a_2, ..., a_d\}$.
Procedure: Function TreeGenerate(D, A). **Output**: A decision tree.

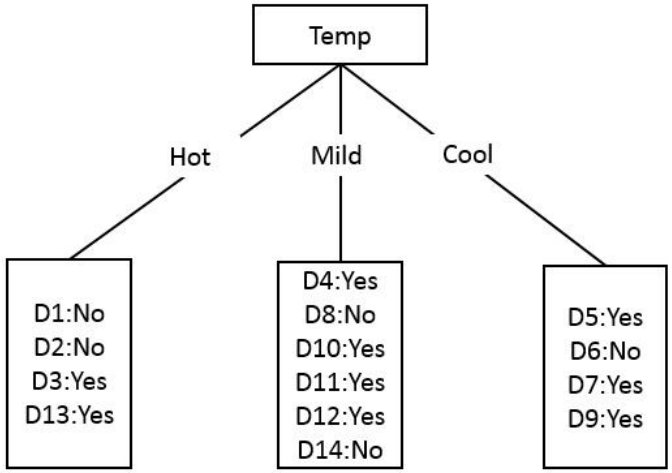
```
1  Generate node;
2  if all the samples in D belong to class C then
3  |   mark this node as class C leaf node; return
4  end
5  if A = ∅ OR samples in D have the same value on A then
6  |   mark this node as leaf node, and the class should be the most frequent
   |   occurrence class; return
7  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 = ∅ 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 \ {a_*})
15 |   end
16 end
```

Decision Tree Example









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:

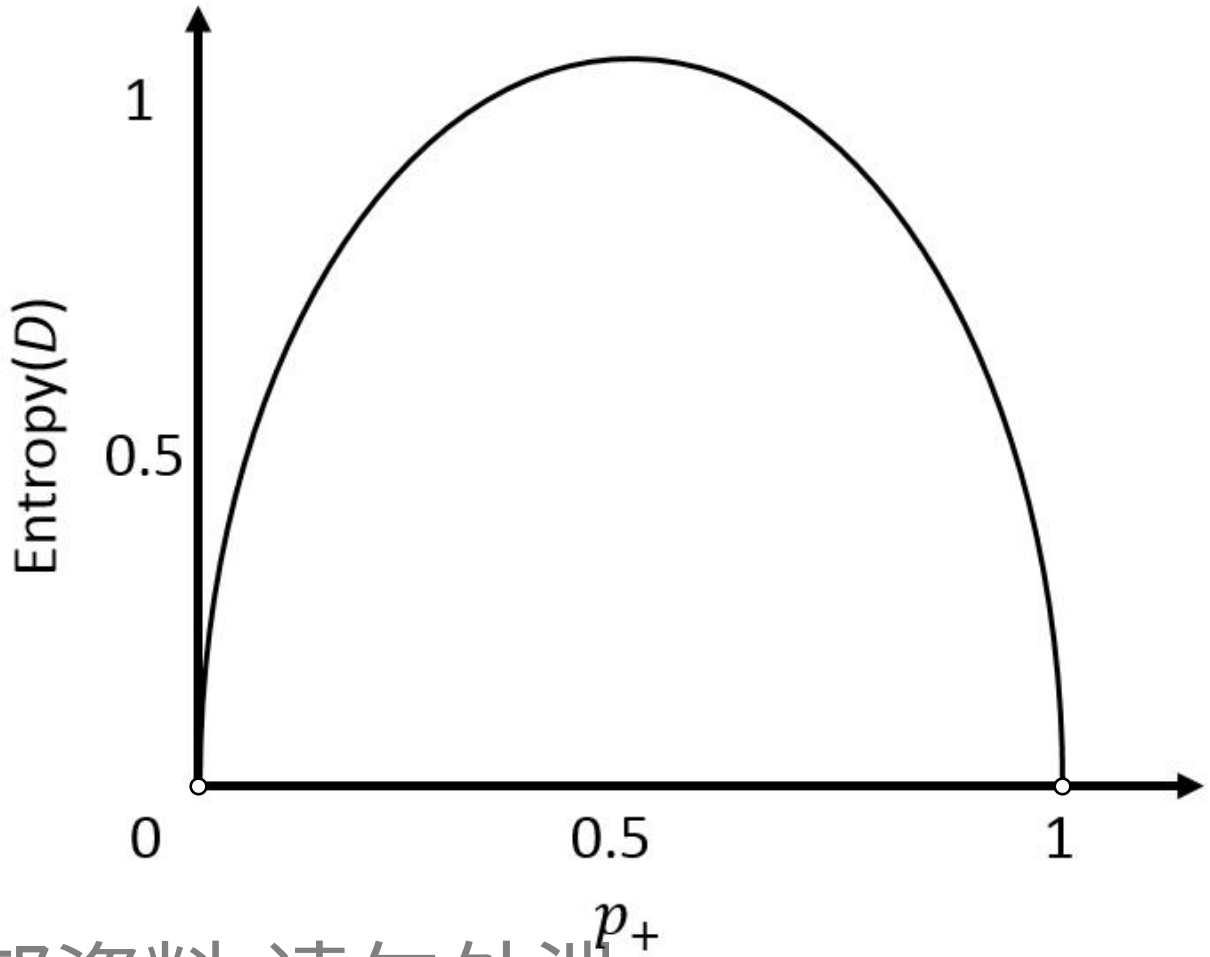
- D is a collection of 14 examples with 9 positive and 5 negative examples
- Entropy of D relative to the boolean classification:

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

- 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

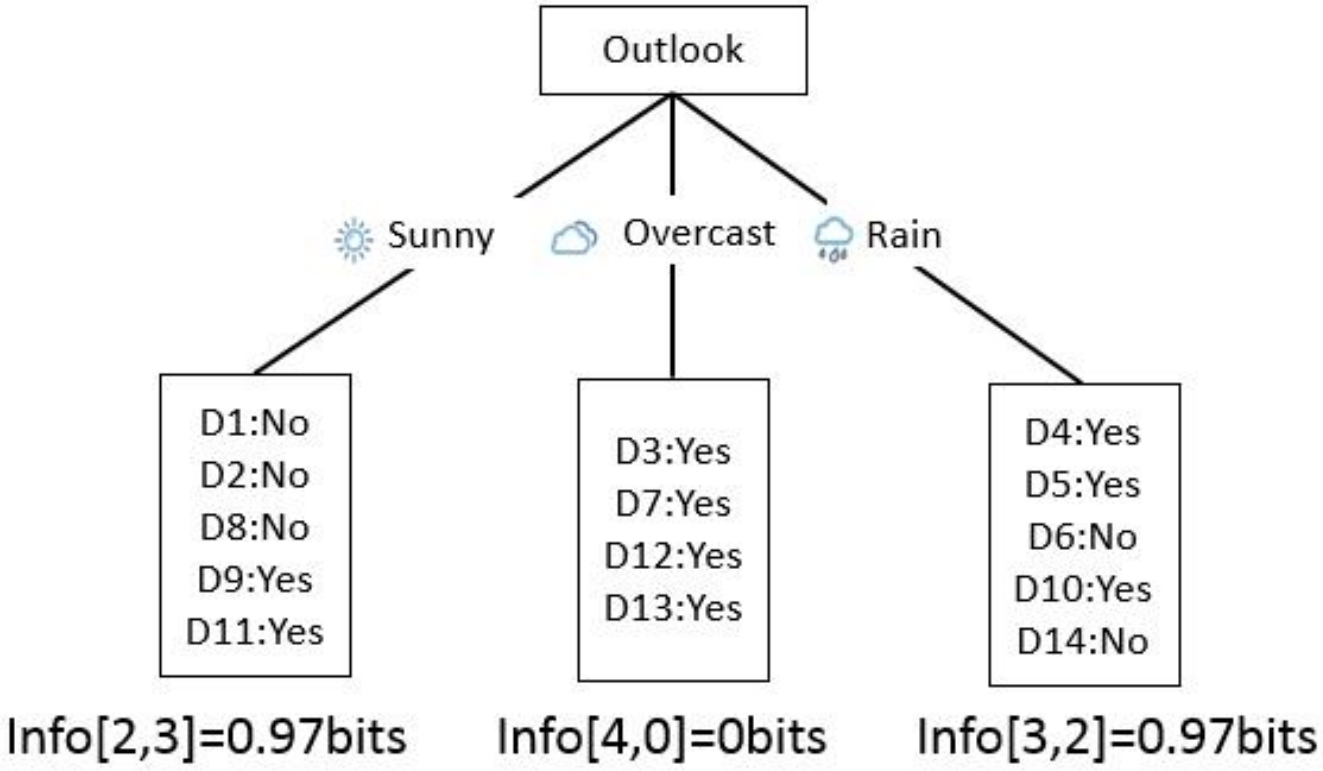
- Entropy measures the (im)purity of a collection
- Information gain of attribute A is the reduction in entropy caused by partitioning the set of examples D

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

where $\text{Values}(A)$ 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

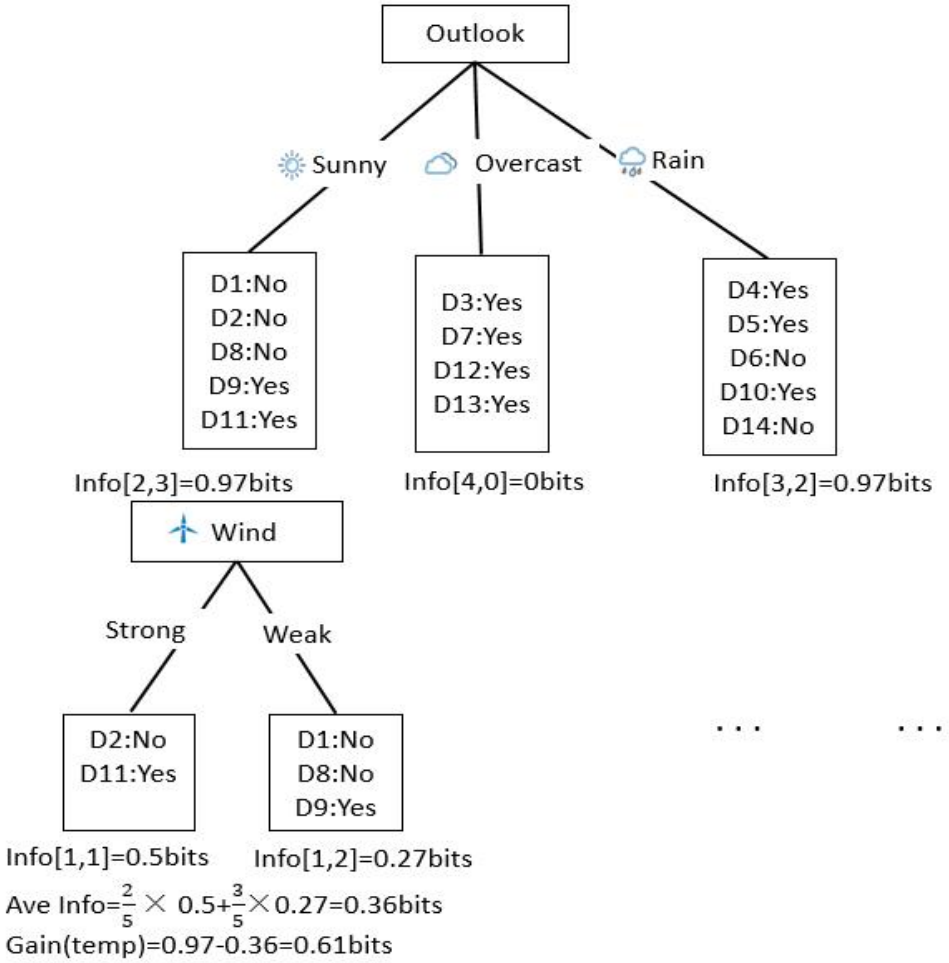


$$\text{Info}[2,3] = \text{entropy}(2,3) = -\frac{2}{5}\log_2\frac{2}{5} - \frac{3}{5}\log_2\frac{3}{5} = 0.97\text{bits}$$

Information Gain for Each Attribute

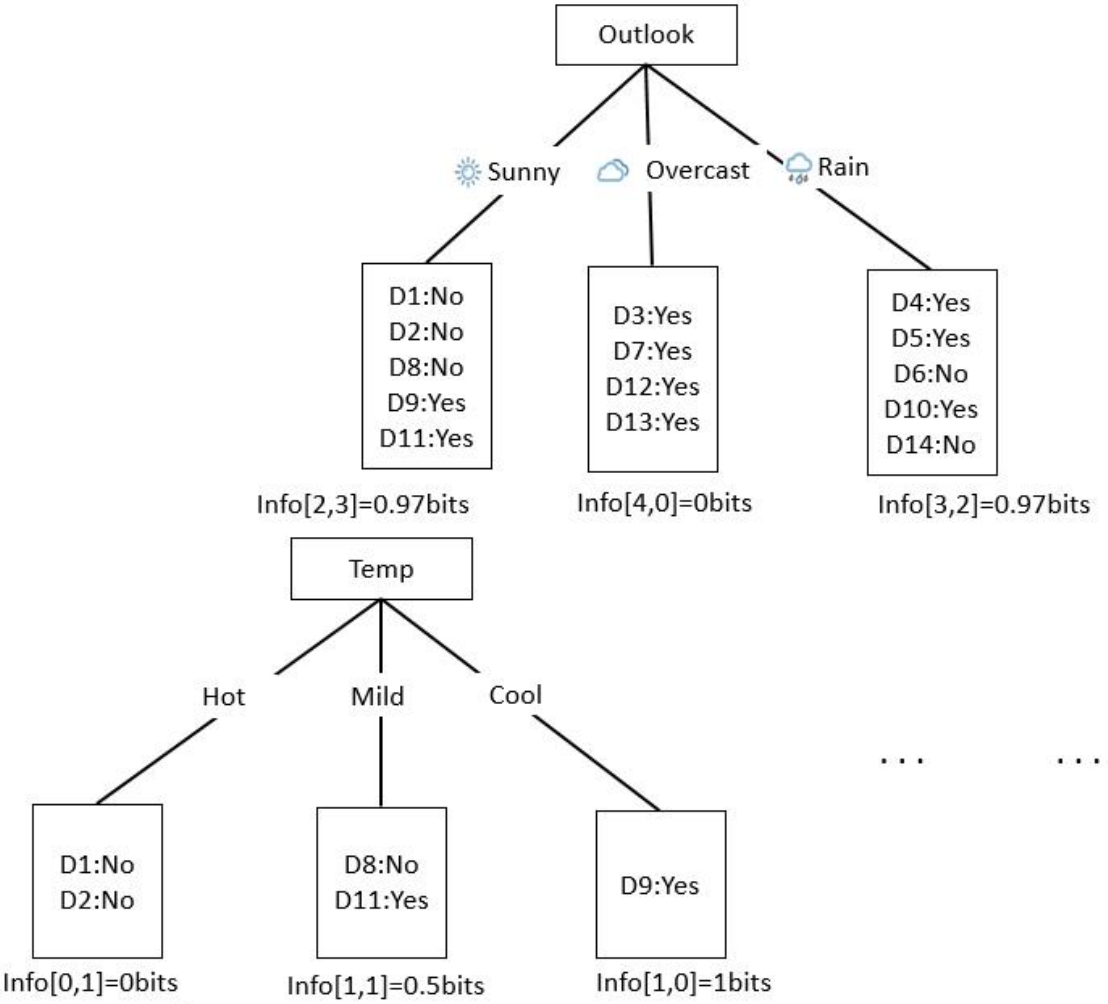
- $\text{Gain}(\text{outlook}) = 0.94 - 0.693 = 0.247$
- $\text{Gain}(\text{temperature}) = 0.94 - 0.911 = 0.029$
- $\text{Gain}(\text{humidity}) = 0.94 - 0.788 = 0.152$
- $\text{Gain}(\text{windy}) = 0.94 - 0.892 = 0.048$
- $\text{argmax}_A\{0.247,\ 0.029,\ 0.152,\ 0.048\} =$ outlook
- Select outlook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

Expanded Tree: Play Tennis for Outlook = Sunny

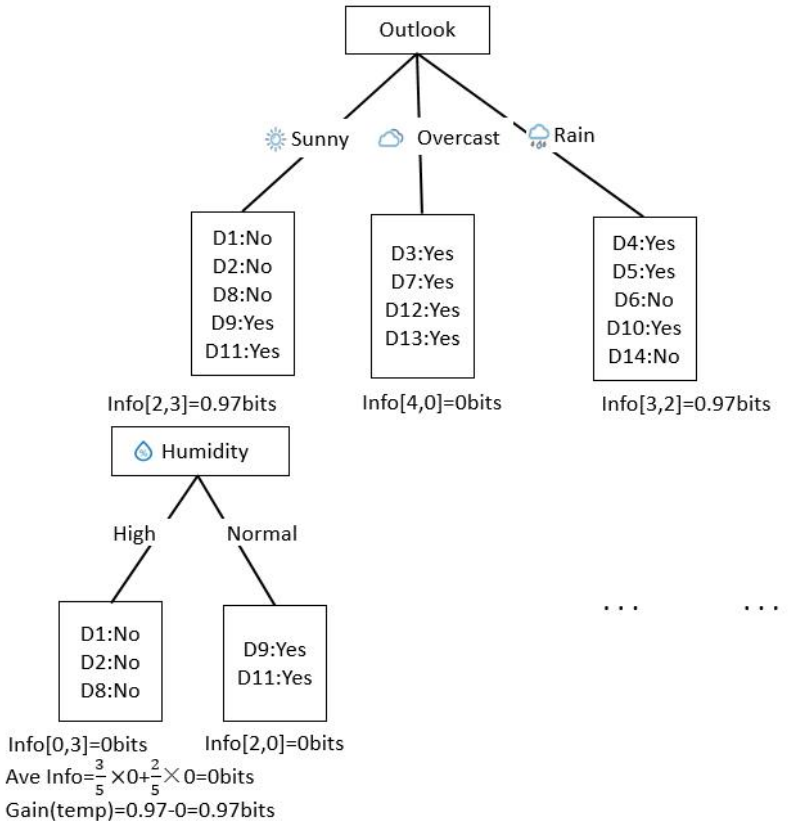


- Where *temp* contains wind, humidity and temperature

Expanded Tree: Play Tennis for Outlook = Sunny

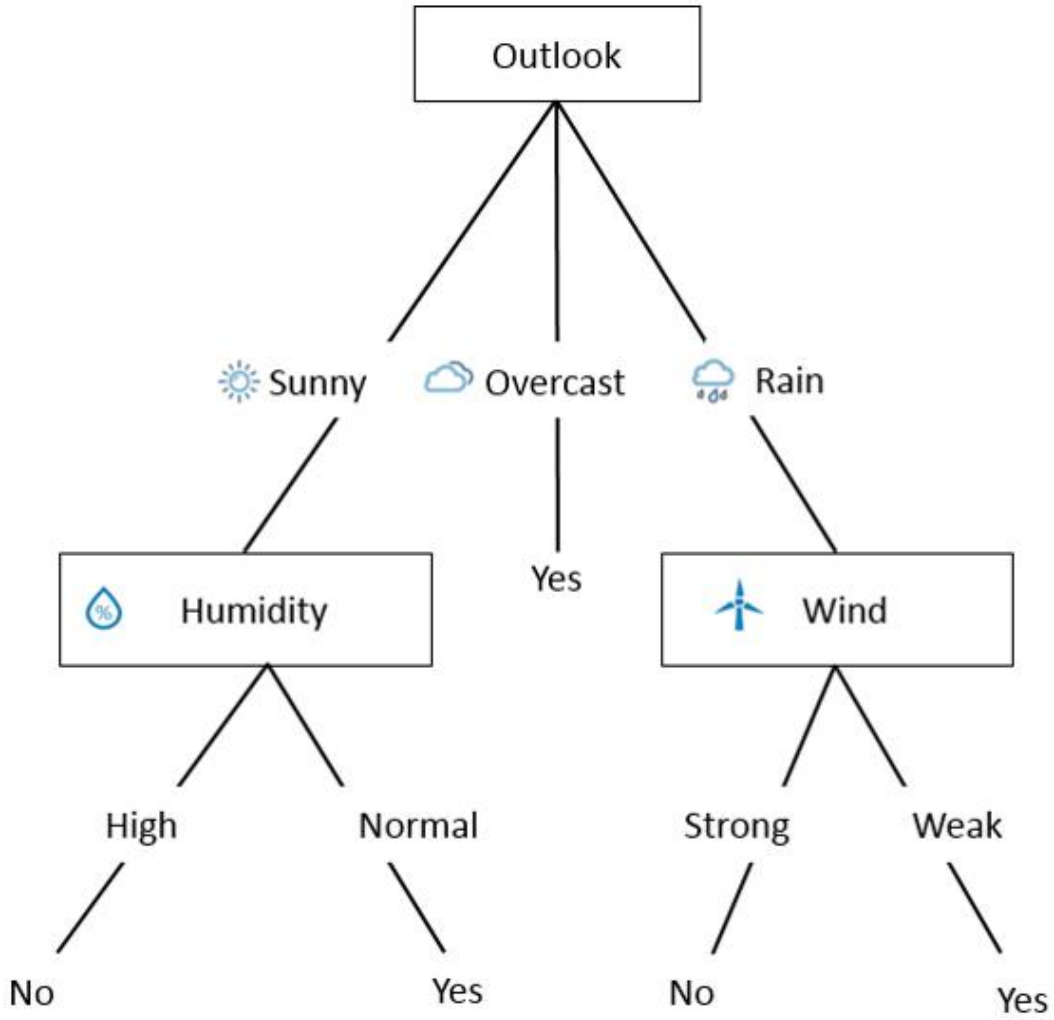


Expanded Tree: Play Tennis for Outlook = Sunny



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

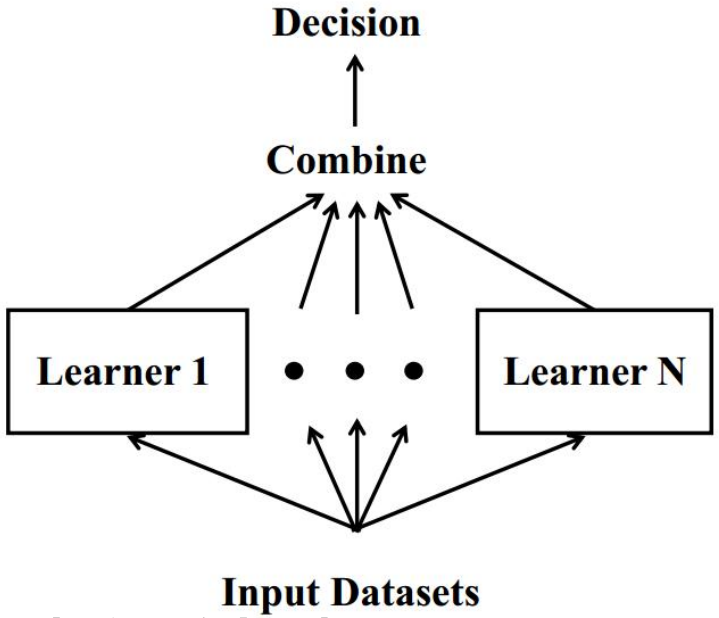
Decision Tree for Weather Data



Contents

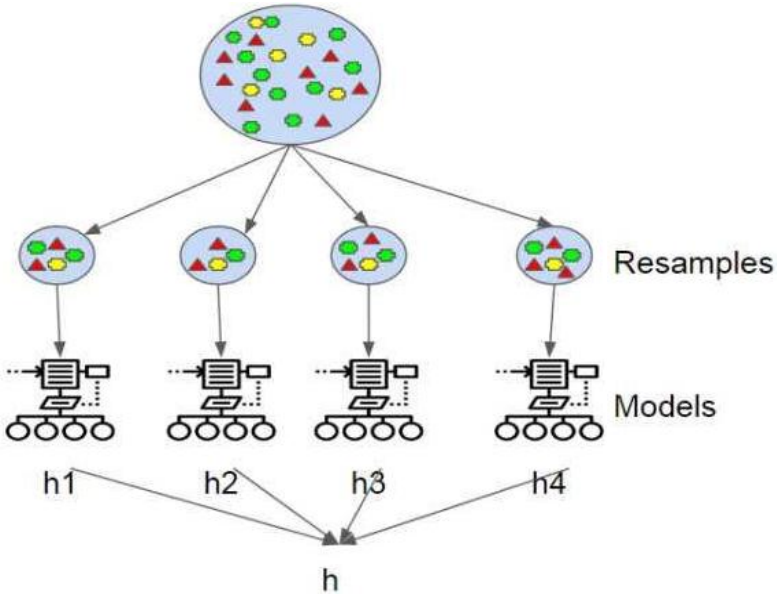
Ensemble Learning

- 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

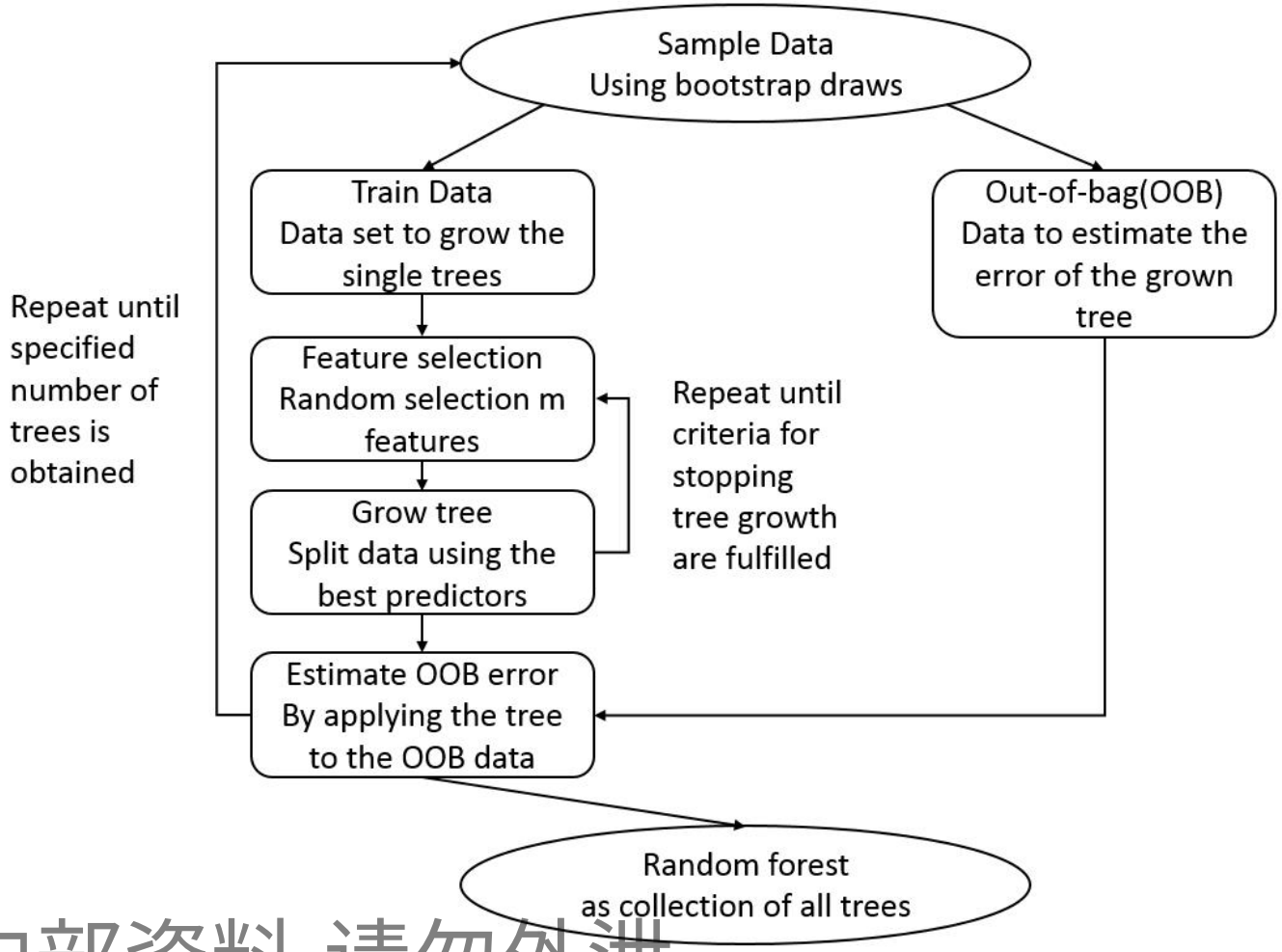
- Random forest is an extension of bagging using decision tree as base learner
- Randomly select m out of p features to get the optimal partition feature

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:



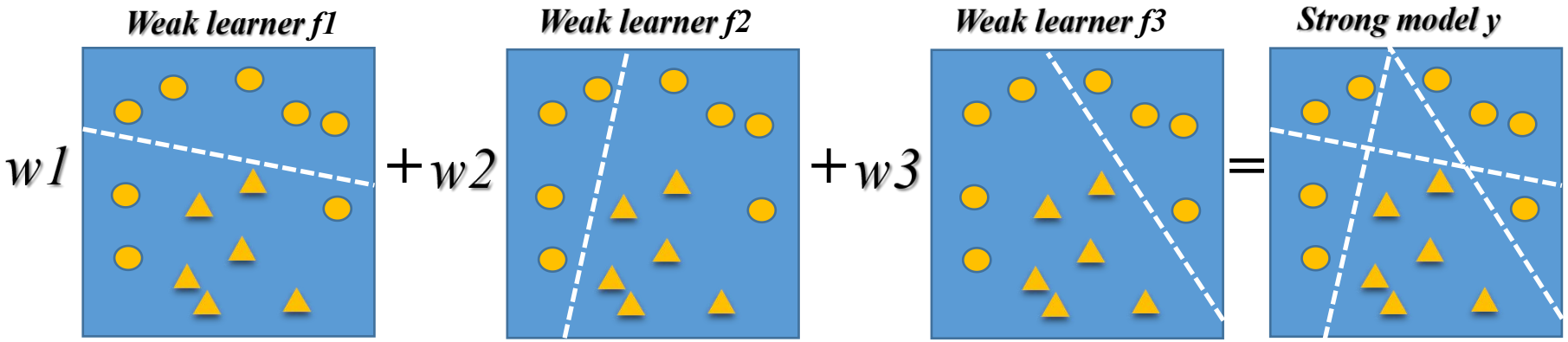
Contents

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

AdaBoost: How does it work?

- Learns a series of base classifiers from the data
- Combines base learners linearly
- Makes strong predictions based on combined learners



Algorithm: AdaBoost

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

1 **Initialize** the weight vector: w_1 (□)=$1/n$,□ =1,2,…,□ ;
2 **for** $t = 1, ..., T$ **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 α_t of $h_t(x)$

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

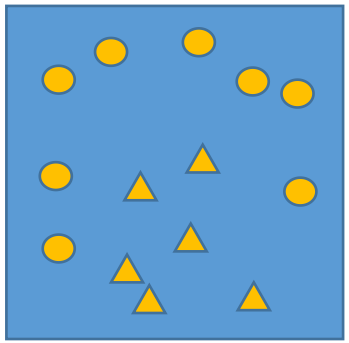
7 Update the weights of each data point

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

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

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

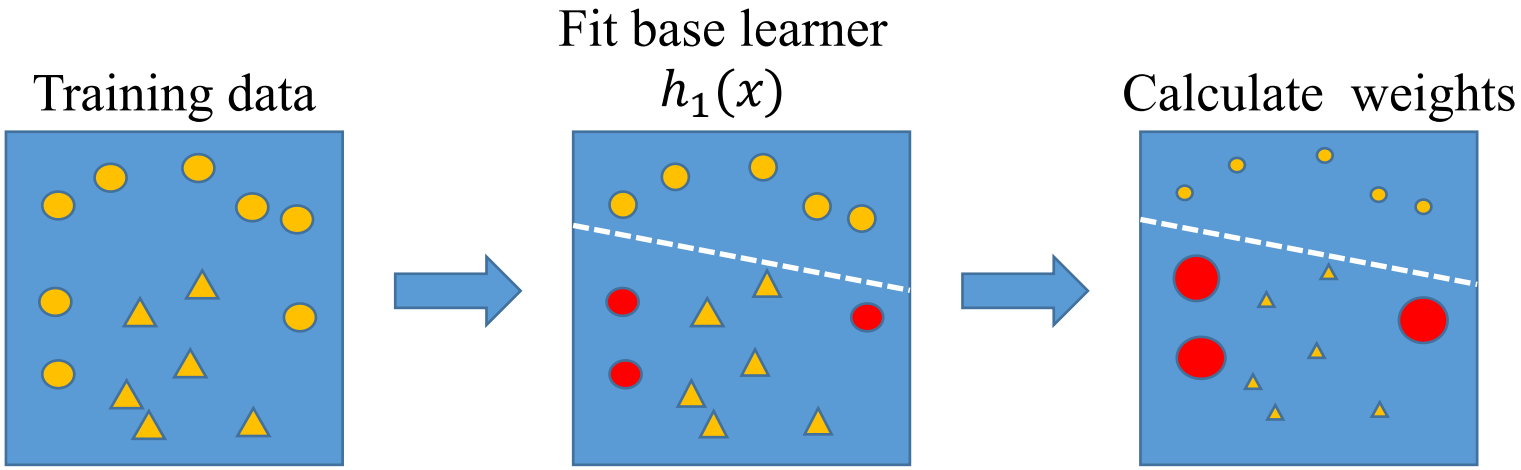
where n is the number of data points

AdaBoost: Iterations of Algorithm

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

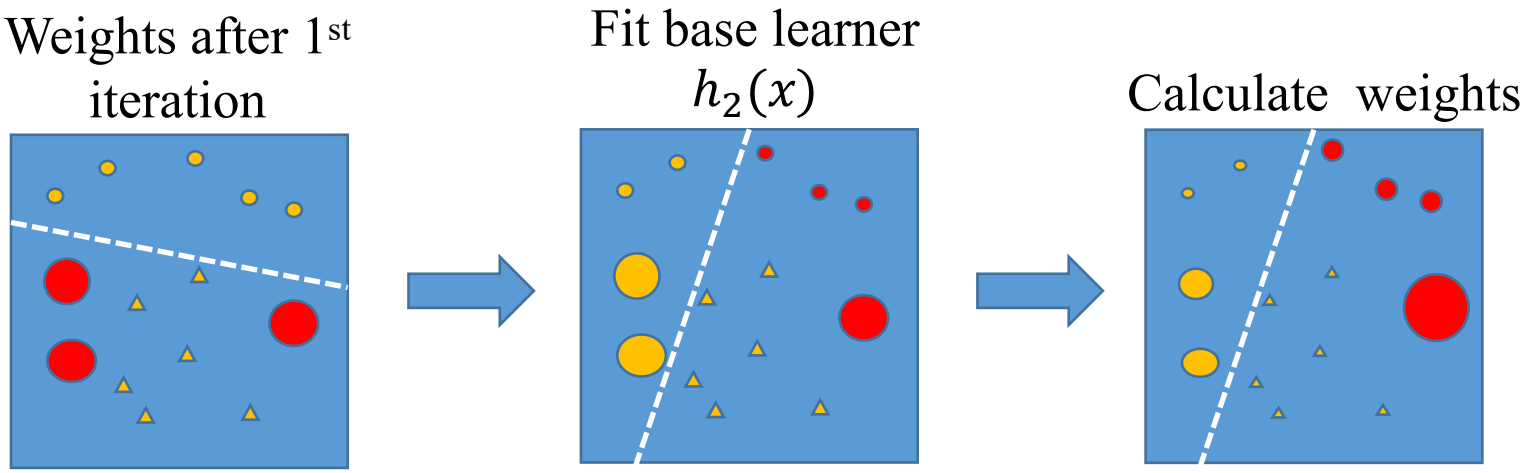
- Fit base learner $h_t(x)$ to data points
- Calculate the classification error rate e_t of $h_t(x)$
- Calculate the weight α_t of $h_t(x)$
- Update the weights of each data point

AdaBoost: Iteration 1



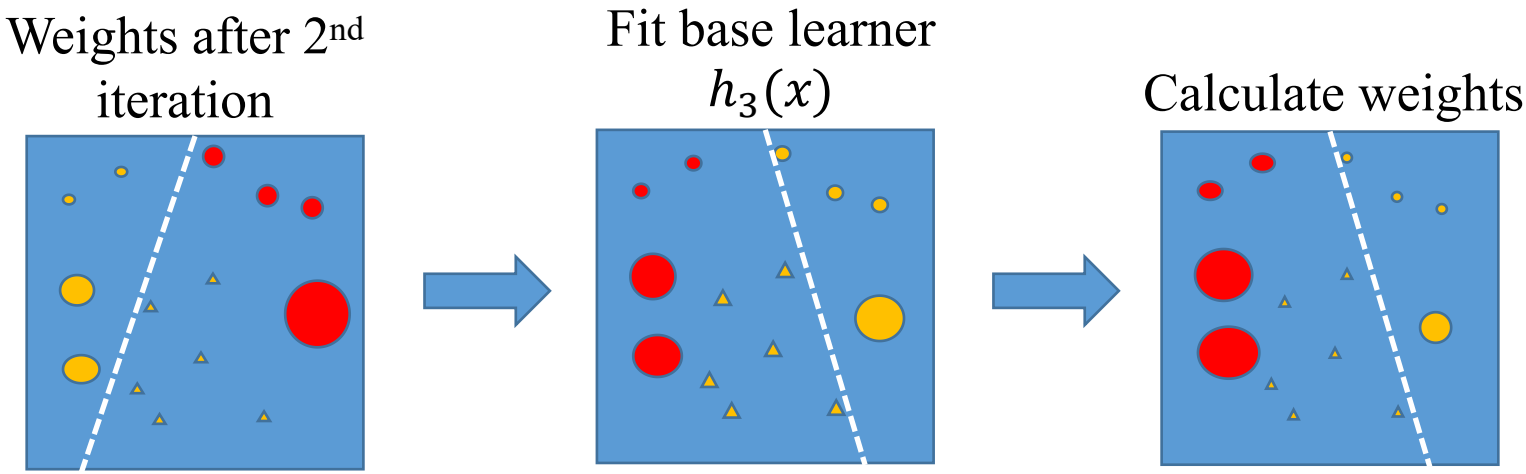
- Initially all data points have the same weight $1/n$
- The class correctly classified will be given less weights in the next iteration, and higher weights for misclassified class

AdaBoost: Iteration 2



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

AdaBoost: Iteration 3



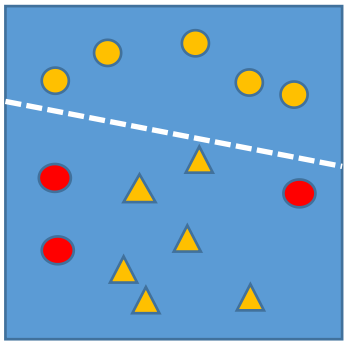
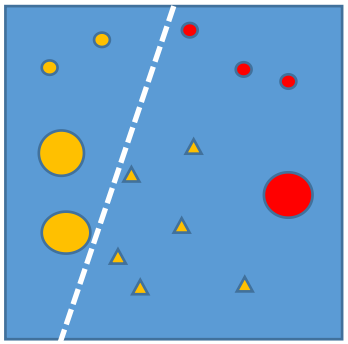
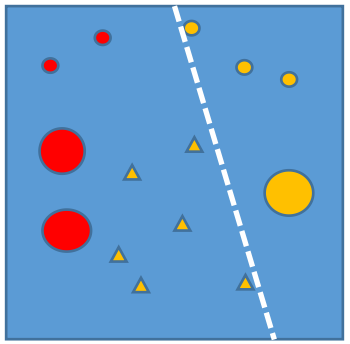
…continue iterating until either:

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

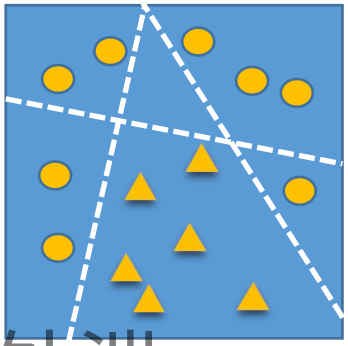
AdaBoost: Final Model

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

base learner $h_1(x)$ base learner $h_2(x)$ base learner $h_3(x)$

α_1  $+ \alpha_2$  $+ \alpha_3$ 

strong model $H(x)$

$=$ 

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

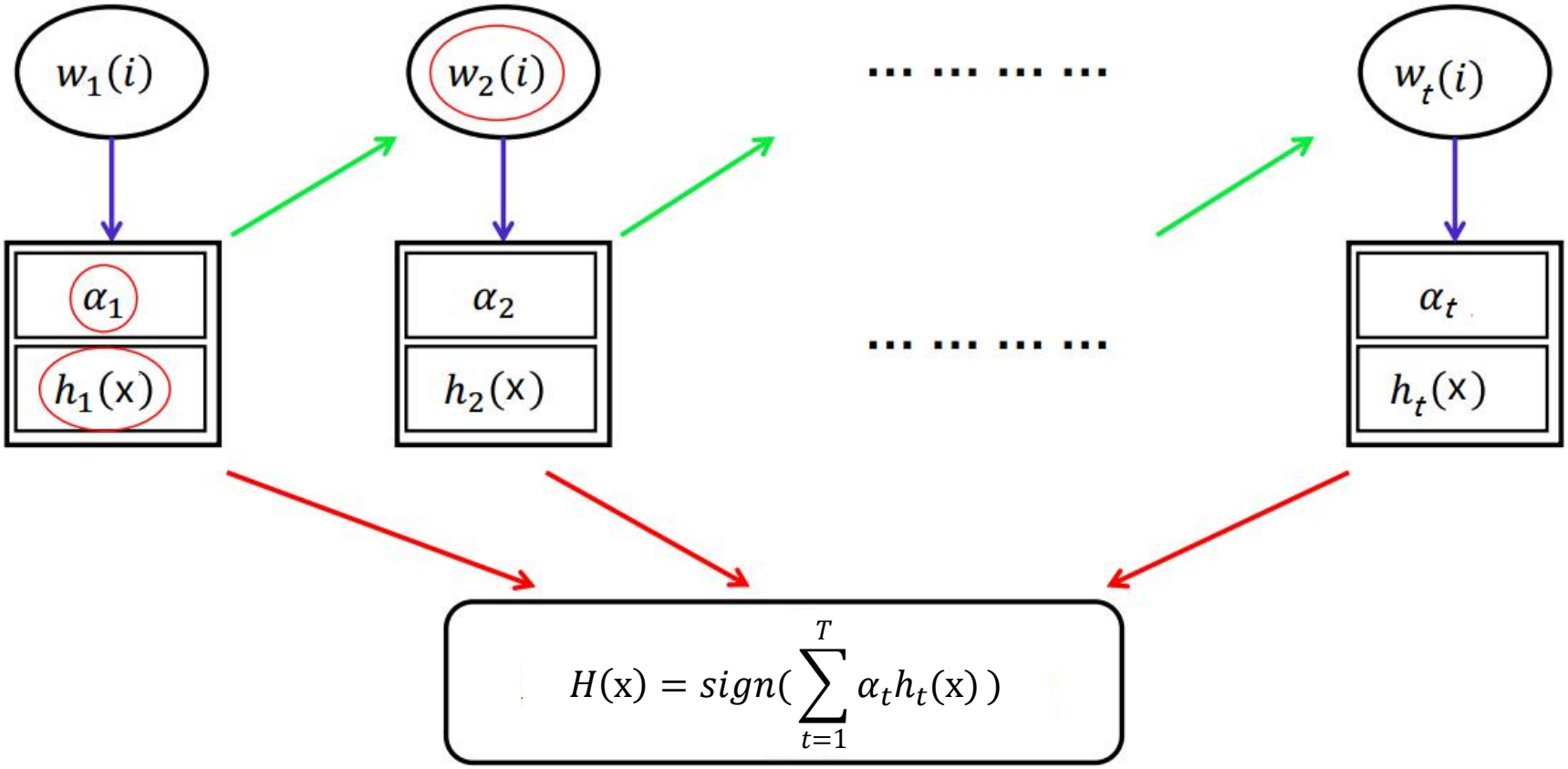
- Ensemble learner

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

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 $h_1(\mathrm{x})$, α_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

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

- $w_2(i),\ i = 1, ..., 10$ 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

Contents

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

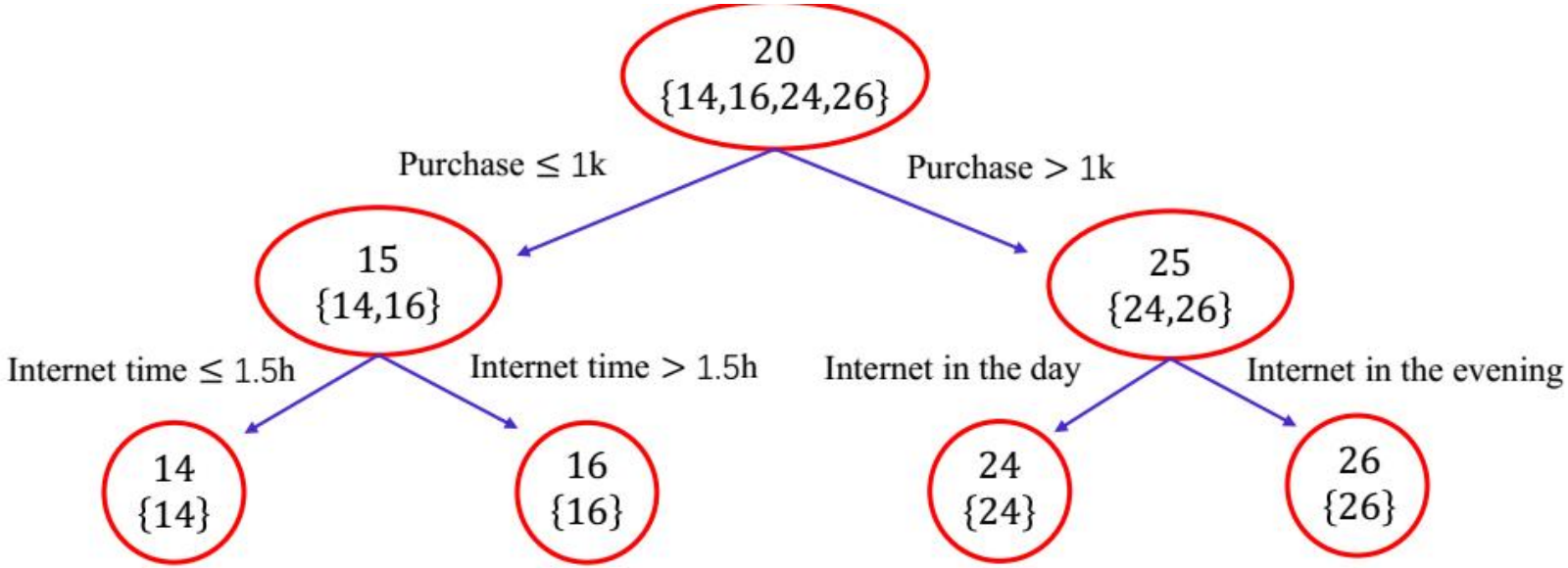
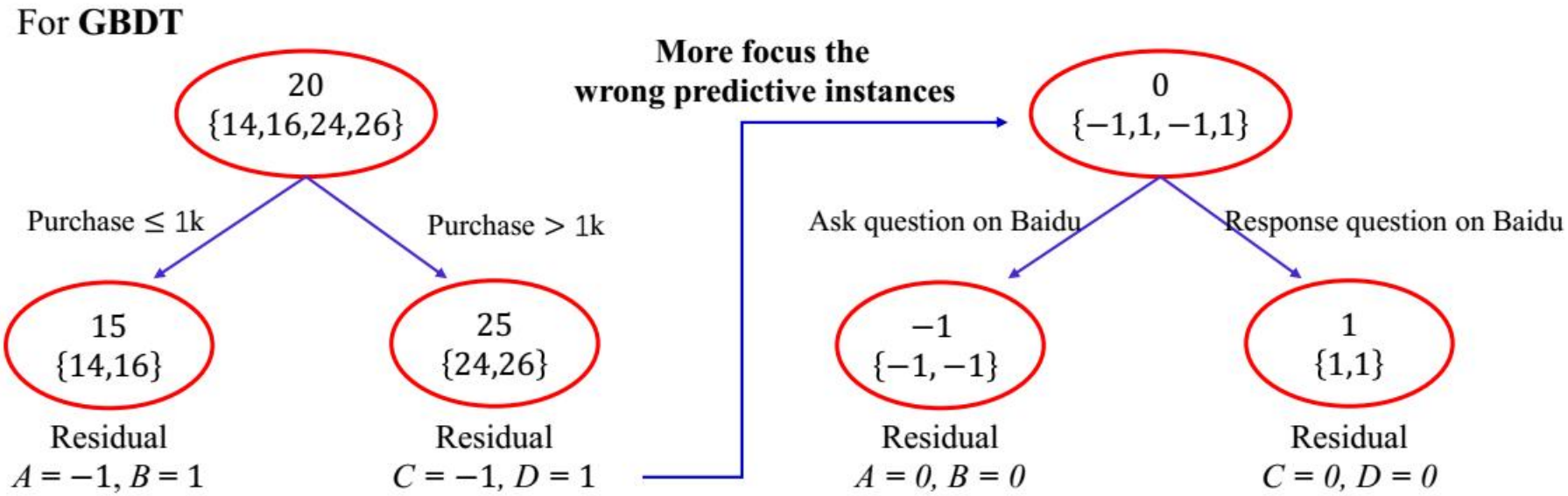


Figure: Single regression tree

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 $\lvert y_i - f(x_i)\rvert \le \delta_m$ $\delta_m \text{sign}[y_i - f(x_i)]$ 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: $D = \{(x_1, y_1), ..., (x_n, y_n)\}$, **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** $m = 1,2, ..., M$ **do**

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

3 $r_{im} = -\left[\frac{\partial L(y_i, f_{m-1}(x_i))}{\partial f_{m-1}(x_i)}\right]$

4 Fit a regression tree to targets r_{im} giving terminal regions

5 $R_{jm},\ j = 1,2, ..., J_m$

6 **end**

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

8 $\mu_{jm} = \text{argmin}_\mu \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \mu),\ j = 1,2, ..., J_m$

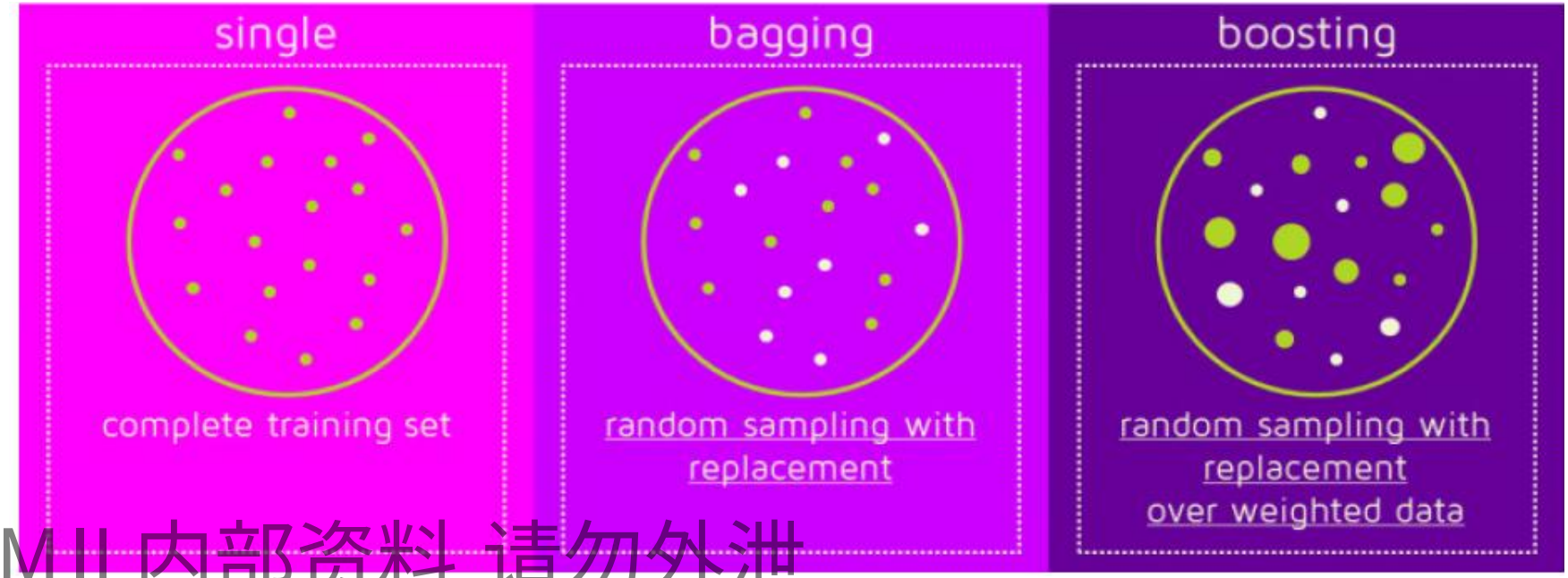
9 Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \mu j_m (x \in R_{jm})$

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)?



Thank You