2019 EE448, Big Data Mining, Lecture 6

Supervised Learning
(Part III)

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http://wnzhang.net/teaching/ee448/index.html

Content of Supervised Learning

- Introduction to Machine Learning
- Linear Models
- Support Vector Machines
- Neural Networks
- Tree Models
- Ensemble Methods

Content of This Lecture

- Tree Models
- Ensemble Methods

ML Task: Function Approximation

- Problem setting
  - Instance feature space $\mathcal{X}$
  - Instance label space $\mathcal{Y}$
  - Unknown underlying function (target) $f : \mathcal{X} \mapsto \mathcal{Y}$
  - Set of function hypothesis $H = \{h | h : \mathcal{X} \mapsto \mathcal{Y}\}$

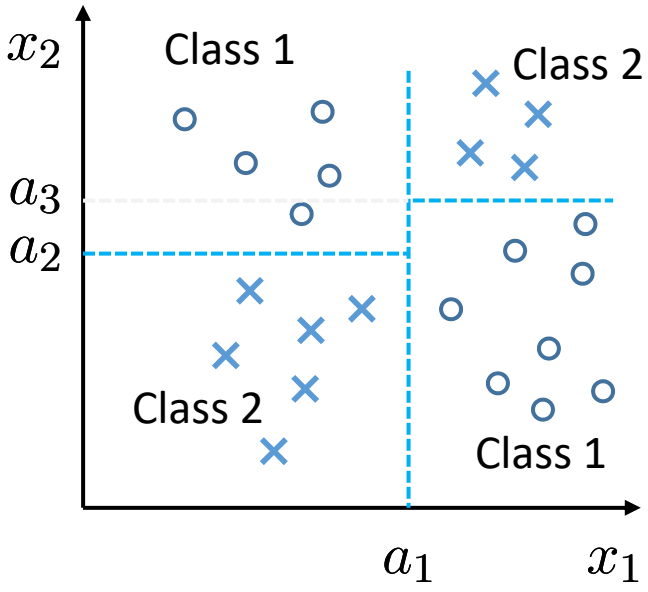
- Input: training data generated from the unknown

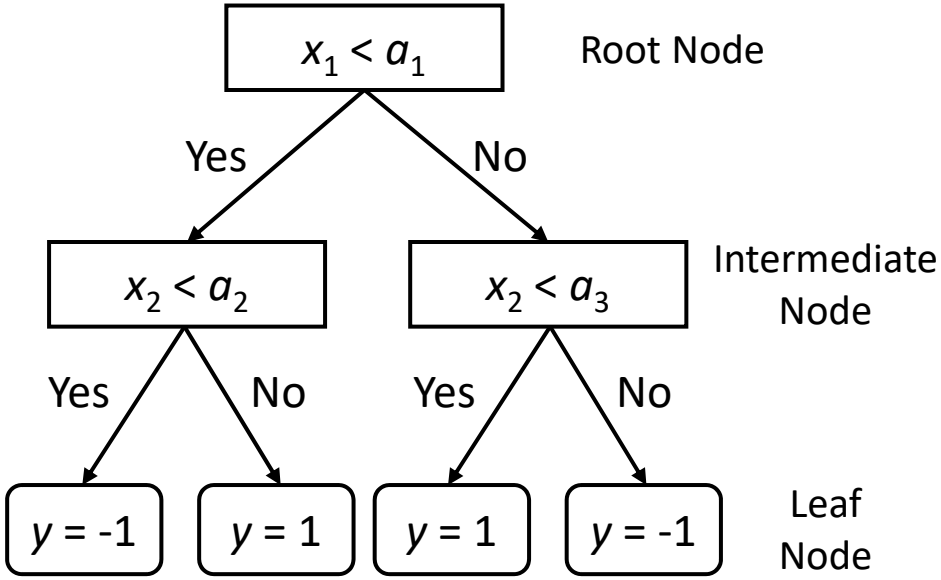
$$\{(x^{(i)}, y^{(i)})\} = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$$

- Output: a hypothesis $h \in H$ that best approximates f
- Optimize in functional space, not just parameter space

Optimize in Functional Space

- Tree models
  - Intermediate node for splitting data
  - Leaf node for label prediction
- Continuous data example

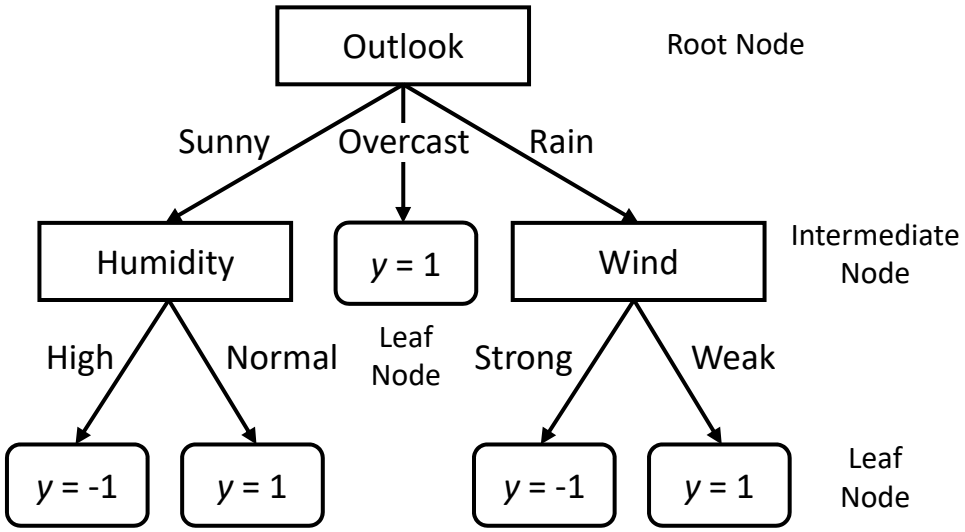




Optimize in Functional Space

- Tree models
  - Intermediate node for splitting data
  - Leaf node for label prediction
- Discrete/categorical data example

Predictors				Response
Outlook	**Temperature**	**Humidity**	**Wind**	**Class Play=Yes Play=No**
Sunny	Hot	High	Weak	No
Sunny	Hot	High	Strong	No
Overcast	Hot	High	Weak	Yes
Rain	Mild	High	Weak	Yes
Rain	Cool	Normal	Weak	Yes
Rain	Cool	Normal	Strong	No
Overcast	Cool	Normal	Strong	Yes
Sunny	Mild	High	Weak	No
Sunny	Cool	Normal	Weak	Yes
Rain	Mild	Normal	Weak	Yes
Sunny	Mild	Normal	Strong	Yes
Overcast	Mild	High	Strong	Yes
Overcast	Hot	Normal	Weak	Yes
Rain	Mild	High	Strong	No



Decision Tree Learning

- Problem setting
  - Instance feature space $\mathcal{X}$
  - Instance label space $\mathcal{Y}$
  - Unknown underlying function (target) $f : \mathcal{X} \mapsto \mathcal{Y}$
  - Set of function hypothesis $H = \{h | h : \mathcal{X} \mapsto \mathcal{Y}\}$

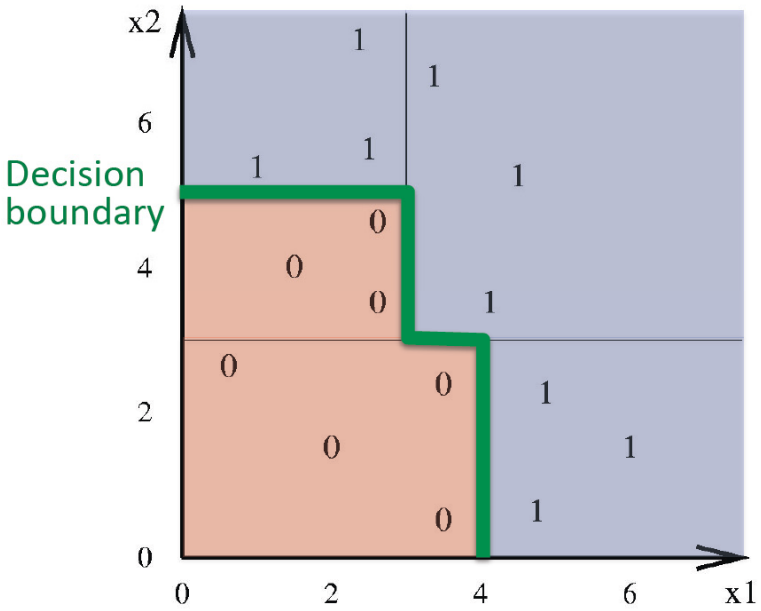
- Input: training data generated from the unknown

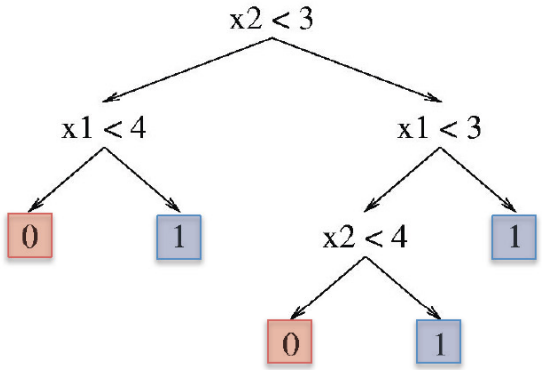
$$\{(x^{(i)}, y^{(i)})\} = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$$

- Output: a hypothesis $h \in H$ that best approximates f
- Here each hypothesis h is a decision tree

Decision Tree – Decision Boundary

- Decision trees divide the feature space into axis-parallel (hyper-)rectangles
- Each rectangular region is labeled with one label
  - or a probabilistic distribution over labels





Slide credit: Eric Eaton

History of Decision-Tree Research

- Hunt and colleagues used exhaustive search decision-tree methods (CLS) to model human concept learning in the 1960's.
- In the late 70's, Quinlan developed ID3 with the information gain heuristic to learn expert systems from examples.
- Simultaneously, Breiman and Friedman and colleagues developed CART (Classification and Regression Trees), similar to ID3.
- In the 1980's a variety of improvements were introduced to handle noise, continuous features, missing features, and improved splitting criteria. Various expert-system development tools results.
- Quinlan's updated decision-tree package (C4.5) released in 1993.
- Sklearn (python)Weka (Java) now include ID3 and C4.5

Slide credit: Raymond J. Mooney

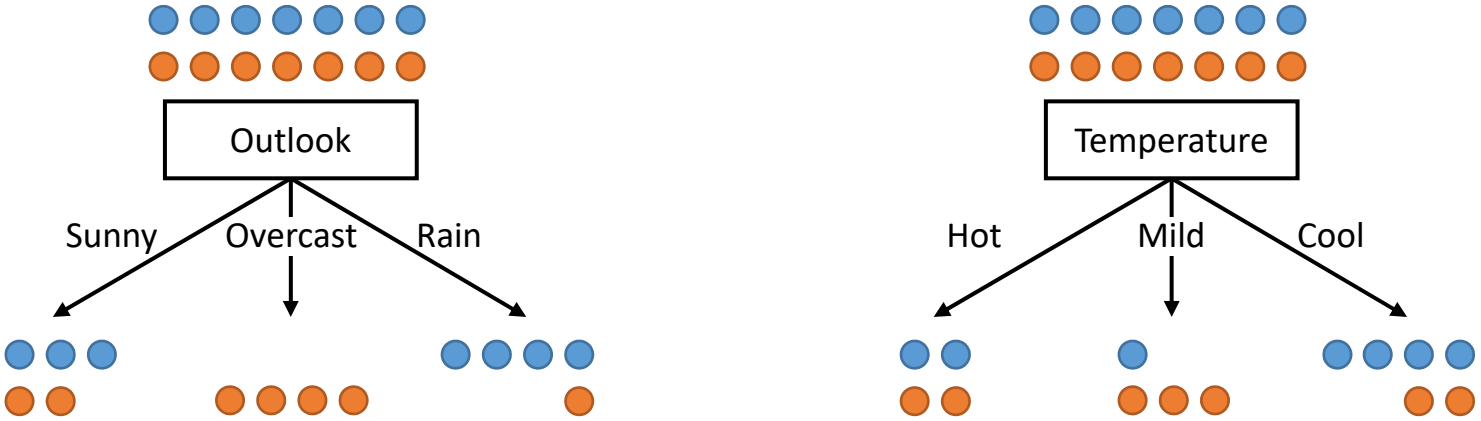
Decision Trees

- Tree models
  - Intermediate node for splitting data
  - Leaf node for label prediction

- Key questions for decision trees
  - How to select node splitting conditions?
  - How to make prediction?
  - How to decide the tree structure?

Node Splitting

- Which node splitting condition to choose?



- Choose the features with higher classification capacity
  - Quantitatively, with higher information gain

Fundamentals of Information Theory

- Entropy (more specifically, Shannon entropy) is the expected value (average) of the information contained in each message.
- Suppose *X* is a random variable with *n* discrete values

$$P(X = x_i) = p_i$$

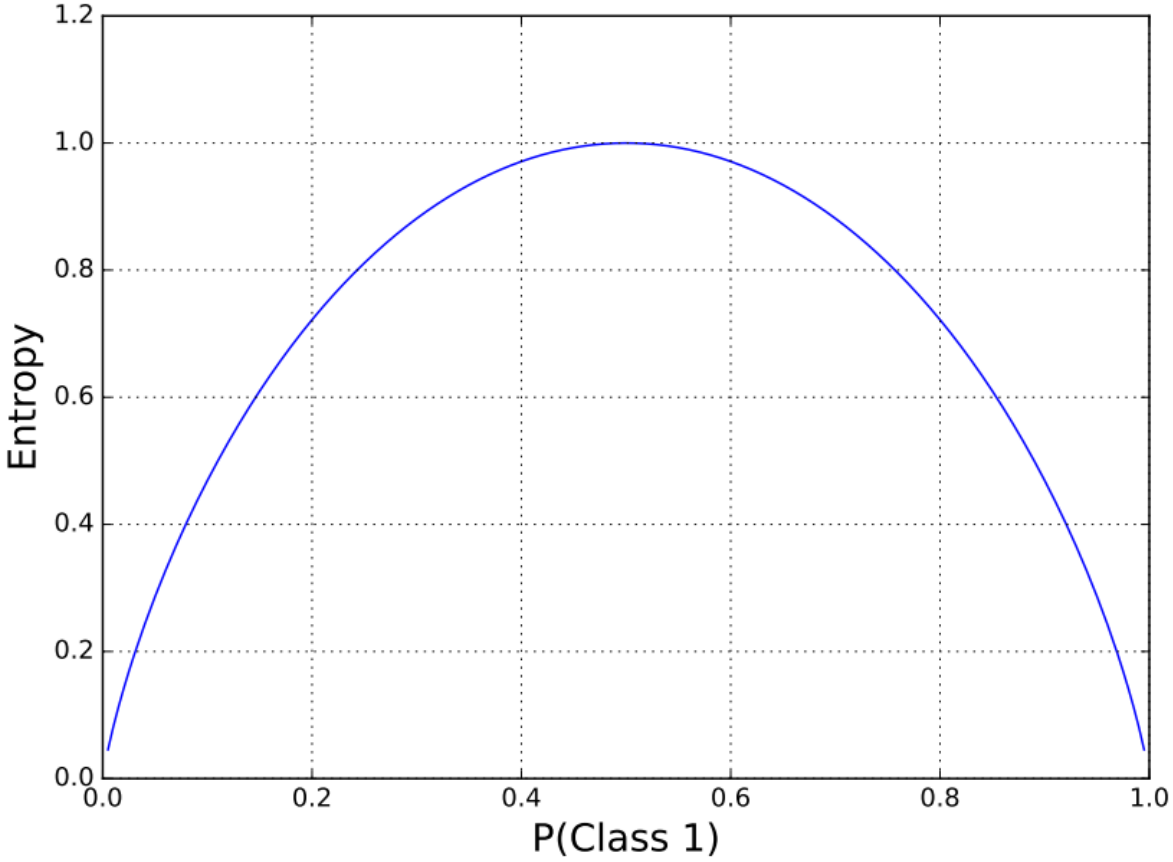
- then its entropy *H*(*X*) is

$$H(X) = -\sum_{i=1}^{n} p_i \log p_i$$

- It is easy to verify

$$H(X) = -\sum_{i=1}^{n} p_i \log p_i \leq -\sum_{i=1}^{n} \frac{1}{n} \log \frac{1}{n} = \log n$$

Illustration of Entropy



- Entropy of binary distribution

$$H(X) = -p_1 \log p_1 - (1 - p_1) \log(1 - p_1)$$

Cross Entropy

- Cross entropy is used to measure the difference between two random variable distributions

$$H(X,Y) = -\sum_{i=1}^{n} P(X=i)\log P(Y=i)$$

- Continuous formulation

$$H(p,q) = -\int p(x)\log q(x)dx$$

- Compared to KL divergence

$$D_{\mathrm{KL}}(p\|q) = \int p(x)\log\frac{p(x)}{q(x)}dx = H(p,q) - H(p)$$

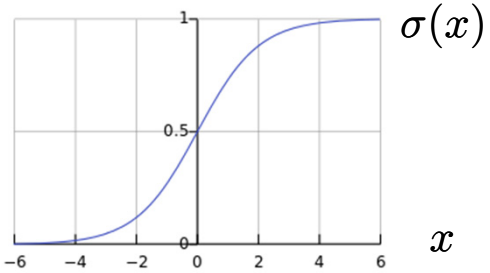
Review

Cross Entropy in Logistic Regression

- Logistic regression is a binary classification model

$$p_\theta(y=1|x) = \sigma(\theta^\top x) = \frac{1}{1+e^{-\theta^\top x}}$$

$$p_\theta(y=0|x) = \frac{e^{-\theta^\top x}}{1+e^{-\theta^\top x}}$$



- Cross entropy loss function

$$\mathcal{L}(y, x, p_\theta) = -y \log \sigma(\theta^\top x) - (1-y)\log(1-\sigma(\theta^\top x))$$

- Gradient

$$\frac{\partial \mathcal{L}(y, x, p_\theta)}{\partial \theta} = -y\frac{1}{\sigma(\theta^\top x)}\sigma(z)(1-\sigma(z))x - (1-y)\frac{-1}{1-\sigma(\theta^\top x)}\sigma(z)(1-\sigma(z))x$$

$$= (\sigma(\theta^\top x) - y)x$$

$$\theta \leftarrow \theta + (y - \sigma(\theta^\top x))x$$

$$\frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1-\sigma(z))$$

Conditional Entropy

- Entropy $H(X) = -\sum_{i=1}^{n} P(X=i) \log P(X=i)$
- Specific conditional entropy of *X* given *Y* = *v*

$$H(X|Y=v) = -\sum_{i=1}^{n} P(X=i|Y=v) \log P(X=i|Y=v)$$

- Specific conditional entropy of *X* given *Y*

$$H(X|Y) = \sum_{v \in \text{values}(Y)} P(Y=v) H(X|Y=v)$$

- Information Gain or Mutual Information of *X* given *Y*

$$\begin{aligned} I(X,Y) &= H(X) - H(X|Y) = H(Y) - H(Y|X) \\ &= H(X) + H(Y) - H(X,Y) \end{aligned}$$

Information Gain

- Information Gain or Mutual Information of *X* given *Y*

$$
\begin{aligned}
&I(X,Y) = H(X) - H(X|Y) \\
&= -\sum_v P(X=v)\log P(X=v) + \sum_u P(Y=u)\sum_v P(X=v|Y=u)\log P(X=v|Y=u) \\
&= -\sum_v P(X=v)\log P(X=v) + \sum_u \sum_v P(X=v,Y=u)\log P(X=v|Y=u) \\
&= -\sum_v P(X=v)\log P(X=v) + \sum_u \sum_v P(X=v,Y=u)[\log P(X=v,Y=u) - \log P(Y=u)] \\
&= -\sum_v P(X=v)\log P(X=v) - \sum_v P(Y=v)\log P(Y=v) + \sum_{u,v} P(X=v,Y=u)\log P(X=v,Y=u) \\
&= H(X) + H(Y) - H(X,Y)
\end{aligned}
$$

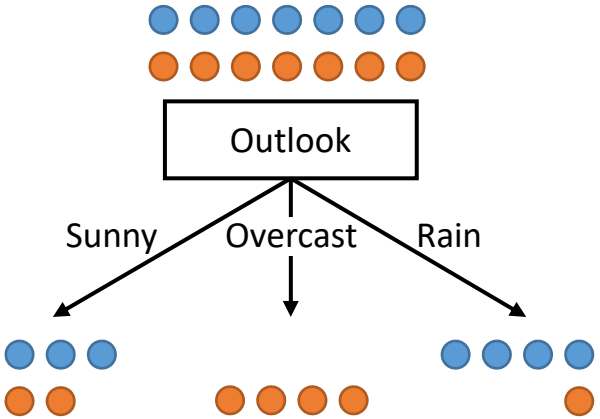
Entropy of (*X*,*Y*) instead of cross entropy

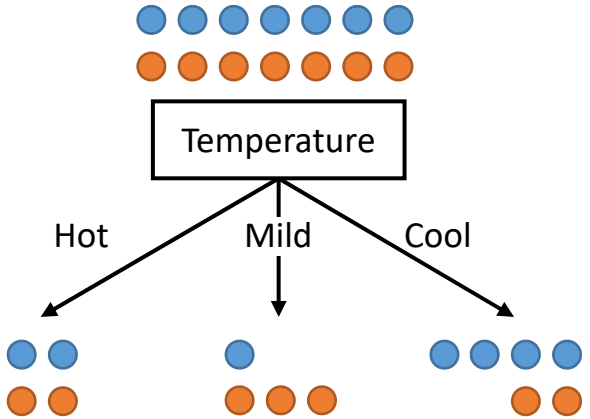
Node Splitting

- Information gain

$$H(X|Y=v) = -\sum_{i=1}^{n} P(X=i|Y=v)\log P(X=i|Y=v)$$

$$H(X|Y) = \sum_{v\in \text{values}(Y)} P(Y=v)H(X|Y=v)$$





$$H(X|Y=S) = -\frac{3}{5}\log\frac{3}{5} - \frac{2}{5}\log\frac{2}{5} = 0.9710$$

$$H(X|Y=O) = -\frac{4}{4}\log\frac{4}{4} = 0$$

$$H(X|Y=R) = -\frac{4}{5}\log\frac{4}{5} - \frac{1}{5}\log\frac{1}{5} = 0.7219$$

$$H(X|Y) = \frac{5}{14}\times 0.9710 + \frac{4}{14}\times 0 + \frac{5}{14}\times 0.7219 = 0.6046$$

$$I(X,Y) = H(X) - H(X|Y) = 1 - 0.6046 = 0.3954$$

$$H(X|Y=H) = -\frac{2}{4}\log\frac{2}{4} - \frac{2}{4}\log\frac{2}{4} = 1$$

$$H(X|Y=M) = -\frac{1}{4}\log\frac{1}{4} - \frac{3}{4}\log\frac{3}{4} = 0.8113$$

$$H(X|Y=C) = -\frac{4}{6}\log\frac{4}{6} - \frac{2}{6}\log\frac{2}{6} = 0.9183$$

$$H(X|Y) = \frac{4}{14}\times 1 + \frac{4}{14}\times 0.8113 + \frac{5}{14}\times 0.9183 = 0.9111$$

$$I(X,Y) = H(X) - H(X|Y) = 1 - 0.9111 = 0.0889$$

Information Gain Ratio

- The ratio between information gain and the entropy

$$I_R(X,Y) = \frac{I(X,Y)}{H_Y(X)} = \frac{H(X) - H(X|Y)}{H_Y(X)}$$

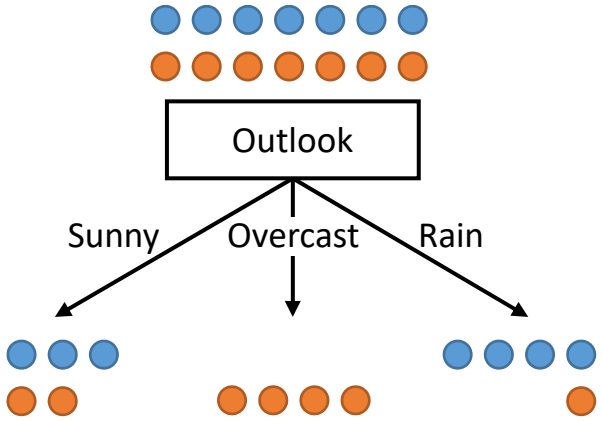
- where the entropy (of *Y*) is

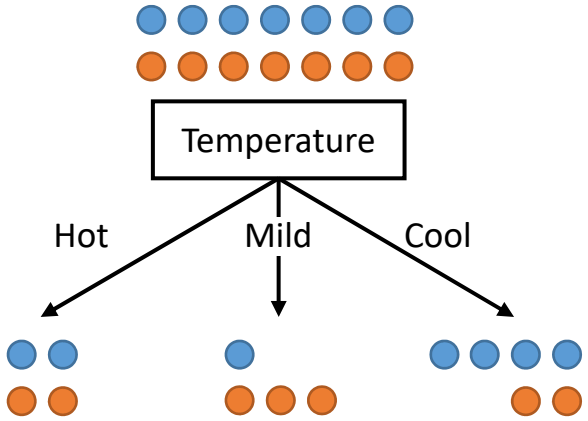
$$H_Y(X) = -\sum_{v \in \text{values}(Y)} \frac{|X_{y=v}|}{|X|} \log \frac{|X_{y=v}|}{|X|}$$

- where $|X_{y=v}|$ is the number of observations with the feature *y=v*

Node Splitting

- Information gain ratio $I_R(X,Y) = \frac{I(X,Y)}{H_Y(X)} = \frac{H(X) - H(X|Y)}{H_Y(X)}$





$$I(X,Y) = H(X) - H(X|Y) = 1 - 0.6046 = 0.3954$$

$$H_Y(X) = -\frac{4}{14}\log\frac{4}{14} - \frac{5}{14}\log\frac{5}{14} - \frac{5}{14}\log\frac{5}{14} = 1.5774$$

$$I_R(X,Y) = \frac{0.3954}{1.5774} = 0.2507$$

$$I(X,Y) = H(X) - H(X|Y) = 1 - 0.9111 = 0.0889$$

$$H_Y(X) = -\frac{4}{14}\log\frac{4}{14} - \frac{4}{14}\log\frac{4}{14} - \frac{6}{14}\log\frac{6}{14} = 1.5567$$

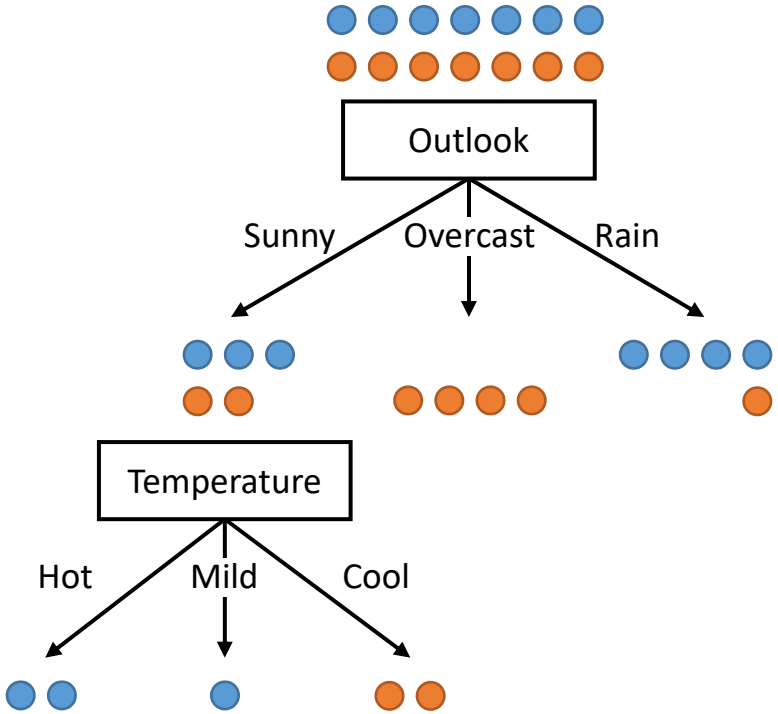
$$I_R(X,Y) = \frac{0.0889}{1.5567} = 0.0571$$

Decision Tree Building: ID3 Algorithm

- Algorithm framework
  - Start from the root node with all data
  - For each node, calculate the information gain of all possible features
  - Choose the feature with the highest information gain
  - Split the data of the node according to the feature
  - Do the above recursively for each leaf node, until
    - There is no information gain for the leaf node
    - Or there is no feature to select

Decision Tree Building: ID3 Algorithm

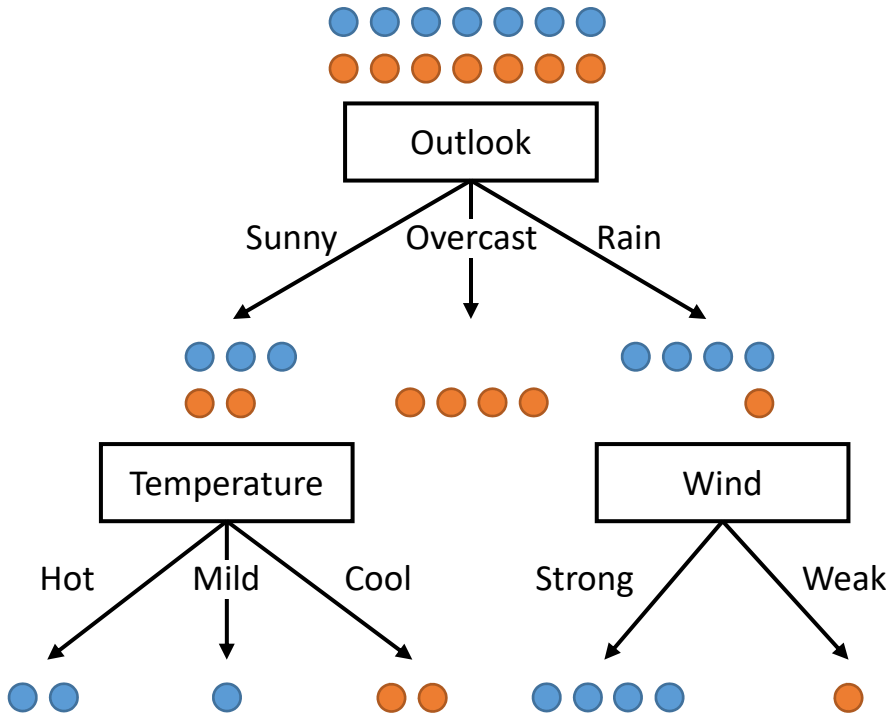
- An example decision tree from ID3



- Each path only involves a feature at most once

Decision Tree Building: ID3 Algorithm

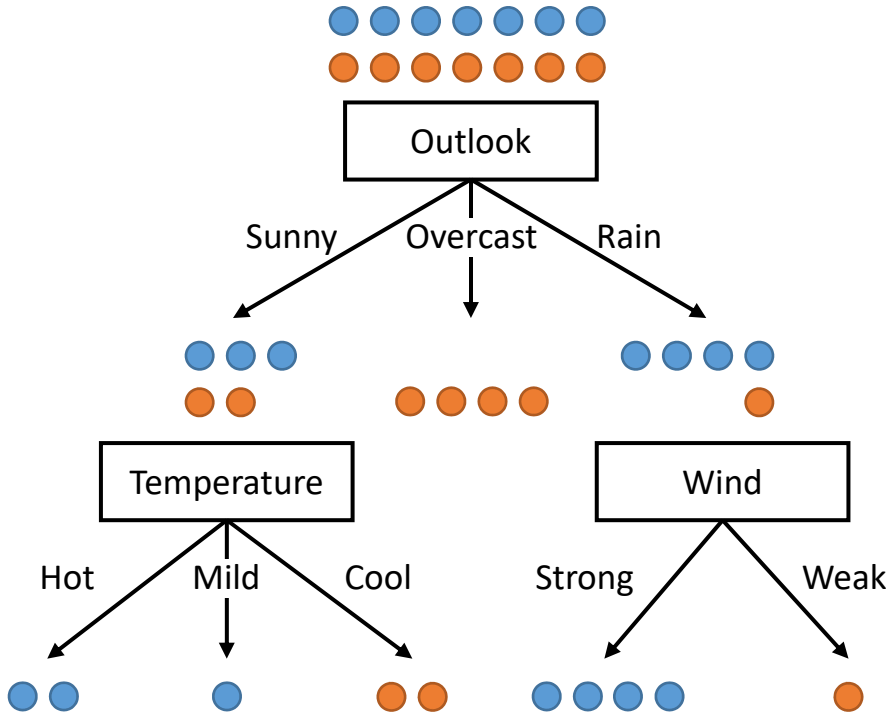
- An example decision tree from ID3



- How about this tree, yielding perfect partition?

Overfitting

- Tree model can approximate any finite data by just growing a leaf node for each instance



Decision Tree Training Objective

- Cost function of a tree *T* over training data

$$C(T) = \sum_{t=1}^{|T|} N_t H_t(T)$$

where for the leaf node *t*

- $H_t(T)$ is the empirical entropy
- N_t is the instance number, N_{tk} is the instance number of class *k*

$$H_t(T) = -\sum_k \frac{N_{tk}}{N_t} \log \frac{N_{tk}}{N_t}$$

- Training objective: find a tree to minimize the cost

$$\min_T C(T) = \sum_{t=1}^{|T|} N_t H_t(T)$$

Decision Tree Regularization

- Cost function over training data

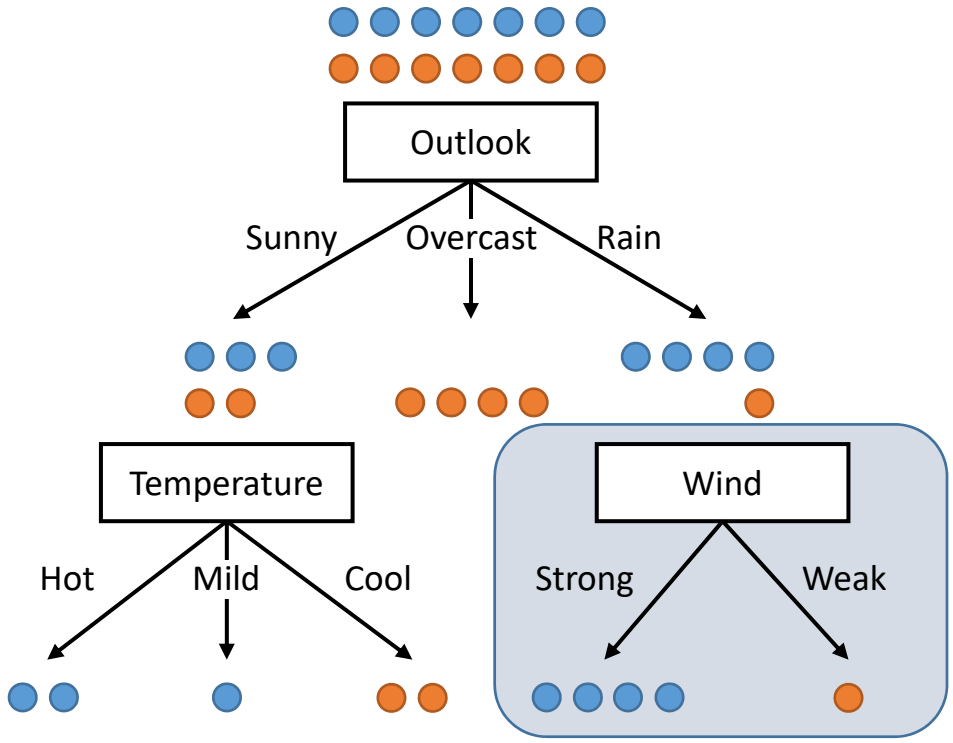
$$C(T) = \sum_{t=1}^{|T|} N_t H_t(T) + \lambda |T|$$

where

- $|T|$ is the number of leaf nodes of the tree T
- λ is the hyperparameter of regularization

Decision Tree Building: ID3 Algorithm

- An example decision tree from ID3



Whether to split this node?

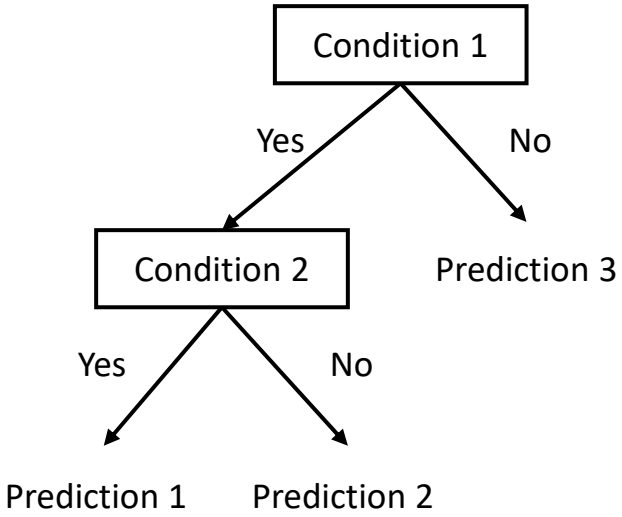
- Calculate the cost function difference. $C(T) = \sum_{t=1}^{|T|} N_t H_t(T) + \lambda |T|$

Summary of ID3

- A classic and straightforward algorithm of training decision trees
  - Work on discrete/categorical data
  - One branch for each value/category of the feature
- Algorithm C4.5 is similar and more advanced to ID3
  - Splitting the node according to information gain ratio
- Splitting branch number depends on the number of different categorical values of the feature
  - Might lead to very broad tree

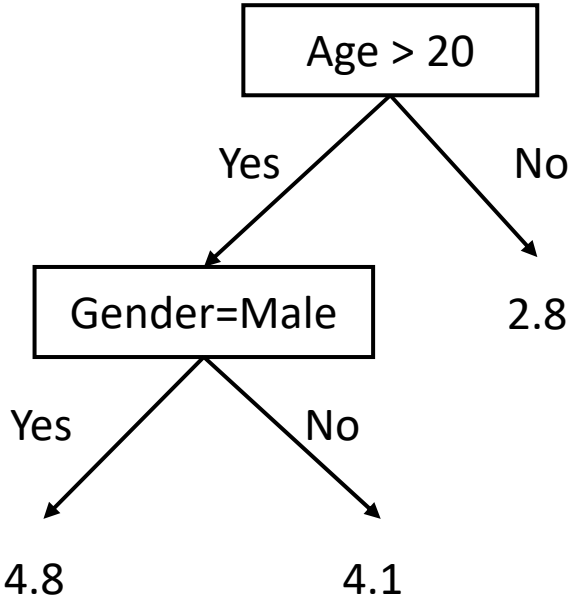
CART Algorithm

- Classification and Regression Tree (CART)
  - Proposed by Leo Breiman et al. in 1984
  - Binary splitting (yes or no for the splitting condition)
  - Can work on continuous/numeric features
  - Can repeatedly use the same feature (with different splitting)



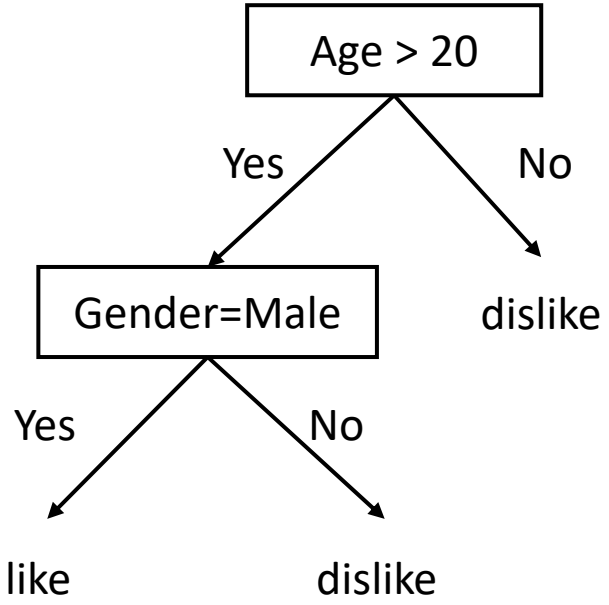
CART Algorithm

- Regression Tree
  - Output the predicted value



For example: predict the user's rating to a movie

- Classification Tree
  - Output the predicted class



For example: predict whether the user like a move

Regression Tree

- Let the training dataset with continuous targets *y*

$$D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$$

- Suppose a regression tree has divided the space into *M* regions R_1, R_2, …, R_M, with c_m as the prediction for region R_m

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m)$$

- Loss function for (x_i, y_i)

$$\frac{1}{2}(y_i - f(x_i))^2$$

- It is easy to see the optimal prediction for region *m* is

$$\hat{c}_m = \text{avg}(y_i | x_i \in R_m)$$

Regression Tree

- How to find the optimal splitting regions?
- How to find the optimal splitting conditions?
  - Defined by a threshold value *s* on variable *j*
  - Lead to two regions

$$R_1(j,s) = \{x | x^{(j)} \leq s\} \qquad R_2(j,s) = \{x | x^{(j)} > s\}$$

- Training based on current splitting

$$\min_{j,s} \left[\min_{c_1} \sum_{x \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x \in R_2(j,s)} (y_i - c_2)^2 \right]$$

$$\hat{c}_m = \text{avg}(y_i | x_i \in R_m)$$

Regression Tree Algorithm

- INPUT: training data *D*
- OUTPUT: regression tree *f(x)*
- Repeat until stop condition satisfied:
  - Find the optimal splitting (*j*,*s*)

$$\min_{j,s}\left[\min_{c_1}\sum_{x\in R_1(j,s)}(y_i-c_1)^2+\min_{c_2}\sum_{x\in R_2(j,s)}(y_i-c_2)^2\right]$$

  - Calculate the prediction value of the new region R_1, R_2

$$\hat{c}_m=\text{avg}(y_i|x_i\in R_m)$$

- Return the regression tree

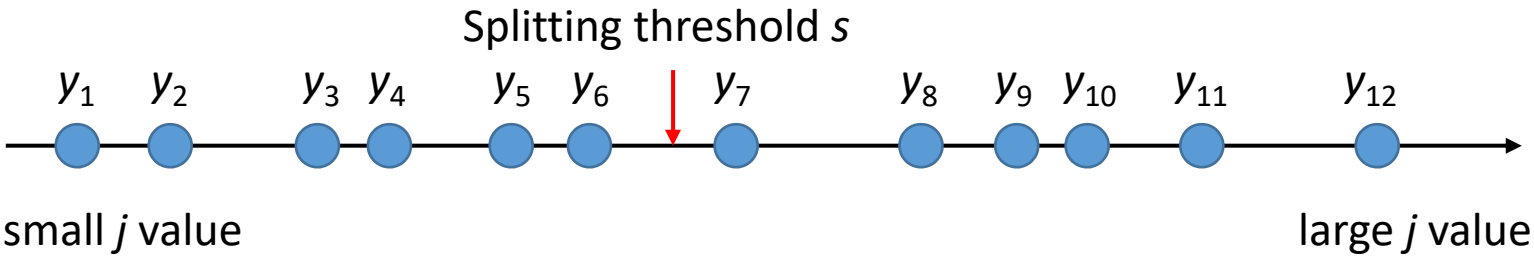
$$f(x)=\sum_{m=1}^{M}\hat{c}_m I(x\in R_m)$$

Regression Tree Algorithm

- How to efficiently find the optimal splitting (*j*,*s*)?

$$\min_{j,s}\left[\min_{c_1}\sum_{x\in R_1(j,s)}(y_i-c_1)^2+\min_{c_2}\sum_{x\in R_2(j,s)}(y_i-c_2)^2\right]$$

- Sort the data ascendingly according to feature *j* value



$$\text{loss}=\sum_{i=1}^{6}(y_i-c_1)^2+\sum_{i=7}^{12}(y_i-c_2)^2$$

Online updated

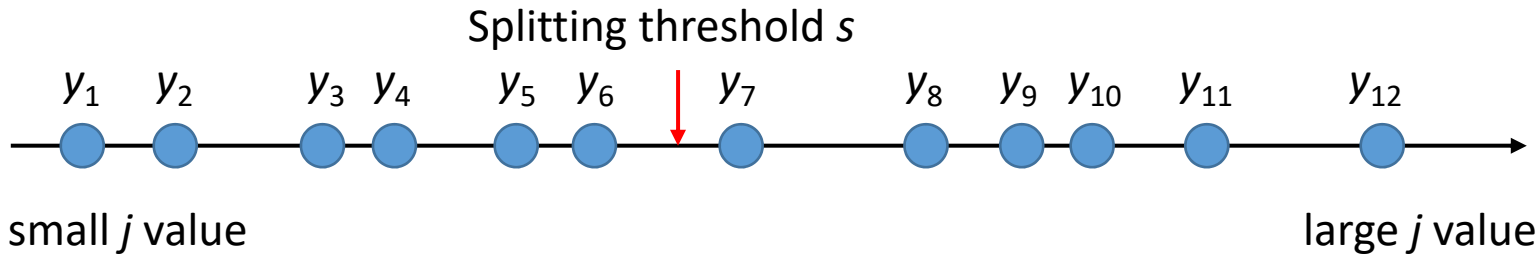
$$=\sum_{i=1}^{6}y_i^2-\frac{1}{6}\Big(\sum_{i=1}^{6}y_i\Big)^2+\sum_{i=7}^{12}y_i^2-\frac{1}{6}\Big(\sum_{i=7}^{12}y_i\Big)^2=-\frac{1}{6}\Big(\sum_{i=1}^{6}y_i\Big)^2-\frac{1}{6}\Big(\sum_{i=7}^{12}y_i\Big)^2+C$$

Regression Tree Algorithm

- How to efficiently find the optimal splitting (*j*,*s*)?

$$\min_{j,s}\left[\min_{c_1}\sum_{x\in R_1(j,s)}(y_i-c_1)^2+\min_{c_2}\sum_{x\in R_2(j,s)}(y_i-c_2)^2\right]$$

- Sort the data ascendingly according to feature *j* value



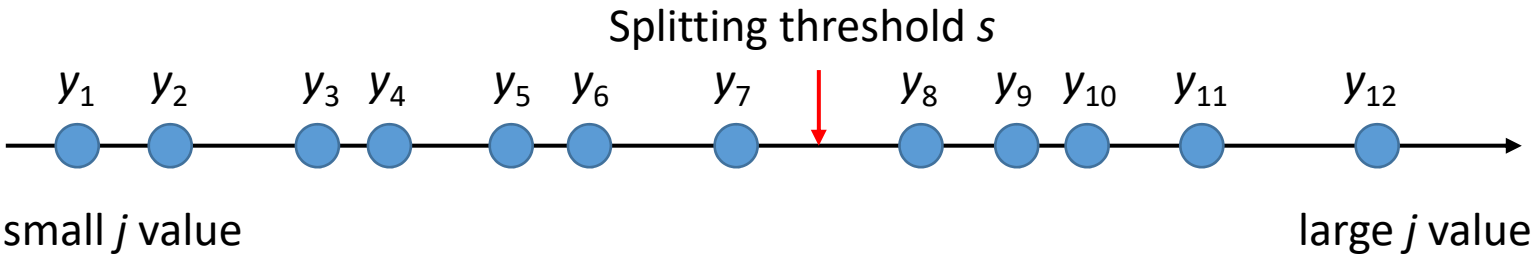
$$\text{loss}_{6,7}=-\frac{1}{6}\Big(\sum_{i=1}^{6}y_i\Big)^2-\frac{1}{6}\Big(\sum_{i=7}^{12}y_i\Big)^2+C$$

Regression Tree Algorithm

- How to efficiently find the optimal splitting (*j*,*s*)?

$$\min_{j,s}\left[\min_{c_1}\sum_{x\in R_1(j,s)}(y_i-c_1)^2+\min_{c_2}\sum_{x\in R_2(j,s)}(y_i-c_2)^2\right]$$

- Sort the data ascendingly according to feature *j* value



$$\text{loss}_{6,7}=-\frac{1}{6}\Big(\sum_{i=1}^{6}y_i\Big)^2-\frac{1}{6}\Big(\sum_{i=7}^{12}y_i\Big)^2+C$$

$$\text{loss}_{7,8}=-\frac{1}{7}\Big(\sum_{i=1}^{7}y_i\Big)^2-\frac{1}{5}\Big(\sum_{i=8}^{12}y_i\Big)^2+C$$

- Maintain and online update in *O*(1) Time

$$\text{Sum}(R_1)=\sum_{i=1}^{k}y_i \qquad \text{Sum}(R_2)=\sum_{i=k+1}^{n}y_i$$

- *O*(n) in total for checking one feature

Classification Tree

- The training dataset with categorical targets *y*

$$D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$$

- Suppose a regression tree has divided the space into *M* regions R_1, R_2, …, R_M, with c_m as the prediction for region R_m

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m)$$

- Here the leaf node prediction c_m is the category distribution

$$\hat{c}_m = \{P(y_k | x_i \in R_m)\}_{k=1\ldots K}$$

- c_m is solved by counting categories

$$P(y_k | x_i \in R_m) = \frac{C_m^k}{C_m}$$

instances in leaf *m* with cat *k*

instances in leaf *m*

Classification Tree

- How to find the optimal splitting regions?
- How to find the optimal splitting conditions?
  - For continuous feature *j*, defined by a threshold value *s*
    - Yield two regions

$$R_1(j,s) = \{x | x^{(j)} \leq s\} \qquad R_2(j,s) = \{x | x^{(j)} > s\}$$

  - For categorical feature *j*, select a category *a*
    - Yield two regions

$$R_1(j,s) = \{x | x^{(j)} = a\} \qquad R_2(j,s) = \{x | x^{(j)} \neq a\}$$

  - How to select? Argmin Gini impurity.

Gini Impurity

- In classification problem
  - suppose there are *K* classes
  - let p_k be the probability of an instance with the class *k*
  - the Gini impurity index is

$$\text{Gini}(p) = \sum_{k=1}^{K} p_k(1 - p_k) = 1 - \sum_{k=1}^{K} p_k^2$$

- Given the training dataset *D*, the Gini impurity is

$$\text{Gini}(D) = 1 - \sum_{k=1}^{K} \left(\frac{|D^k|}{|D|} \right)^2$$

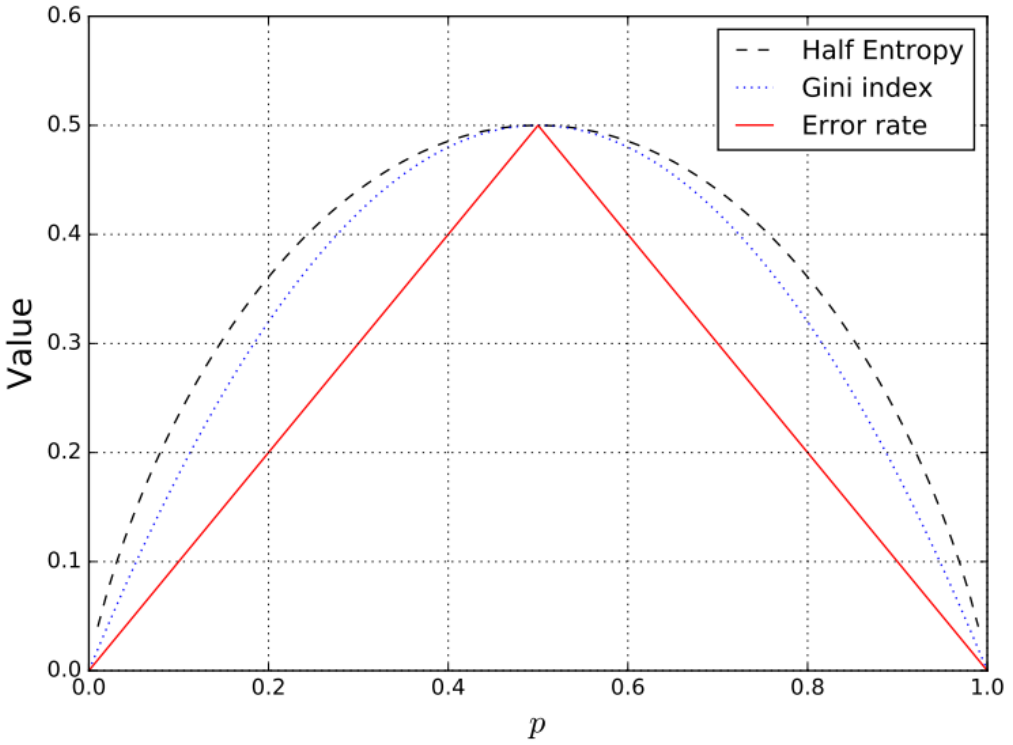
$|D^k|$: # instances in *D* with cat *k*

$|D|$: # instances in *D*

Gini Impurity

- For binary classification problem
  - let *p* be the probability of an instance with the class 1
  - Gini impurity is $\mathrm{Gini}(p) = 2p(1-p)$
  - Entropy is $H(p) = -p\log p - (1-p)\log(1-p)$

Gini impurity and entropy are quite similar in representing classification error rate.



Gini Impurity

- With a categorical feature *j* and one of its categories *a*
  - The two split regions R_1, R_2

$$R_1(j,a) = \{x | x^{(j)} = a\} \qquad R_2(j,a) = \{x | x^{(j)} \neq a\}$$

$$D_j^1 = \{(x,y) | x^{(j)} = a\} \qquad D_j^2 = \{(x,y) | x^{(j)} \neq a\}$$

  - The Gini impurity of feature *j* with the selected category *a*

$$\text{Gini}(D_j, j = a) = \frac{|D_j^1|}{|D_j|}\text{Gini}(D_j^1) + \frac{|D_j^2|}{|D_j|}\text{Gini}(D_j^2)$$

Classification Tree Algorithm

- INPUT: training data *D*
- OUTPUT: classification tree *f(x)*
- Repeat until stop condition satisfied:
  - Find the optimal splitting (*j*,a)

$$\min_{j,a} \text{Gini}(D_j, j = a)$$

  - Calculate the prediction distribution of the new region R_1, R_2

$$\hat{c}_m = \{P(y_k | x_i \in R_m)\}_{k=1...K}$$

- Return the classification tree

$$f(x) = \sum_{m=1}^{M} \hat{c}_m I(x \in R_m)$$

1. Node instance number is small
2. Gini impurity is small
3. No more feature

Classification Tree Output

- Class label output
  - Output the class with the highest conditional probability

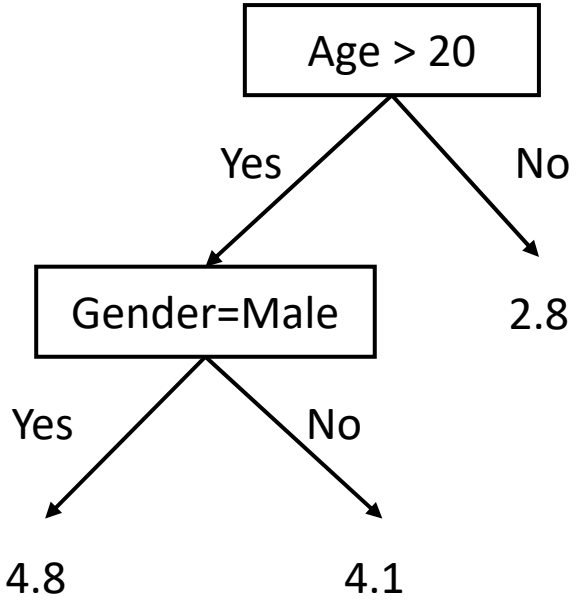
$$f(x) = \arg\max_{y_k} \sum_{m=1}^{M} I(x \in R_m) P(y_k | x_i \in R_m)$$

- Probabilistic distribution output

$$f(x) = \sum_{m=1}^{M} \hat{c}_m I(x \in R_m)$$

$$\hat{c}_m = \{P(y_k | x_i \in R_m)\}_{k=1 \ldots K}$$

Converting a Tree to Rules



For example: predict the user's rating to a movie

```
IF Age > 20:
  IF Gender = Male:
    return 4.8
  ELSE:
    return 4.1
ELSE:
  return 2.8
```

Decision tree model is easy to be visualized, explained and debugged.

Learning Model Comparison

Characteristic	Neural Nets	SVM	Trees	MARS	k-NN, Kernels
Natural handling of data of "mixed" type	▼	▼	▲	▲	▼
Handling of missing values	▼	▼	▲	▲	▲
Robustness to outliers in input space	▼	▼	▲	▼	▲
Insensitive to monotone transformations of inputs	▼	▼	▲	▼	▼
Computational scalability (large N)	▼	▼	▲	▲	▼
Ability to deal with irrelevant inputs	▼	▼	▲	▲	▼
Ability to extract linear combinations of features	▲	▲	▼	▼	◆
Interpretability	▼	▼	◆	▲	▼
Predictive power	▲	▲	▼	◆	▲

[Table 10.3 from Hastie et al. Elements of Statistical Learning, 2nd Edition]

Content of This Lecture

- Tree Models
- Ensemble Methods

Ensemble Learning

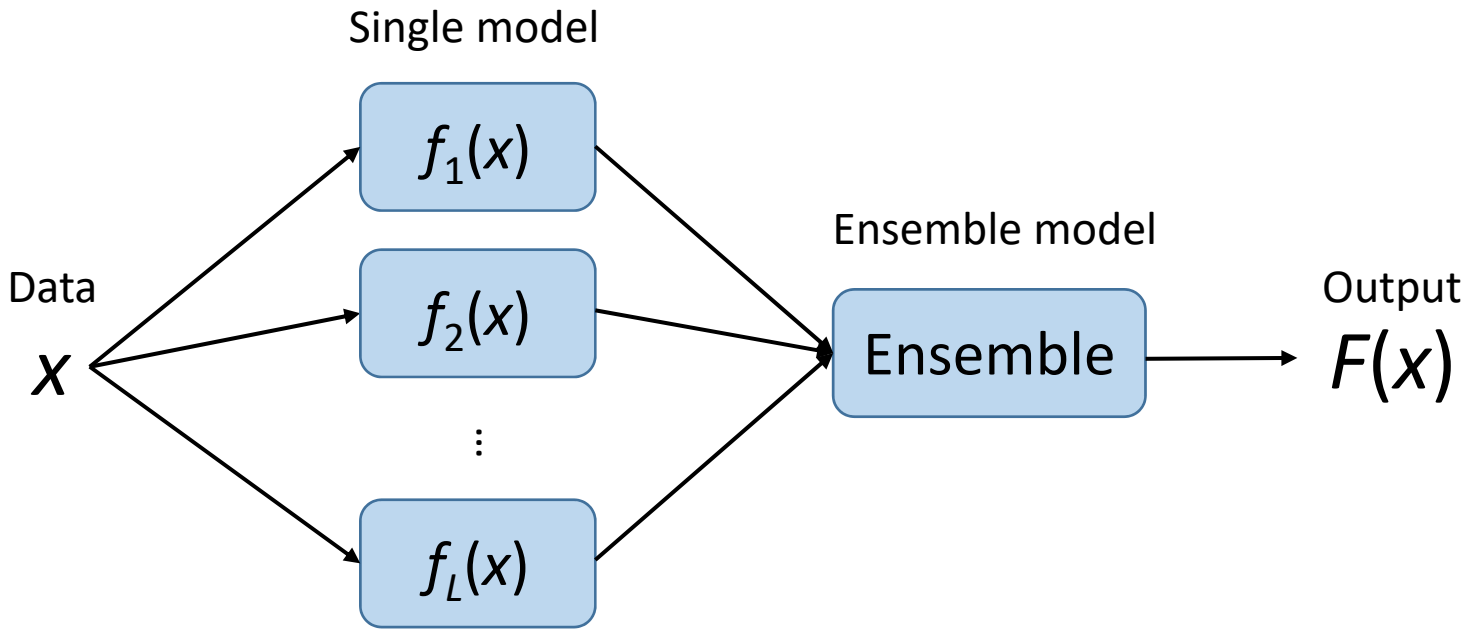
Bagging

Random Forest

Ensemble Learning

- Consider a set of predictors $f_1, \ldots, f_L$
  - Different predictors have different performance across data
- Idea: construct a predictor $F(x)$ that combines the individual decisions of $f_1, \ldots, f_L$
  - E.g., could have the member predictor vote
  - E.g., could use different members for different region of the data space
  - Works well if the member each has low error rates
- Successful ensembles require diversity
  - Predictors should make different mistakes
  - Encourage to involve different types of predictors

Ensemble Learning



- Although complex, ensemble learning probably offers the most sophisticated output and the best empirical performance!

Practical Application in Competitions

- Netflix Prize Competition
  - Task: predict the user's rating on a movie, given some users' ratings on some movies
  - Called 'collaborative filtering' (we will have a lecture about it later)

- Winner solution
  - BellKor's Pragmatic Chaos – an ensemble of more than 800 predictors

Yehuda Koren

[Yehuda Koren. The BellKor Solution to the Netflix Grand Prize. 2009.]

Practical Application in Competitions

- KDD-Cup 2011 Yahoo! Music Recommendation
  - Task: predict the user's rating on a music, given some users' ratings on some music
    - With music information like album, artist, genre IDs
- Winner solution
  - From A graduate course of National Taiwan University - an ensemble of 221 predictors

A Linear Ensemble of Individual and Blended Models for Music Rating Prediction

Po-Lung Chen, Chen-Tse Tsai, Yao-Nan Chen, Ku-Chun Chou, Chun-Liang Li, Cheng-Hao Tsai, Kuan-Wei Wu, Yu-Cheng Chou, Chung-Yi Li, Wei-Shih Lin, Shu-Hao Yu, Rong-Bing Chiu, Chieh-Yen Lin, Chien-Chih Wang, Po-Wei Wang, Wei-Lun Su, Chen-Hung Wu, Tsung-Ting Kuo, Todd G. McKenzie, Ya-Hsuan Chang, Chun-Sung Ferng, Chia-Mau Ni, Hsuan-Tien Lin, Chih-Jen Lin, Shou-De Lin

{R99922038, R98922028, R99922008, R99922095, B97018, B97705004, B96018, B96115, B96069, B96113, B95076, B97114, B97042, D98922007, B97058, B96110, B96055, D97944007, D97041, B96025, R99922054, B96092, HTLIN, CJLIN, SDLIN}@CSIE.NTU.EDU.TW

Department of Computer Science and Information Engineering, National Taiwan University

Practical Application in Competitions

- KDD-Cup 2011 Yahoo! Music Recommendation
  - Task: predict the user's rating on a music, given some users' ratings on some music
    - With music information like album, artist, genre IDs
- 3rd place solution
  - SJTU-HKUST joint team, an ensemble of 16 predictors

Informative Ensemble of Multi-Resolution Dynamic Factorization Models

Tianqi Chen*, Zhao Zheng, Qiuxia Lu, Xiao Jiang, Yuqiang Chen, Weinan Zhang
Kailong Chen and Yong Yu
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800 Dongchuan Road, Shanghai 200240 China
{tqchen, zhengzhao,luqiuxia,jiangxiao,yuqiangchen,wnzhang,chenkl,yyu}@apex.sjtu.edu.cn

Nathan N. Liu†, Bin Cao, Luheng He and Qiang Yang
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Clear Water Bay, Hong Kong
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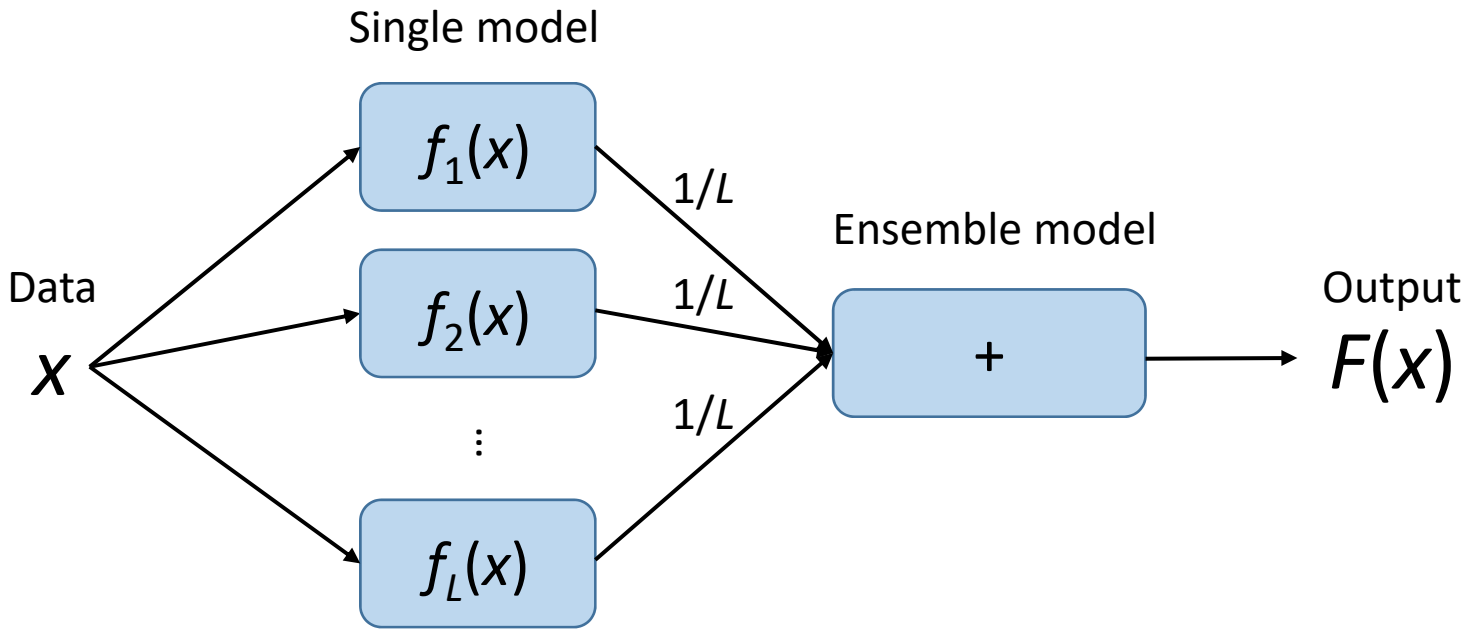
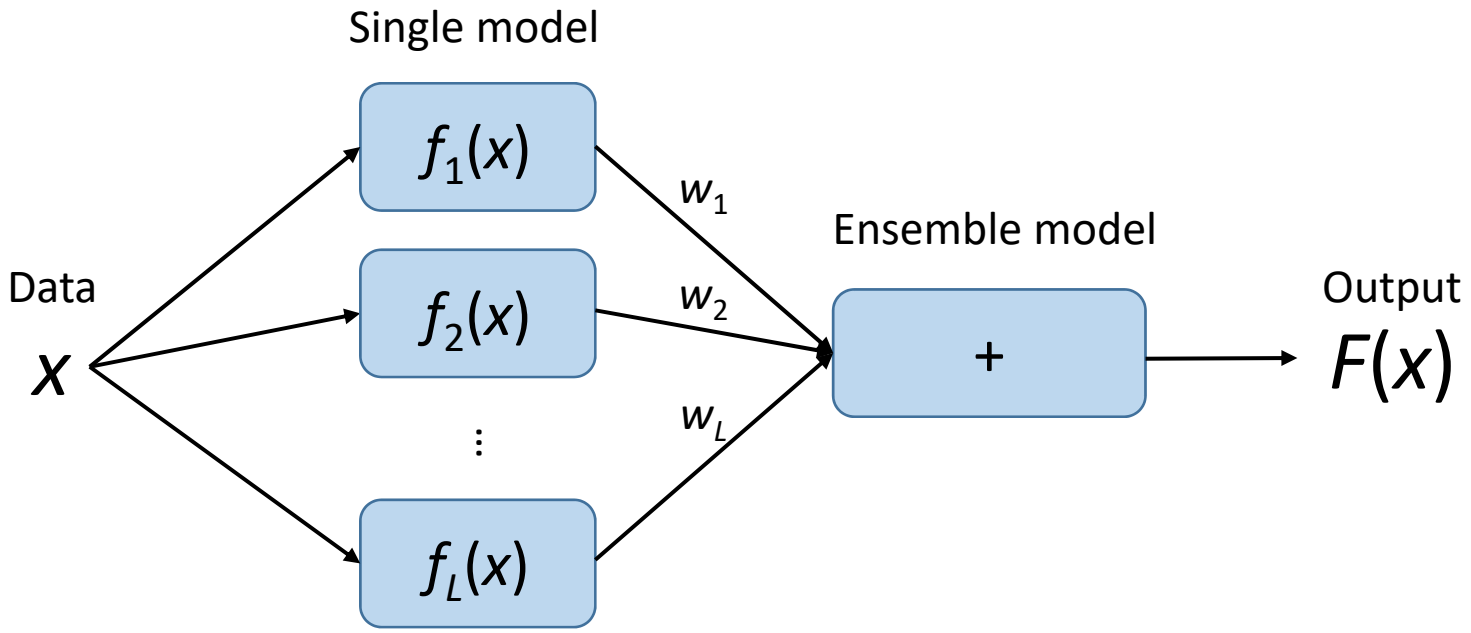
Combining Predictor: Averaging



$$F(x) = \frac{1}{L}\sum_{i=1}^{L} f_i(x)$$

- Averaging for regression; voting for classification

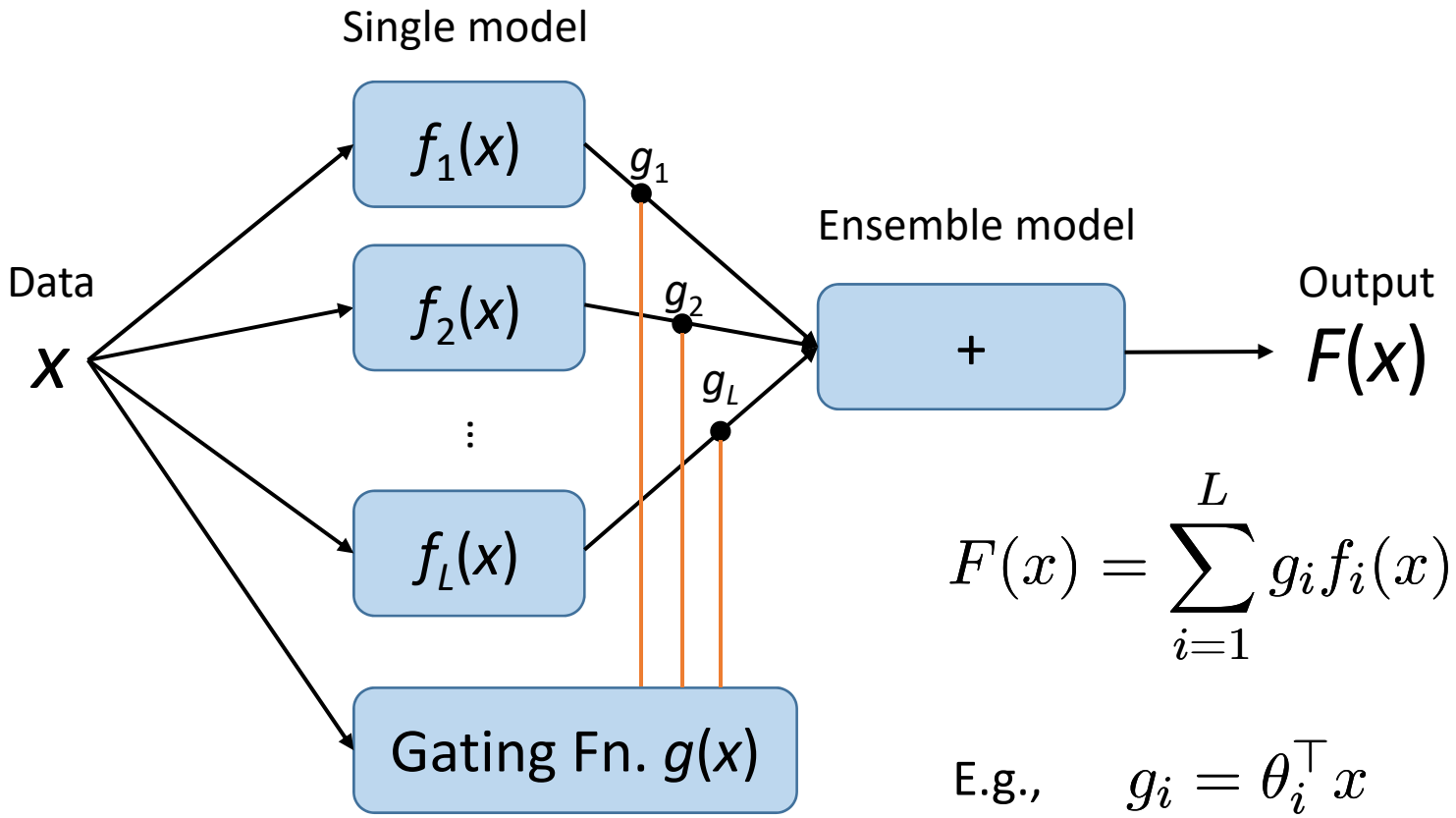
Combining Predictor: Weighted Avg



$$F(x) = \sum_{i=1}^{L} w_i f_i(x)$$

- Just like linear regression or classification
- Note: single model will not be updated when training ensemble model

Combining Predictor: Gating



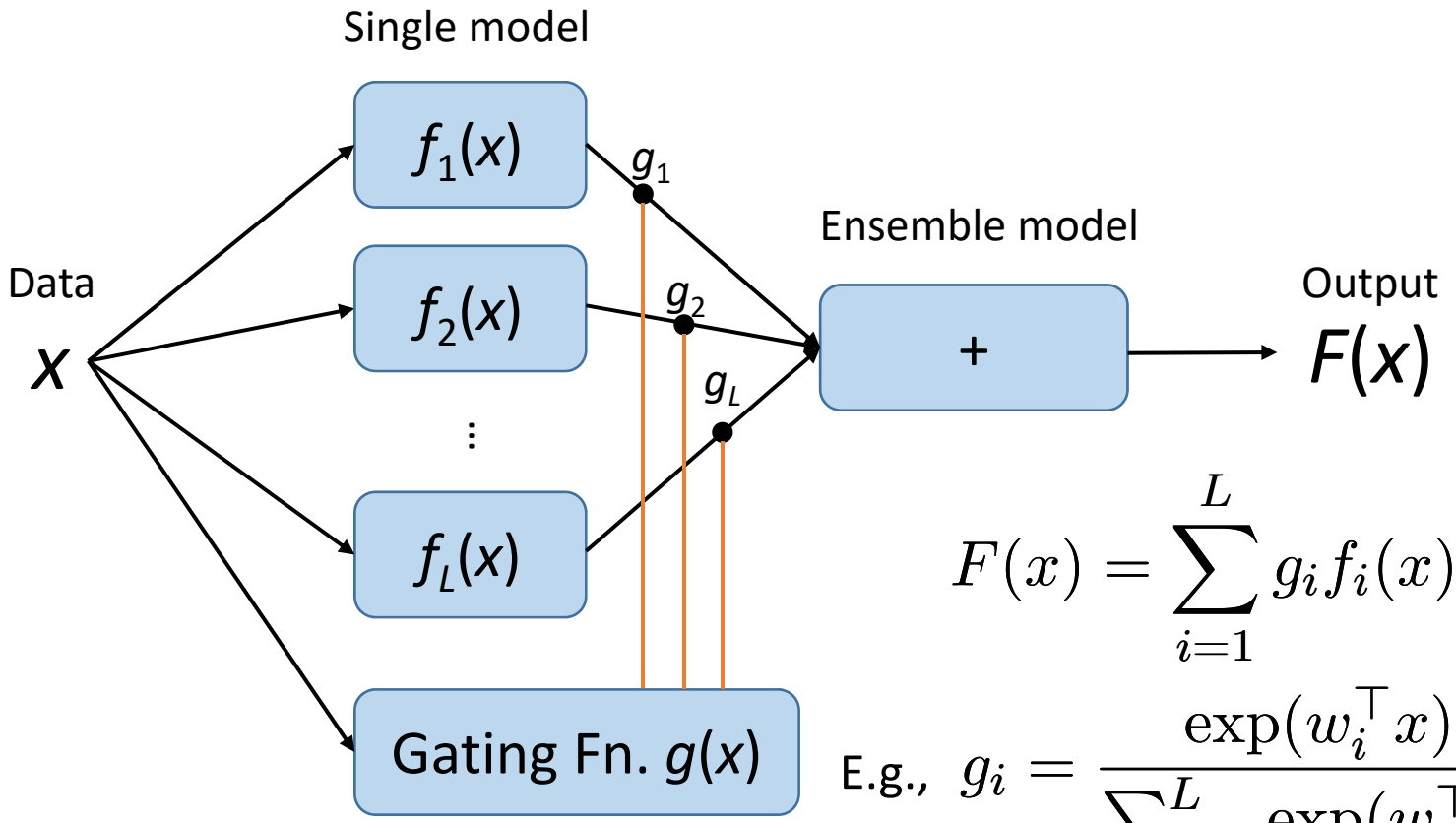
$$F(x) = \sum_{i=1}^{L} g_i f_i(x)$$

E.g., $g_i = \theta_i^\top x$

Design different learnable gating functions

- Just like linear regression or classification
- Note: single model will not be updated when training ensemble model

Combining Predictor: Gating



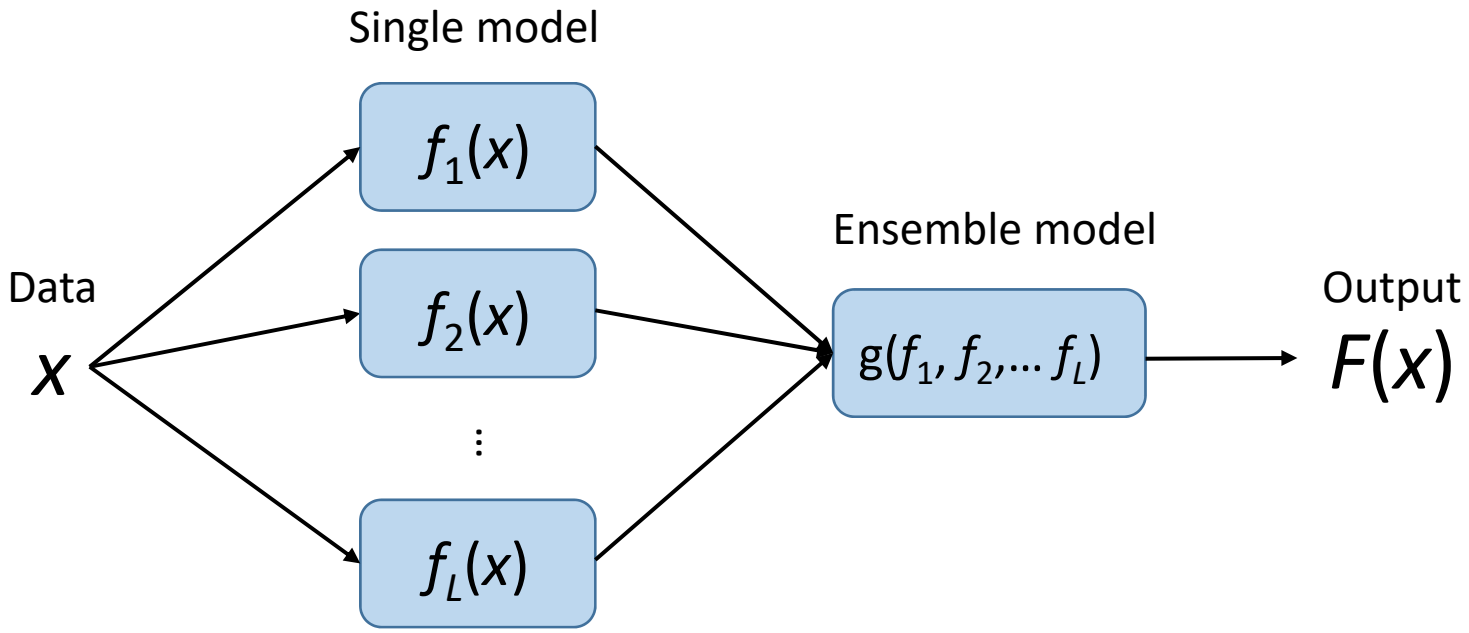
$$F(x) = \sum_{i=1}^{L} g_i f_i(x)$$

E.g., $g_i = \frac{\exp(w_i^\top x)}{\sum_{j=1}^{L} \exp(w_i^\top x)}$

Design different learnable gating functions

- Just like linear regression or classification
- Note: single model will not be updated when training ensemble model

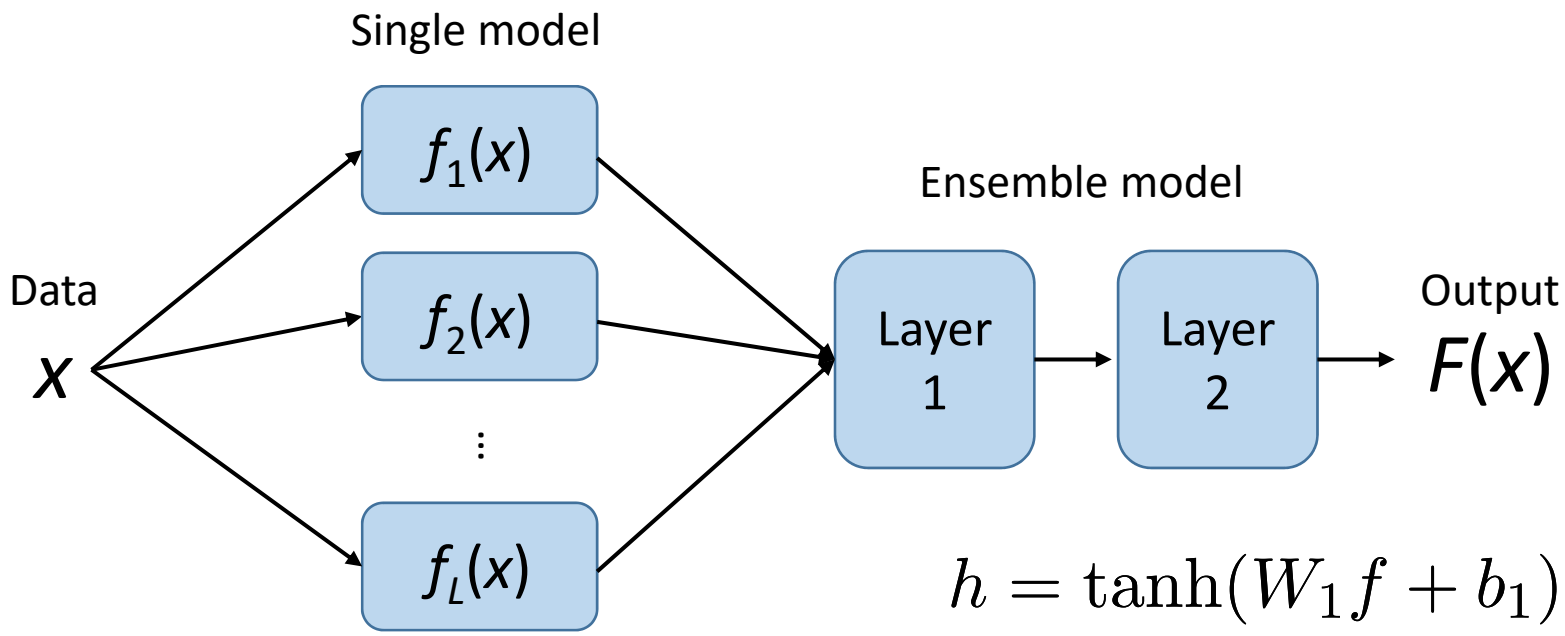
Combining Predictor: Stacking



$$F(x) = g(f_1(x), f_2(x), \ldots, f_L(x))$$

- This is the general formulation of an ensemble

Combining Predictor: Multi-Layer

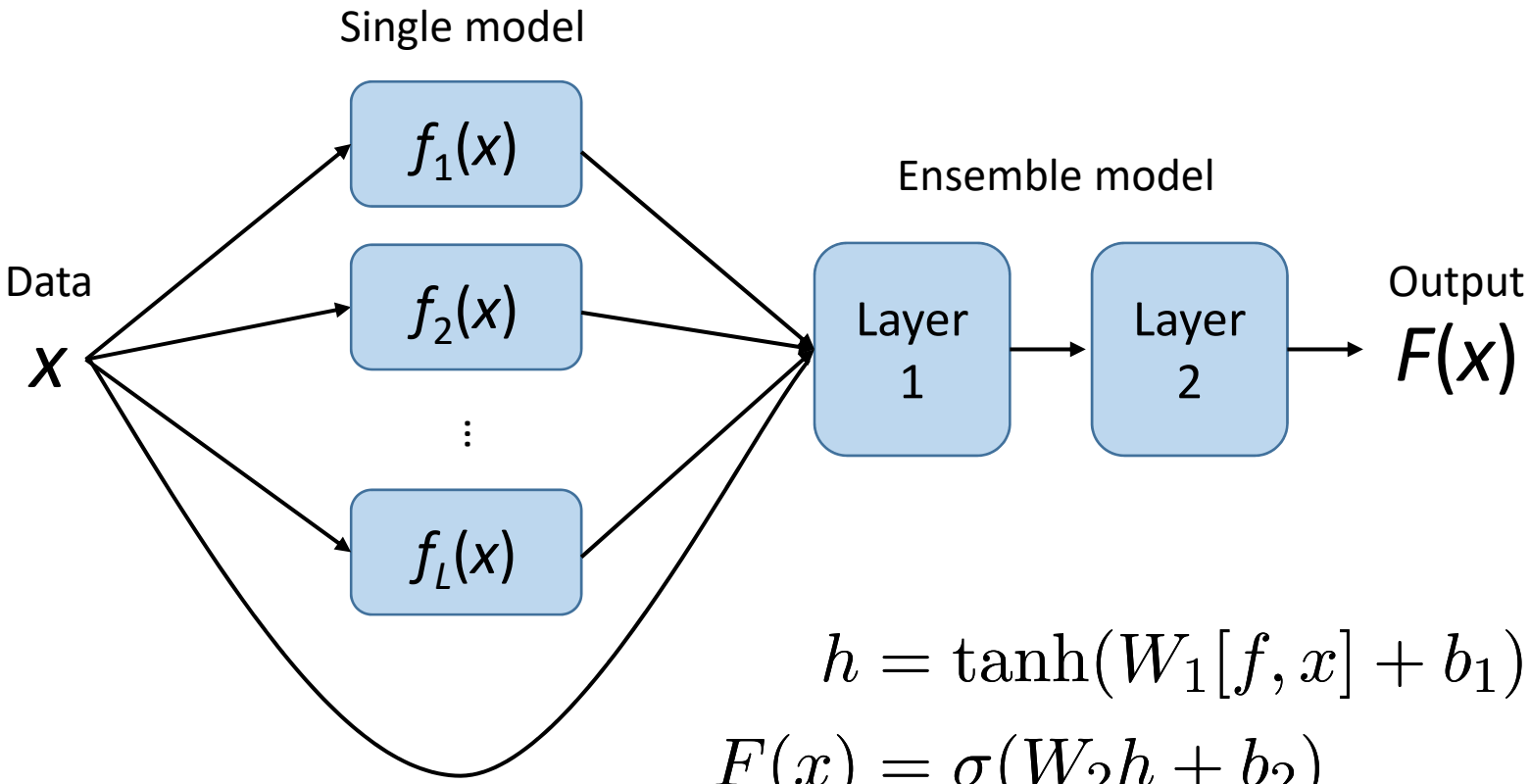


$$h = \tanh(W_1 f + b_1)$$

$$F(x) = \sigma(W_2 h + b_2)$$

- Use neural networks as the ensemble model

Combining Predictor: Multi-Layer

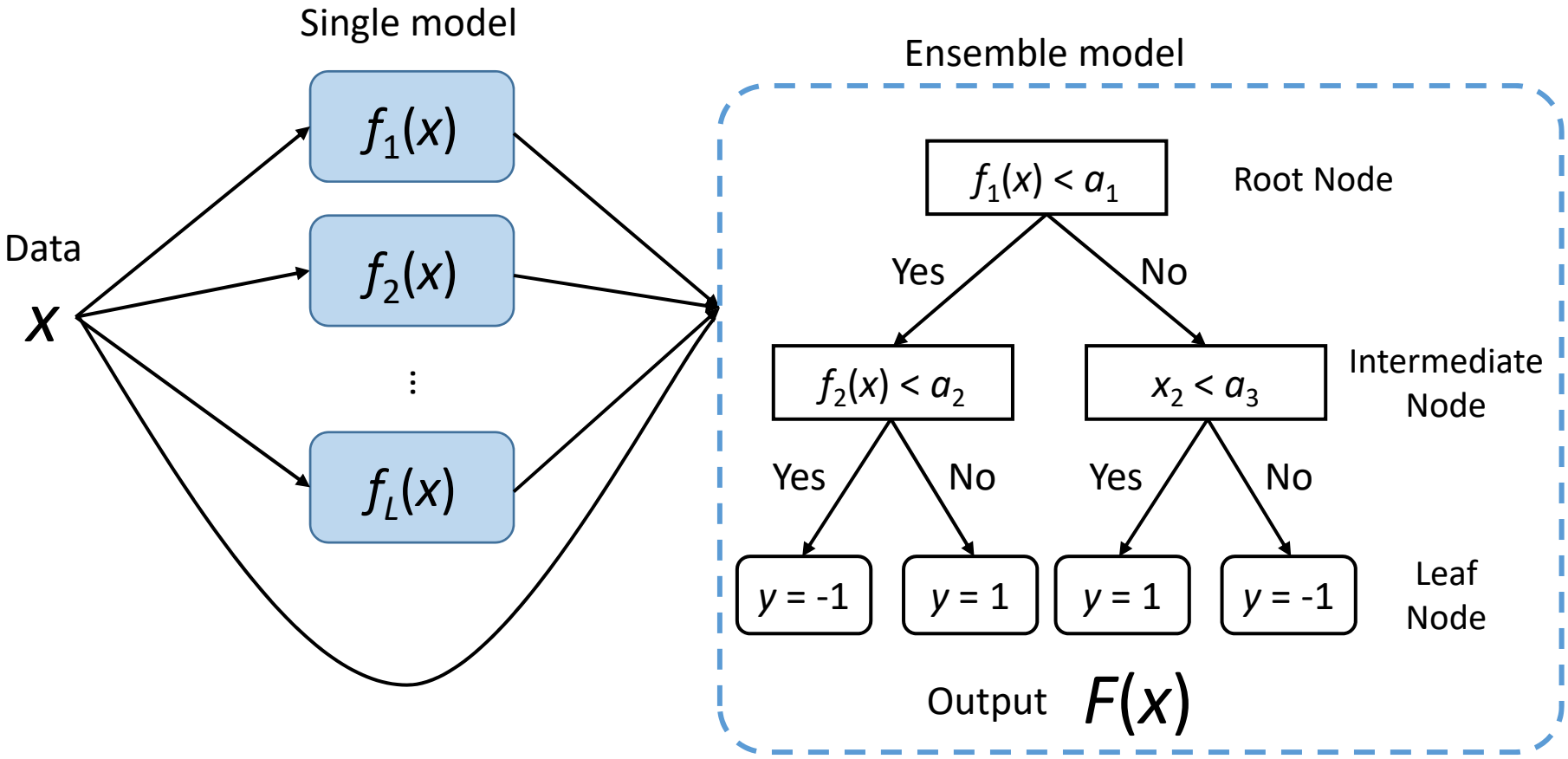


$$h = \tanh(W_1[f, x] + b_1)$$

$$F(x) = \sigma(W_2 h + b_2)$$

- Use neural networks as the ensemble model
- Incorporate *x* into the first hidden layer (as gating)

Combining Predictor: Tree Models



- Use decision trees as the ensemble model
- Splitting according to the value of *f*'s and *x*

Diversity for Ensemble Input

- Successful ensembles require diversity
  - Predictors may make different mistakes
  - Encourage to
    - involve different types of predictors
    - vary the training sets
    - vary the feature sets

Cause of the Mistake	**Diversification Strategy**
Pattern was difficult	Try different models
Overfitting	Vary the training sets
Some features are noisy	Vary the set of input features

[Based on slide by Leon Bottou]

Ensemble Learning

Bagging

Random Forest

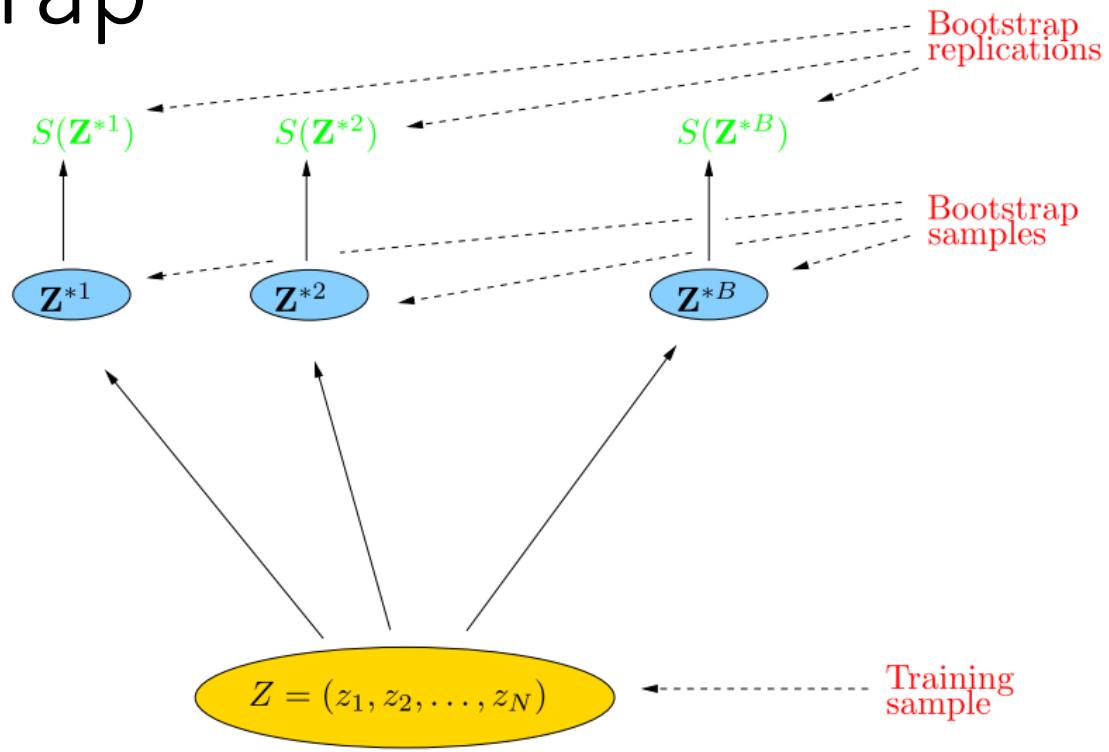
Manipulating the Training Data

- Bootstrap replication
  - Given *n* training samples *Z*, construct a new training set *Z** by sampling *n* instances with replacement
  - Excludes about 37% of the training instances

$$P\{\text{observation } i \in \text{bootstrap samples}\} = 1 - \left(1 - \frac{1}{N}\right)^N$$
$$\simeq 1 - e^{-1} = 0.632$$

- Bagging (Bootstrap Aggregating)
  - Create bootstrap replicates of training set
  - Train a predictor for each replicate
  - Validate the predictor using out-of-bootstrap data
  - Average output of all predictors

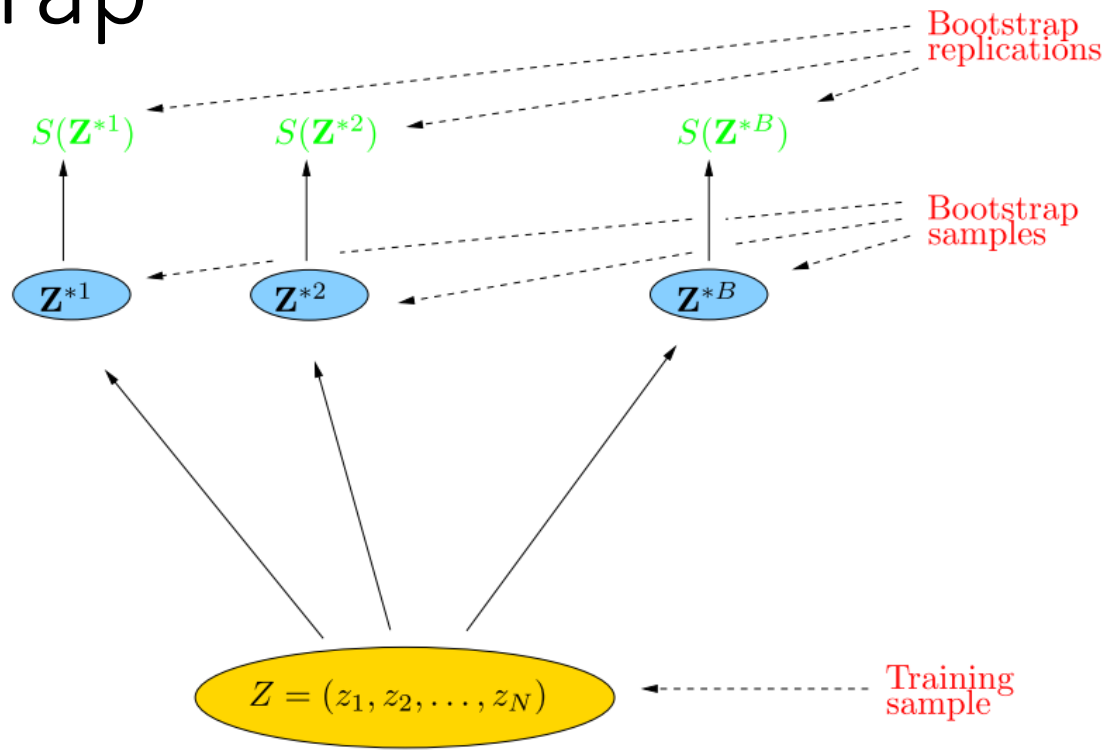
Bootstrap



- Basic idea
  - Randomly draw datasets with replacement from the training data
  - Each replicate with the same size as the training set
  - Evaluate any statistics *S*() over the replicates
    - For example, variance

$$\hat{\mathrm{Var}}[S(\boldsymbol{Z})] = \frac{1}{B-1}\sum_{b=1}^{B}(S(\boldsymbol{Z}^{*b}) - \bar{S}^{*})^2$$

Bootstrap



- Basic idea
  - Randomly draw datasets with replacement from the training data
  - Each replicate with the same size as the training set
  - Evaluate any statistics *S*() over the replicates
    - For example, model error

$$\hat{\mathrm{Err}}_{\mathrm{boot}} = \frac{1}{B}\frac{1}{N}\sum_{b=1}^{B}\sum_{i=1}^{N} L(y_i, \hat{f}^{*b}(x_i))$$

Bootstrap for Model Evaluation

- If we directly evaluate the model using the whole training data

$$\hat{\mathrm{Err}}_{\mathrm{boot}} = \frac{1}{B}\frac{1}{N}\sum_{b=1}^{B}\sum_{i=1}^{N} L(y_i, \hat{f}^{*b}(x_i))$$

- As the probability of a data instance in the bootstrap samples is

$$P\{\text{observation } i \in \text{bootstrap samples}\} = 1 - \left(1 - \frac{1}{N}\right)^N$$
$$\simeq 1 - e^{-1} = 0.632$$

- If validate on training data, it is much likely to overfit
  - For example in a binary classification problem where *y* is indeed independent with *x*
    - Correct error rate: 0.5
    - Above bootstrap error rate: 0.632*0 + (1-0.632)*0.5=0.184

Leave-One-Out Bootstrap

- Build a bootstrap replicate with one instance *i* out, then evaluate the model using instance *i*

$$\hat{\mathrm{Err}}^{(1)} = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{|C^{-i}|}\sum_{b\in C^{-i}} L(y_i, \hat{f}^{*b}(x_i))$$

  - C^{-i} is the set of indices of the bootstrap samples *b* that do not contain the instance *i*
  - For some instance *i*, the set C^{-i} could be null set, just ignore such cases

- We shall come back to the model evaluation and select in later lectures.

Bootstrap for Model Parameters

- Sec 8.4 of Hastie et al. The elements of statistical learning.

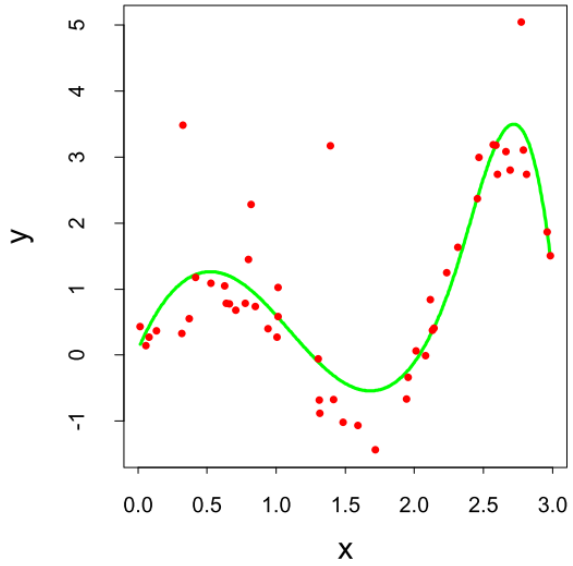
- Bootstrap mean is approximately a posterior average.

Bagging: Bootstrap Aggregating

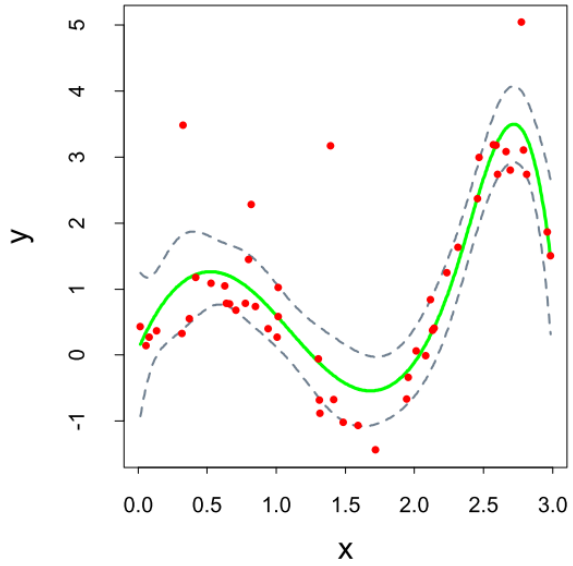
- Bootstrap replication
  - Given *n* training samples $Z = \{(x_1,y_1), (x_2,y_2),\ldots,(x_n,y_n)\}$, construct a new training set Z^* by sampling *n* instances with replacement
  - Construct *B* bootstrap samples Z^{*b} , $b = 1,2,\ldots,B$
  - Train a set of predictors $\hat{f}^{*1}(x), \hat{f}^{*2}(x), \ldots, \hat{f}^{*B}(x)$

- Bagging average the predictions

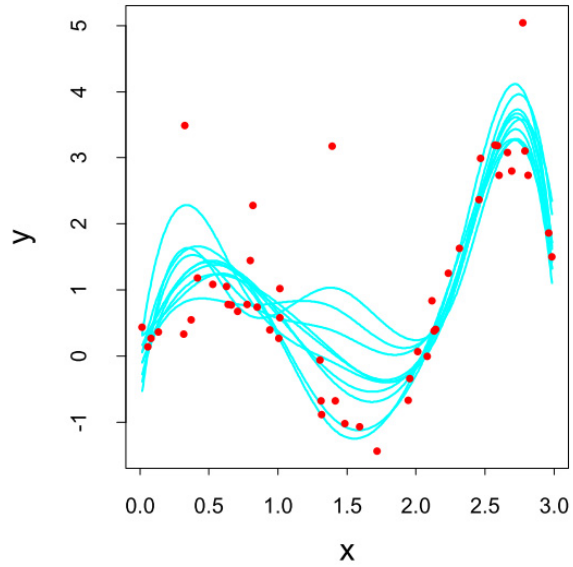
$$\hat{f}_{\text{bag}}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}^{*b}(x)$$



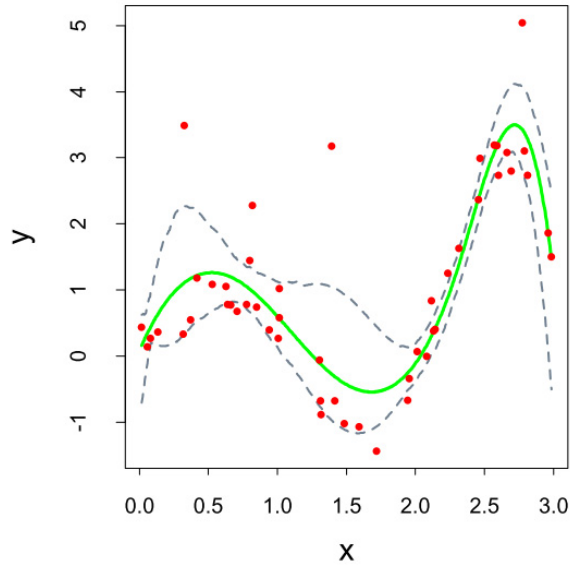
B-spline smooth of data



B-spline smooth plus and minus 1.96 × standard error bands

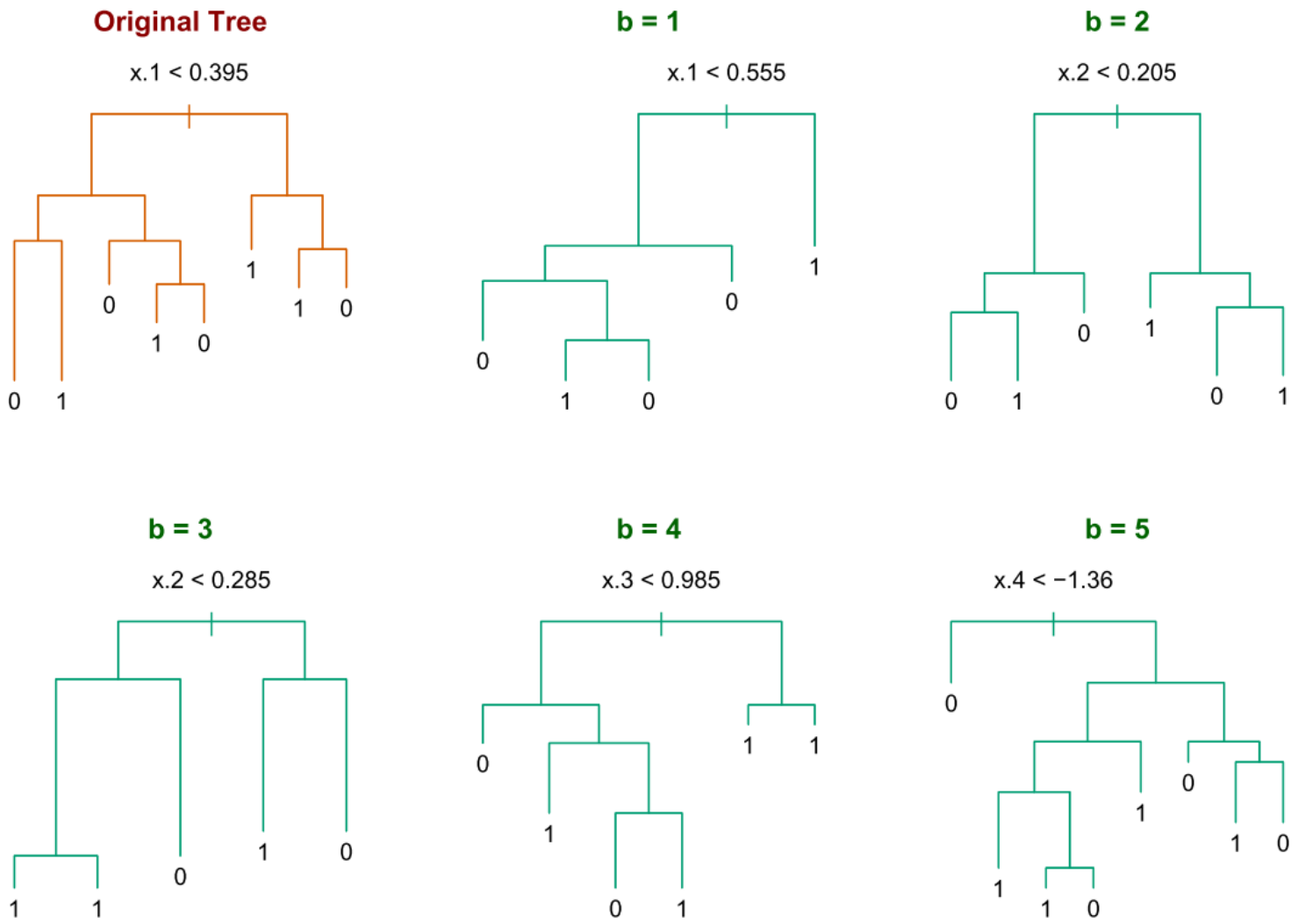


Ten bootstrap replicates of the B-spline smooth.



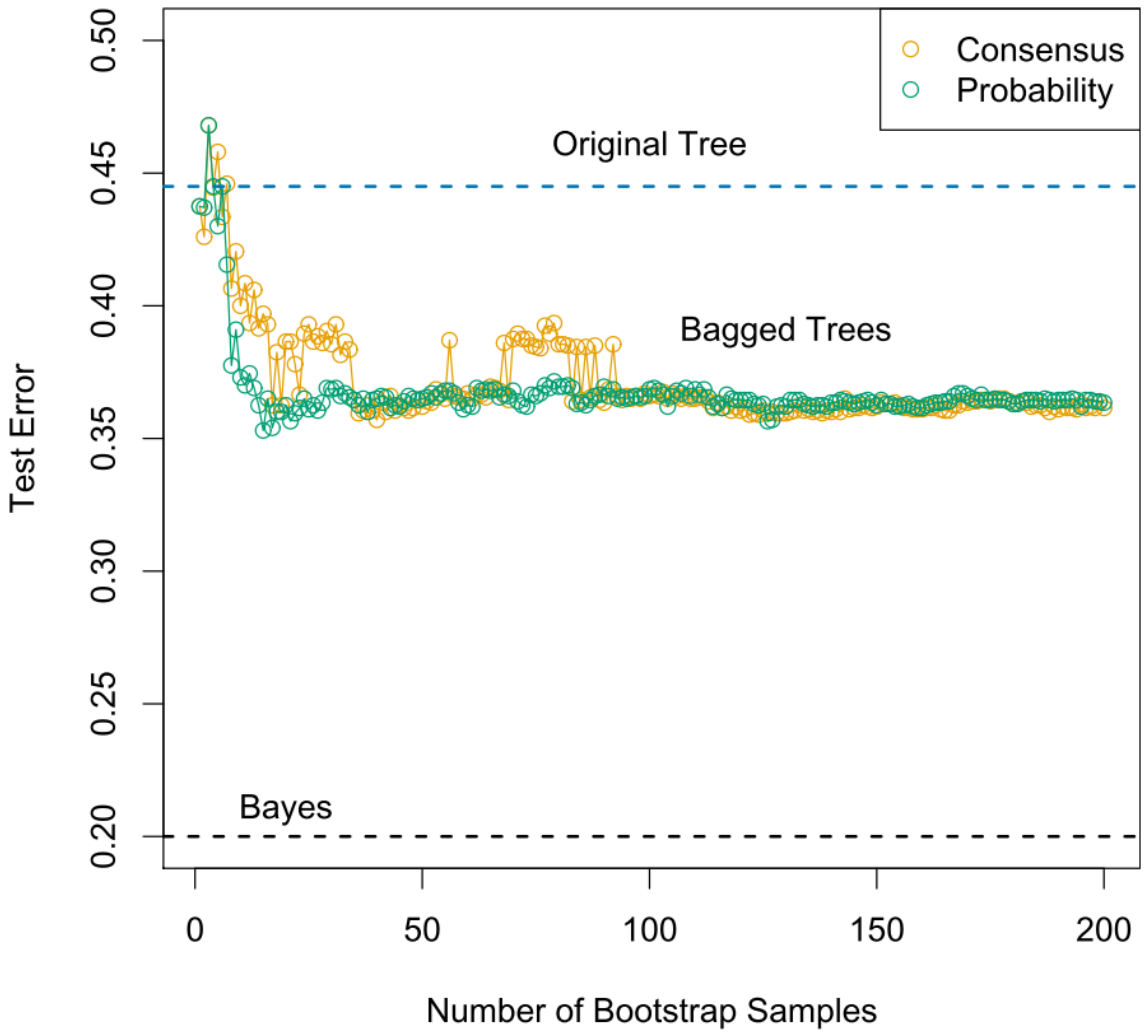
B-spline smooth with 95% standard error bands computed from the bootstrap distribution

Fig 8.2 of Hastie et al. The elements of statistical learning.



Bagging trees on simulated dataset. The top left panel shows the original tree. 5 trees grown on bootstrap samples are shown. For each tree, the top split is annotated.

Fig 8.9 of Hastie et al. The elements of statistical learning.



For classification bagging, consensus vote vs. class probability averaging

Fig 8.10 of Hastie et al. The elements of statistical learning.

Why Bagging Works

- Bias-Variance Decomposition
  - Assume $Y = f(X) + \epsilon$ where $\mathbb{E}[\epsilon] = 0 \quad \mathrm{Var}[\epsilon] = \sigma_\epsilon^2$
  - Then the expected prediction error at an input point x_0

$$\begin{aligned}\mathrm{Err}(x_0) &= \mathbb{E}[(Y - \hat{f}(x_0))^2 | X = x_0] \\ &= \sigma_\epsilon^2 + [\mathbb{E}[\hat{f}(x_0)] - f(x_0)]^2 + \mathbb{E}[\hat{f}(x_0) - \mathbb{E}[\hat{f}(x_0)]]^2 \\ &= \sigma_\epsilon^2 + \mathrm{Bias}^2(\hat{f}(x_0)) + \mathrm{Var}(\hat{f}(x_0))\end{aligned}$$

- Bagging works by reducing the variance with the same bias as the original model (trained over the whole data)
  - Works especially well based on low-bias and high-variance prediction models

Ensemble Learning

Bagging

Random Forest

The Problem of Bagging

- Bagging works by reducing the variance with the same bias as the original model (trained over the whole data)
  - Works especially based on low-bias and high-variance prediction models

- If the variables (with variance σ^2) are i.d. (identically distributed but not necessarily independent) with positive correlation ρ, the variance of the average is

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

- Which reduces to $\rho\sigma^2$, even if the bootstrap sample size goes to infinity

The Problem of Bagging

- Bagging works by reducing the variance with the same bias as the original model (trained over the whole data)
  - Works especially based on low-bias and high-variance prediction models
- Problem: the models trained from bootstrap samples are probably positively correlated

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

Random Forest

- Breiman, Leo. "Random forests." *Machine learning* 45.1 (2001): 532.
- Random forest is a substantial modification of bagging that builds a large collection of de-correlated trees, and then average them.

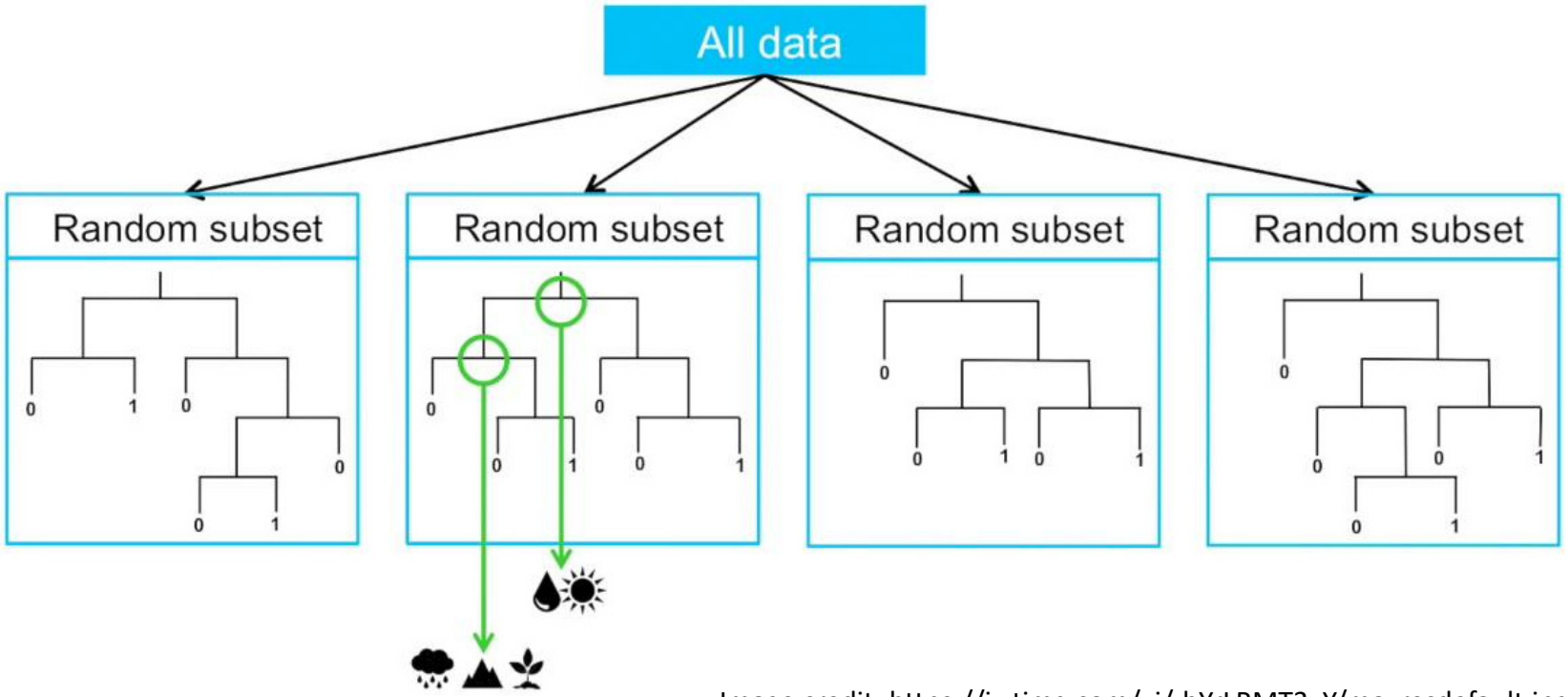
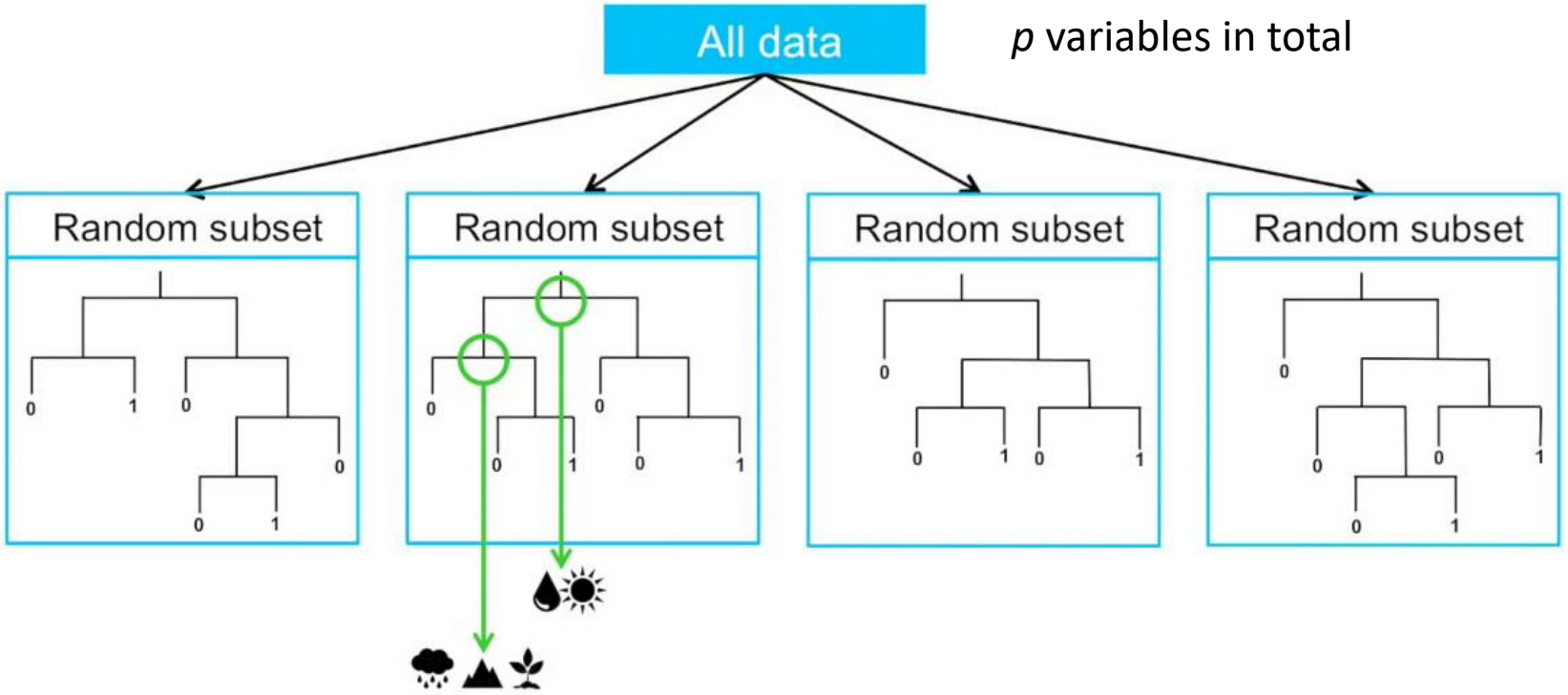


Image credit: https://i.ytimg.com/vi/-bYrLRMT3vY/maxresdefault.jpg

Tree De-correlation in Random Forest



- Before each tree node split, select $m \leq p$ variables at random as candidates of splitting
  - Typically values $m = \sqrt{p}$ or even low as 1

Random Forest Algorithm

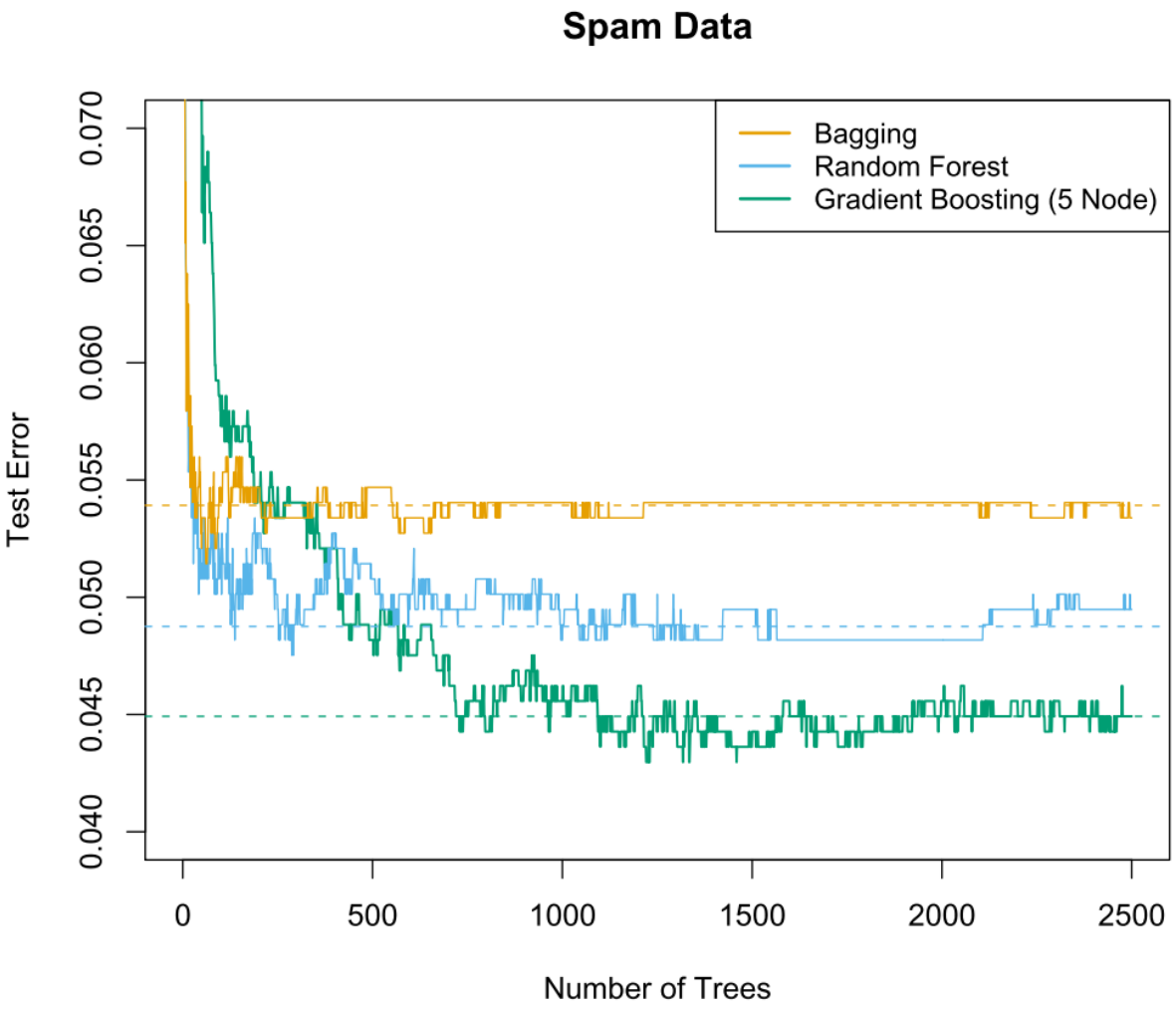
- For b = 1 to B:
  a) Draw a bootstrap sample Z^* of size n from training data
  b) Grow a random-forest tree T_b to the bootstrap data, by recursively repeating the following steps for each leaf node of the tree, until the minimum node size is reached
     I. Select m variables at random from the p variables
     II. Pick the best variable & split-point among the m
     III. Split the node into two child nodes
- Output the ensemble of trees $\{T_b\}_{b=1\ldots B}$
- To make a prediction at a new point x

Regression: prediction average $\hat{f}_{\mathrm{rf}}^{B}(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x)$

Classification: majority voting $\hat{C}_{\mathrm{rf}}^{B}(x) = \text{majority vote } \{\hat{C}_b(x)\}_1^B$

Algorithm 15.1 of Hastie et al. The elements of statistical learning.

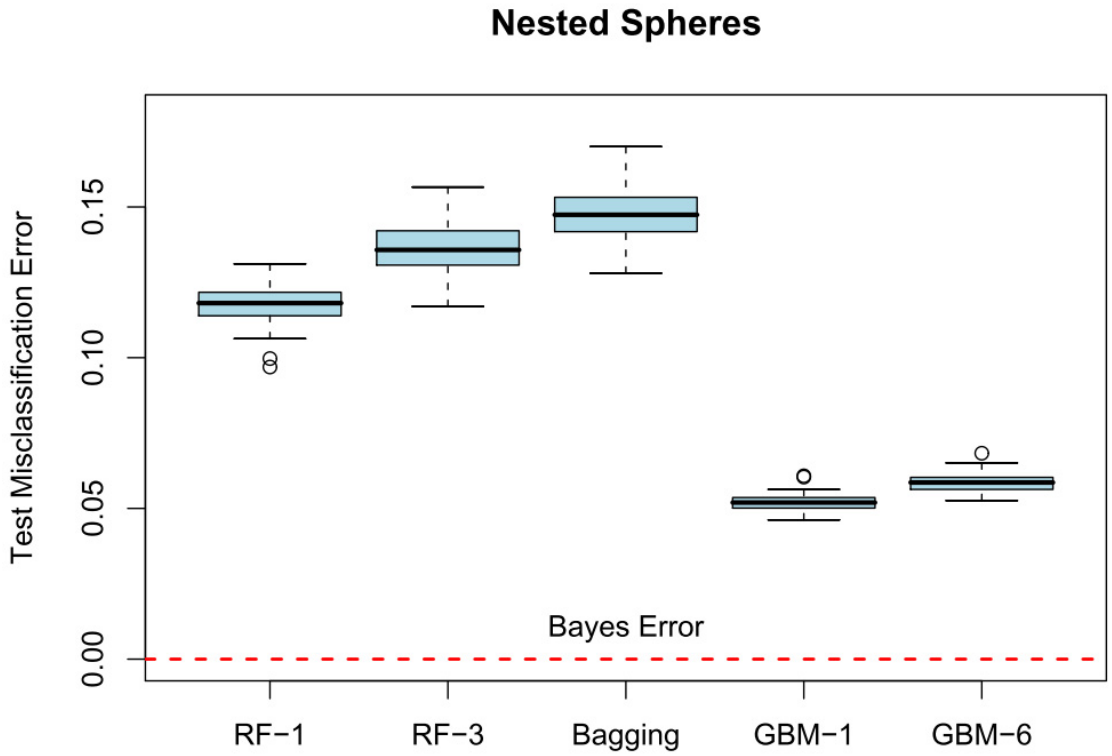
Performance Comparison



1536 test data instances

Fig. 15.1 of Hastie et al. The elements of statistical learning.

Performance Comparison



- Nest spheres data $Y = \begin{cases} 1 & \text{if } \sum_{j=1}^{10} X_j^2 > 9.34 \\ -1 & \text{otherwise} \end{cases}$
- RF-*m*: *m* means the randomly selected variables for each splitting

Fig. 15.2 of Hastie et al. The elements of statistical learning.

For more machine learning details, you can check out my machine learning course at Zhiyuan College

CS420 Machine Learning

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Course webpage:

http://wnzhang.net/teaching/cs420/index.html