INTRODUCTORY APPLIED MACHINE LEARNING

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Today:

- Nearest-neighbor classifiers
- Bayesian classifiers
- Logistic regression
- Ensemble methods

Outline

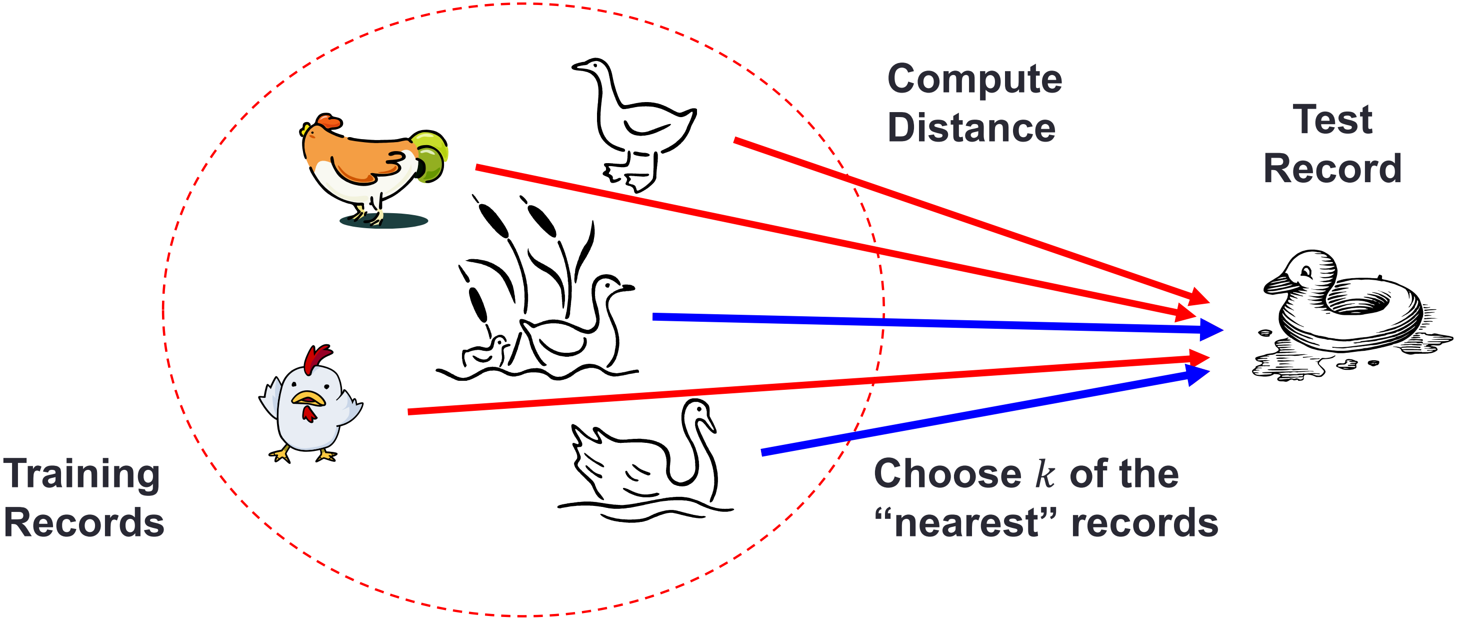
- Goal of the lecture
- K-nearest neighbor
- Naïve Bayesian classification
- Logistic regression
- Bagging
- Boosting

Goals

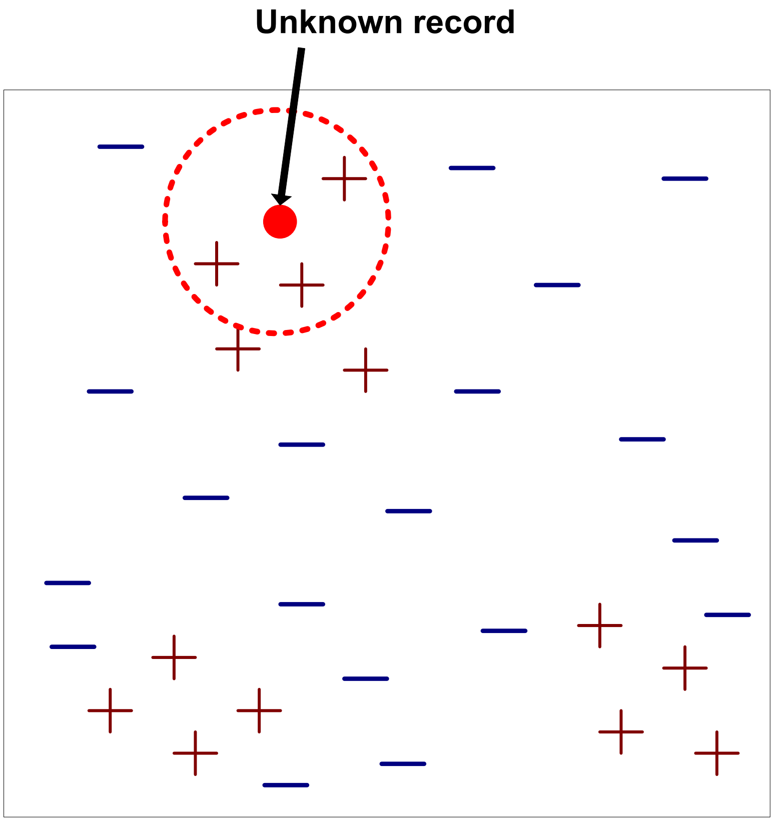
- After this, you should be able to:
  - Build k-nearest neighbor and naïve Bayesian classifiers
  - Build logistic regression models
  - Get basic ideas of ensemble methods
  - Understand the advantages and disadvantages of k-nearest neighbor, naïve Bayesian, logistic regression, and ensemble methods

k-Nearest Neighbor (kNN) Classifier

- An instance-based classifier
- Basic idea: if an animal walks like a duck, quacks like a duck, then it's probably a duck



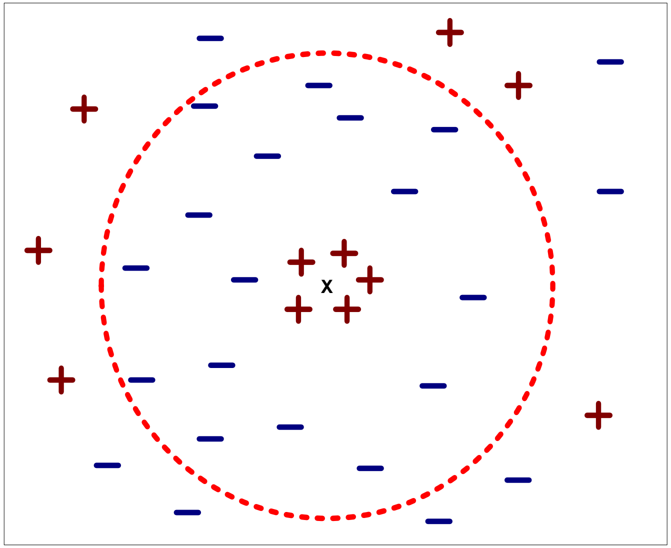
Requirements of kNN



- Uses k “closest” points (nearest neighbors) for performing classification
- Requirements:
  1. The set of stored records
  2. Distance metric to compute distance between records
  3. The value of “k“, the number of nearest neighbors to retrieve

Choice of the k Value

- If k is too small, sensitive to noise points
- If k is too large, neighborhood may include points from other classes



kNN Classification Procedure

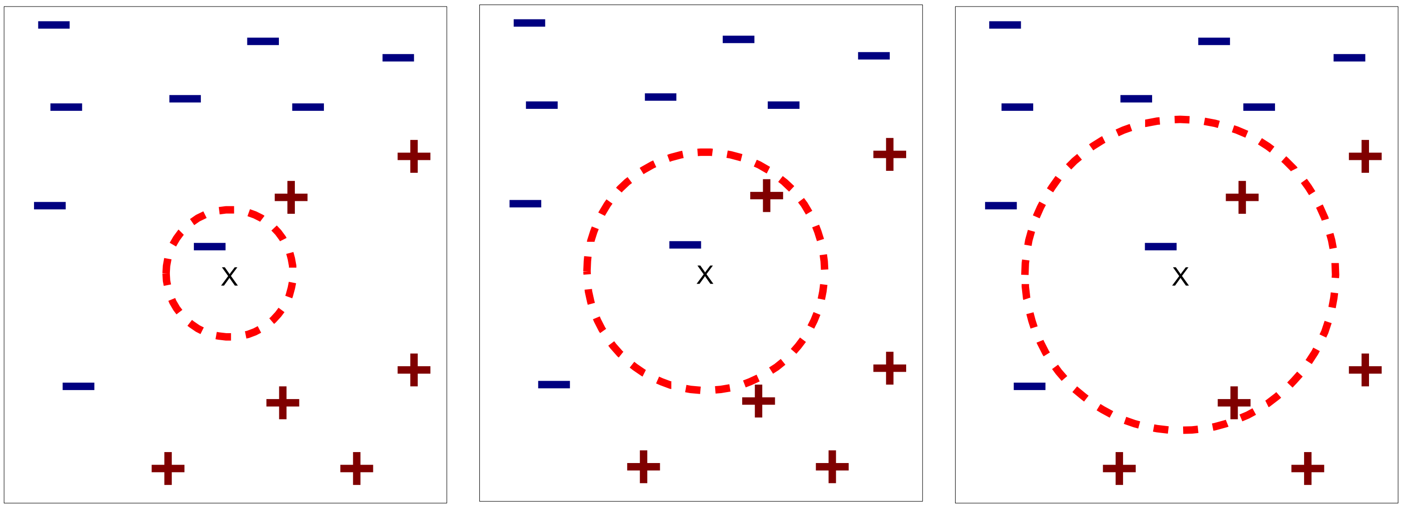
1. Compute the distance $d \in \Re$ between the unknown sample point and neighbor points

   (Typically the Euclidean (L_2) norm is used)
2. Identify k nearest neighbors
3. Take the majority vote of class labels among the k-nearest neighbors

   (Typically the weight factor $w = \frac{1}{d^2} \in \Re$ is used)

The Value of “k“

- k-nearest neighbors of a record x are data points that have the k smallest distance to x

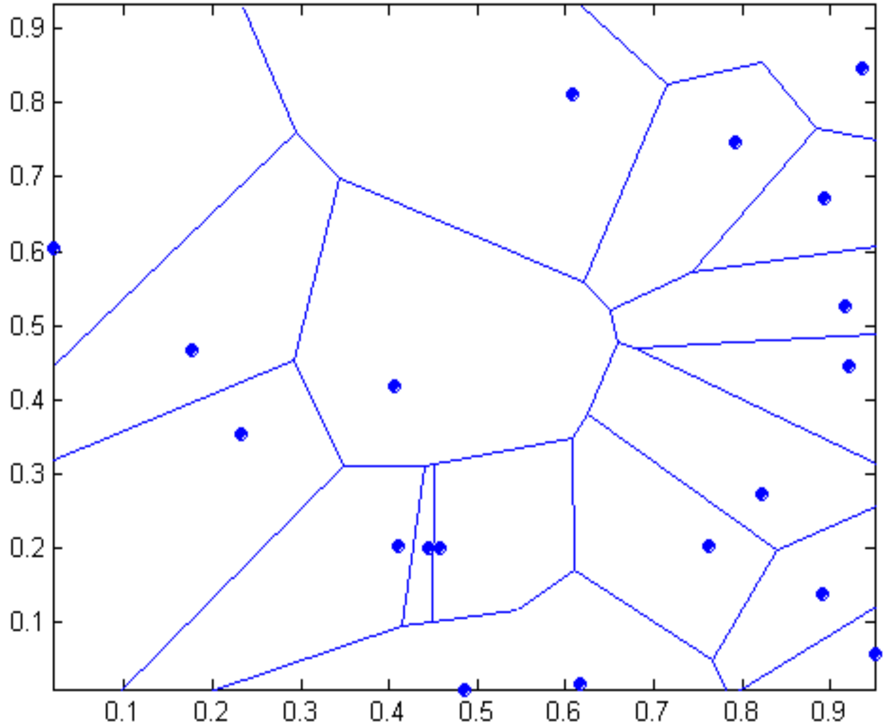


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

Special Case: 1-nearest Neighbor

- Voronoi Diagram:

  decomposition of a space determined by distances to objects



Attribute Normalization

- Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
- Example:
  - Height of a person may vary from 1.5m to 1.8m
  - Weight of a person may vary from 90lb to 300lb
  - Income of a person may vary from $10K to $1M

kNN Summary

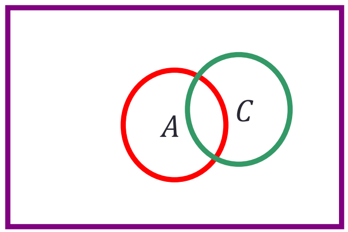
- kNN classifiers do not build models explicitly
- Classifying unknown records are relatively time consuming and computationally intensive
- Highly effective inductive inference method for noisy training data and complex target functions
- Nonparametric architecture

Bayes Theorem

- A probabilistic framework for solving classification problems
- Conditional probability:

$$P(C|A) = \frac{P(A \cap C)}{P(A)}$$

$$P(A|C) = \frac{P(A \cap C)}{P(C)}$$



- Bayes theorem:

prior **likelihood**

posterior

$$P(C|A) = \frac{P(A|C)P(C)}{P(A)}$$

evidence

Example of Bayes Theorem

- Given:
  - A doctor knows that meningitis (M) causes stiff neck (S) 50% of the time
  - Prior probability of any patient having meningitis is 1/50,000
  - Prior probability of any patient having stiff neck is 1/20
- If a patient has stiff neck, what's the probability he/she has meningitis?

$$P(M|S) = \frac{P(S|M)P(M)}{P(S)} = \frac{0.5 \times 1/50000}{1/20} = 0.0002$$

Towards Naïve Bayesian Classification

- Given a training set of attributes $\boldsymbol{x} = (x_1, x_2, \dots, x_K)$ and class y_j, $j = 1 \dots m$
- Consider each attribute and class label as a random variable
- Goal is to predict the class y_j for given $(x_1, x_2, \dots, x_K)$
- This is equivalent to find the value of y_j that maximizes the posteriori $P(y_j|\boldsymbol{x}) = P(y_j|x_1, x_2, \dots, x_K)$

Classification Using Naïve Bayes

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Question: find the evade $y_j = Yes$ or No, given the evidence $\boldsymbol{x} = (No\ refund, Married, Inc = 120K)$
- This is equivalent to find y that maximizes $P(y_j|\boldsymbol{x}) = P(y_j|No\ refund, Married, Inc = 120K)$

Derivation of Naïve Bayes Classifier

- From Bayes theorem:

$$P(y_j|\boldsymbol{x}) = P(y_j|x_1, x_2, \dots, x_K) = \frac{P(x_1, x_2, \dots, x_K|y_j)P(y_j)}{P(x_1, x_2, \dots, x_K)}$$

- Note that $P(\boldsymbol{x}) = P(x_1, x_2, \dots, x_K)$ is constant for all classes
- Choosing the value of y_j that maximizes $P(y_j|x_1, x_2, \dots, x_K)$ is equivalent to choosing the value of y_j that maximizes $P(x_1, x_2, \dots x_K|y_j)P(y_j)$

Derivation of Naïve Bayes Classifier (Cont'd)

- Assume independence among attributes x_i, i.e.,

$$P(x_1, x_2, \dots, x_K | y_j) = P(x_1 | y_j) \times P(x_2 | y_j) \times \cdots \times P(x_K | y_j)$$

- The individual $P(x_i | y_j)$ for all x_i and y_j is easier to be estimated
- The original equation can be reformulated into

$$P(y_j | \boldsymbol{x}) = \frac{P(x_1 | y_j) \times P(x_2 | y_j) \times \cdots \times P(x_K | y_j) P(y_j)}{P(x_1, x_2, \dots, x_n)}$$

- The objective is to find the y_j that maximizes $P(y_j) \prod_{i=1}^{K} P(x_i | y_j)$, i.e.,

$$y = \arg\max_{y} \left[\left(\prod_{i=1}^{K} P(x_i | y_j = y) \right) P(y_j = y) \right]$$

Estimate Probabilities for Discrete Attributes

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Class: $P(y_j) = \frac{N_{y_j}}{N}$

  $$P(No) = \frac{7}{10}, \quad P(Yes) = \frac{3}{10}$$

- Prior/posterior: $P\left(x_i \middle| y_j\right) = \frac{|x_{ij}|}{N_{y_j}}$,

  where $|x_{ij}|$ is number of instances having attribute x_i and belongs to class y_j

- Example:

  $$\begin{cases} P(Status = Married|No) = \frac{4}{7} \\ P(Refund = Yes|Yes) = 0 \end{cases}$$

Estimate Probabilities for Continuous Attributes

- Two Common methods:
  1. Two-way split: $(x < v)$ or $(x > v)$, and choose only one of the two splits as new attribute
  2. Probability density estimation:
     - Assume attribute follows a normal distribution
     - Use data to estimate parameters of distribution, e.g., mean and standard deviation
     - Once probability distribution is known, it can be used to estimate the conditional probability $P(x_i|y_j)$

Estimate Probabilities for Continuous Attributes

Tid	Refund	Marital Status	Taxable Income	Evade
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10	No	Single	90K	Yes

- Normal distribution:

$$P(x_i|y_j) = \frac{1}{\sqrt{2\pi\sigma_{ij}^2}} e^{-\frac{(x_i-\mu_{ij})^2}{2\sigma_{ij}^2}}$$

  for each (x_i, y_j) pair

- Example:

  Let $x_i = Income$, and $y_j = No$

  $\Rightarrow \mu_{ij} = 110$, and $\sigma_{ij}^2 = 2975$

$$P(Income = 120|No) = \frac{1}{\sqrt{2\pi}(54.54)} e^{-\frac{(120-110)^2}{2(2975)}} = 0.0072$$

Example

- Given that $\boldsymbol{x} = (\mathit{No\ refund, Married, Inc} = \mathit{120K})$, find the evade $y_j = Yes$ or No

- Calculate the probability:
  - $P(Refund = Yes|No) = 3/7$
  - $P(Refund = No|No) = 4/7$
  - $P(Refund = Yes|Yes) = 0$
  - $P(Refund = No|Yes) = 1$
  - $P(Marital\ Status = Single|No) = 2/7$
  - $P(Marital\ Status = Divorced|No) = 1/7$
  - $P(Marital\ Status = Married|No) = 4/7$
  - $P(Marital\ Status = Single|Yes) = 2/3$
  - $P(Marital\ Status = Divorced|Yes) = 1/3$
  - $P(Marital\ Status = Married|Yes) = 0$

- Conduct Bayes' classifier:
  - $P(\boldsymbol{x}|No) = P(No\ refund|No) \times P(Married|\ No) \times P(Inc = 120K|\ No)$
    $= 4/7 \times 4/7 \times 0.0072 = 0.0024$
  - $P(\boldsymbol{x}|Yes) = P(No\ Refund|Yes) \times P(Married|Yes) \times P(Inc = 120K|\ Yes)$
    $= 1 \times 0 \times 1.2 \times 10^{-9} = 0$
  - $P(\boldsymbol{x}|No)P(No) > P(\boldsymbol{x}|Yes)P(Yes)$

    $\Rightarrow$ **evade** $= No$

Another Example

Name	Give Birth	Can Fly	Live in Water	Have Legs	Class
human	yes	no	no	yes	mammals
python	no	no	no	no	non-mammals
salmon	no	no	yes	no	non-mammals
whale	yes	no	yes	no	mammals
frog	no	no	sometimes	yes	non-mammals
komodo	no	no	no	yes	non-mammals
bat	yes	yes	no	yes	mammals
pigeon	no	yes	no	yes	non-mammals
cat	yes	no	no	yes	mammals
leopard shark	yes	no	yes	no	non-mammals
turtle	no	no	sometimes	yes	non-mammals
penguin	no	no	sometimes	yes	non-mammals
porcupine	yes	no	no	yes	mammals
eel	no	no	yes	no	non-mammals
salamander	no	no	sometimes	yes	non-mammals
gila monster	no	no	no	yes	non-mammals
platypus	no	no	no	yes	mammals
owl	no	yes	no	yes	non-mammals
dolphin	yes	no	yes	no	mammals
eagle	no	yes	no	yes	non-mammals

M: mammals; N: non-mammals

Give Birth	Can Fly	Live in Water	Have Legs	Class
yes	no	yes	no	?

- Conditional probability:

$$P(\boldsymbol{x}|M) = \frac{6}{7} \times \frac{6}{7} \times \frac{2}{7} \times \frac{2}{7} = 0.06$$

$$P(\boldsymbol{x}|N) = \frac{1}{13} \times \frac{10}{13} \times \frac{3}{13} \times \frac{4}{13}$$
$$= 0.0042$$

$$P(\boldsymbol{x}|M)P(M) = 0.06 \times \frac{7}{20}$$
$$= 0.021$$

$$P(\boldsymbol{x}|N)P(N) = 0.004 \times \frac{13}{20}$$
$$= 0.0027$$

$$P(\boldsymbol{x}|M)P(M) > P(\boldsymbol{x}|N)P(N)$$
$$\Rightarrow \ Mammals$$

Avoiding the Zero-probability Problem

- Naïve Bayesian prediction requires each conditional probability be non-zero; otherwise, the predicted probability will be zero

$$P(\boldsymbol{x}|y_j) = \prod_{i=1}^{K} P(x_i|y_j)$$

- Corrected probability are used

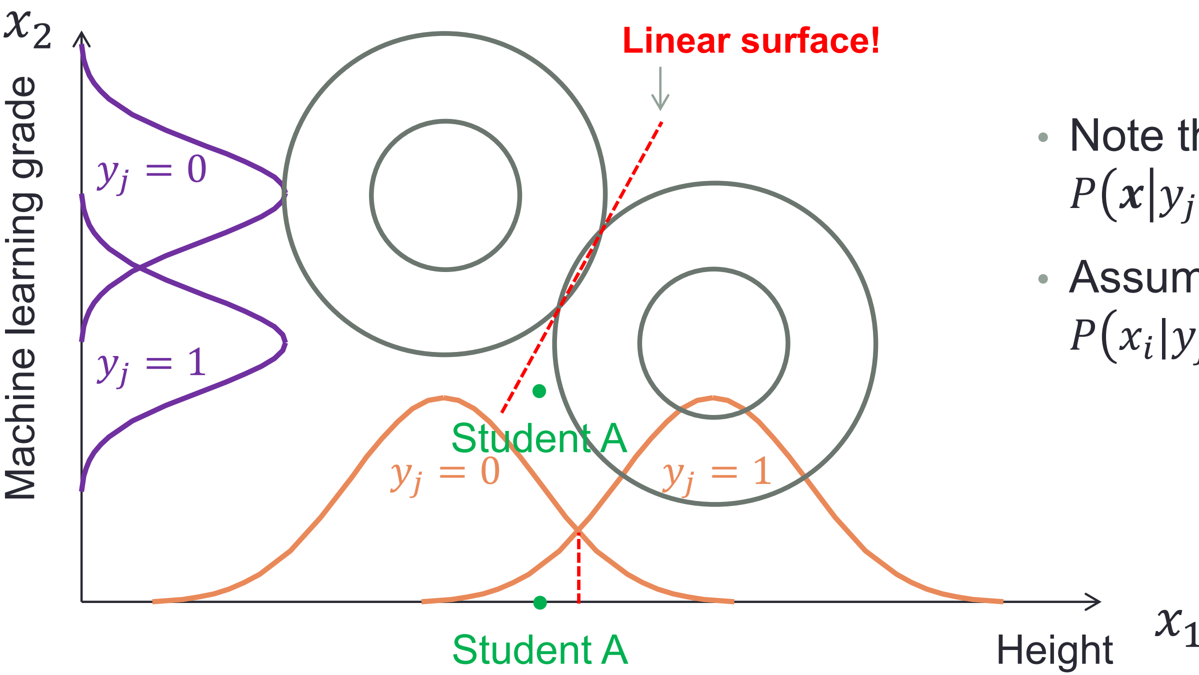
Laplace: $P(x_i|y_j) = \frac{N_{ij}+1}{N_j+|y|}$

m-estimate: $P(x_i|y_j) = \frac{N_{ij}+mp}{N_j+m}$

where $|y|$ is number of classes, p is a predetermined parameter, and m is the equivalent sample size

Geometric Interpretation of Naïve Bayes

- Consider boolean y_j, x_i normally distributed, and $P(y_j = 1) = 0.5$
- Naïve Bayes: $y = \arg\max_{y} P(y_j = y) \prod_{i=1}^{K} P(x_i | y_j = y)$



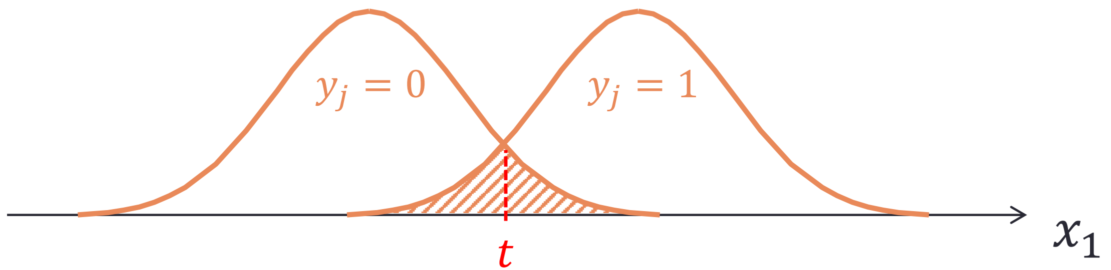
- Note that $P(\boldsymbol{x}|y_j) = \prod_{i=1}^{K} P(x_i|y_j)$
- Assume $P(x_i|y_j) \sim N(\mu_{ij}, \sigma)$

The Minimum Possible Error

- Conditional independence assumption is satisfied
- Assume that we know $P(x_i|y_j)$, and $P(y_j = 1) = 0.5$

$$P(err) = P(\text{pred } y_j = 1 \text{ but } y_j = 0) + P(\text{pred } y_j = 0 \text{ but } y_j = 1)$$

$$= \int_{-\infty}^{t} P(x_1|\, y_j = 1)\, P(\, y_j = 1) + \int_{t}^{\infty} P(x_1|\, y_j = 0)\, P(\, y_j = 0)$$



Naïve Bayes Summary

- Assumption of independently continuous distribution may not hold for some attributes
- Easy to implement
- Robust to isolated noise points
- Can handle missing values by ignoring the instance during probability estimate calculations
- Robust to irrelevant attributes

Logistic Regression Problem Definition

- Objective: estimate $P\left(y_j \middle| \boldsymbol{x}\right) = f(\boldsymbol{x})$ for given $\boldsymbol{x} \in \Re^K$
- Strategy: follow naïve Bayes rule
- Assumptions:
  - y is Boolean (i.e., $y = 1$ or 0)
  - $P(y = 1) = \gamma$ and $P(y = 0) = 1 - \gamma$
  - All x_i are conditionally independent for given y
  - $P\left(x_i \middle| y_j\right) \sim N(\mu_{ij}, \sigma_i)$, i.e., Gaussian distributed

Logistic Regression Derivation

- Bayes rule indicates that

$$\boxed{P(y=1|\boldsymbol{x})} = \frac{P(\boldsymbol{x}|y=1)P(y=1)}{P(\boldsymbol{x}|y=1)P(y=1)+P(\boldsymbol{x}|y=0)P(y=0)}$$

$$= \frac{1}{1+\frac{P(\boldsymbol{x}|y=0)P(y=0)}{P(\boldsymbol{x}|y=1)P(y=1)}} = \frac{1}{1+\exp(\ln\left(\frac{P(\boldsymbol{x}|y=0)P(y=0)}{P(\boldsymbol{x}|y=1)P(y=1)}\right))}$$

$$= \frac{1}{1+\exp(\ln\left(\frac{P(y=0)}{P(y=1)}\right)+\ln\left(\sum_i \frac{P(x_i|y=0)}{P(x_i|y=1)}\right))}$$

$$= \frac{1}{1+\exp(\ln\left(\frac{1-\gamma}{\gamma}\right)+\boxed{\sum_i \ln\left(\frac{P(x_i|y=0)}{P(x_i|y=1)}\right)})}$$

Logistic Regression Derivation (Cont'd)

$$\boxed{\sum_i \ln\left(\frac{P(x_i|y=0)}{P(x_i|y=1)}\right)} = \sum_i \ln\left(\frac{\frac{1}{\sqrt{2\pi\sigma_i^2}}\exp\left(\frac{-(x_i-\mu_{i0})^2}{2\sigma_i^2}\right)}{\frac{1}{\sqrt{2\pi\sigma_i^2}}\exp\left(\frac{-(x_i-\mu_{i1})^2}{2\sigma_i^2}\right)}\right)$$

$$= \sum_i \ln\left(\exp\left(\frac{(x_i-\mu_{i1})^2-(x_i-\mu_{i0})^2}{2\sigma_i^2}\right)\right)$$

$$= \sum_i \frac{(x_i^2-2x_i\mu_{i1}+\mu_{i1}^2)-(x_i^2-2x_i\mu_{i0}+\mu_{i0}^2)}{2\sigma_i^2}$$

$$= \sum_i \left(\frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}x_i + \frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}\right)$$

Logistic Regression Derivation (Cont'd)

$$\boxed{P(y=1|\boldsymbol{x})} = \frac{1}{1+\exp\left(\ln\left(\frac{1-\gamma}{\gamma}\right) + \boxed{\sum_i \left(\frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}x_i + \frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}\right)}\right)}$$

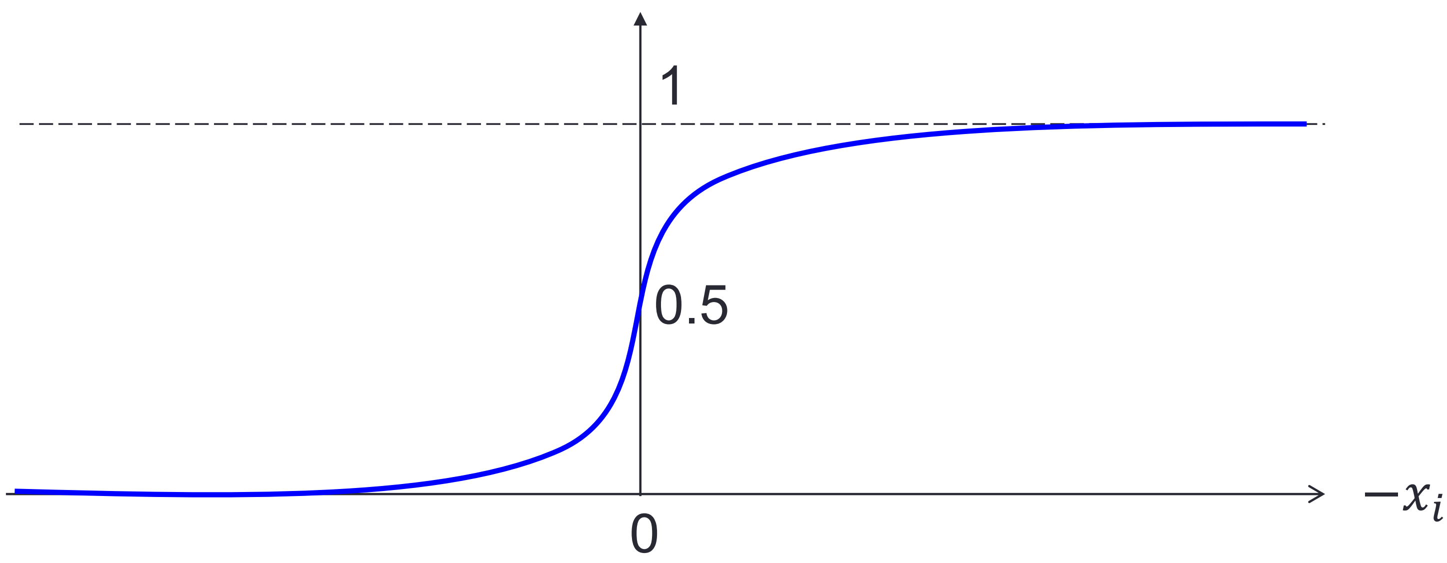
$$= \frac{1}{1+\exp(w_0 + \sum_{i=1}^{K} w_i x_i)}$$ ⇐ *A sigmoid equation!*

where $w_0 = \ln\left(\frac{1-\gamma}{\gamma}\right) + \sum_i \left(\frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}\right),\quad w_i = \frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}$

$$\Rightarrow \quad \underline{P(y=0|\boldsymbol{x})} = 1 - \boxed{P(y=1|\boldsymbol{x})} = \frac{\exp(w_0 + \sum_{i=1}^{K} w_i x_i)}{1+\exp(w_0 + \sum_{i=1}^{K} w_i x_i)}$$

Logistic Function

$$P(y = 1|\boldsymbol{x}) = \frac{1}{1 + \exp(\sum_{i=1}^{K} w_i x_i)}$$



Logistic Regression Derivation (Cont'd)

- This indicates:

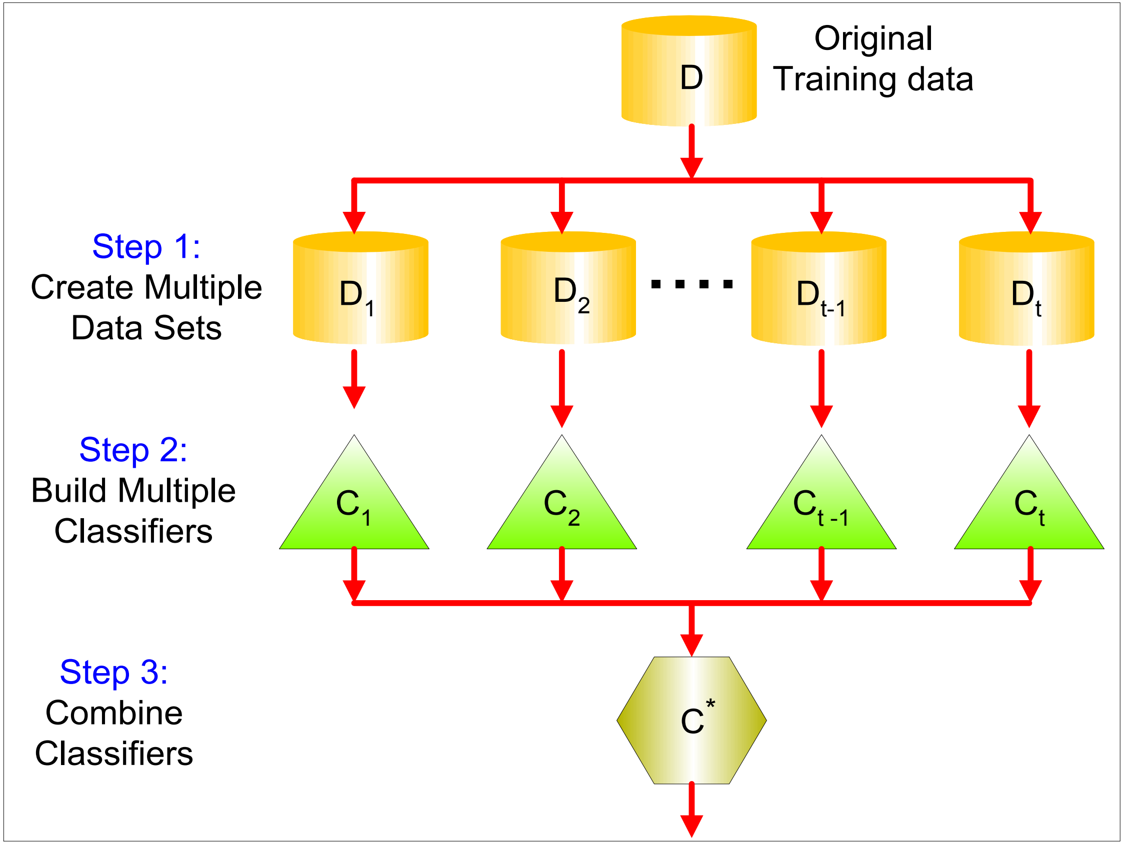
$$\frac{P(y=0|\boldsymbol{x})}{P(y=1|\boldsymbol{x})} = \exp(w_0 + \sum_{i=1}^{K} w_i x_i)$$

which implies

$$\ln\left(\frac{P(y=0|\boldsymbol{x})}{P(y=1|\boldsymbol{x})}\right) = w_0 + \sum_{i=1}^{K} w_i x_i$$

Ensemble Methods

- General idea: combine <u>multiple classifiers</u>



Why Does It Work?

- Suppose there are 25 “base” classifiers
- Each classifier has an error rate $\varepsilon = 0.35$
- Assume classifiers are independent
- The ensemble makes a wrong prediction only if more than half of the base classifiers predict incorrectly
- Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^{i} (1-\varepsilon)^{25-i} = 0.06$$

Typical Ensemble Methods

- Bagging (by Leo Breiman):

  Resampling, i.e., generating new training samples from the original sample set, based on uniform distribution

- Boosting:

  Adaptively changes the weights of samples in resampling to tackle those "hard to classify" samples

Bagging

- Sample with replacement from the original data set according to a uniform probability distribution
- Examples chosen during each bagging:

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

- Build classifier on each bagging sample set
- A particular training data has a probability of $1 - 1/N$ of not being picked, where N is number of samples
- A sample has probability $1 - (1 - 1/N)^N$ of being selected
- The probability is equal to 0.632 if $N \to \infty$, so this method is also called 0.632 bootstrap

Boosting

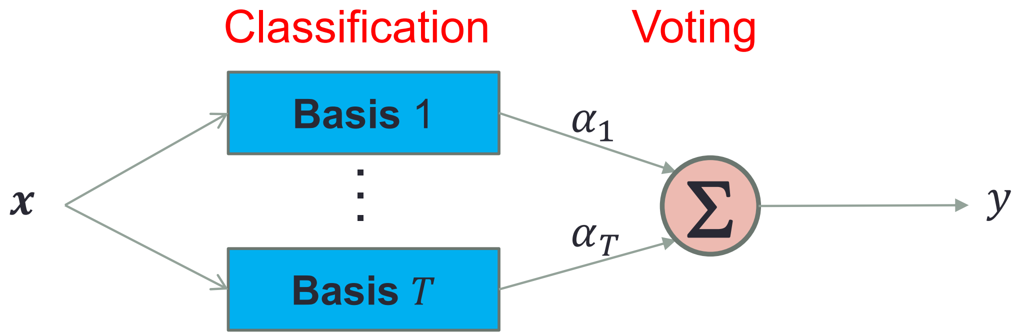
- Sample with replacement from the original data set
- Iteratively change distribution of training data by focusing more on previously misclassified records
- Initially, all n records are assigned equal weights
- Records that are <u>wrongly classified</u> will have their weights increased in the future iteration

Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

Example 4 is hard to classify

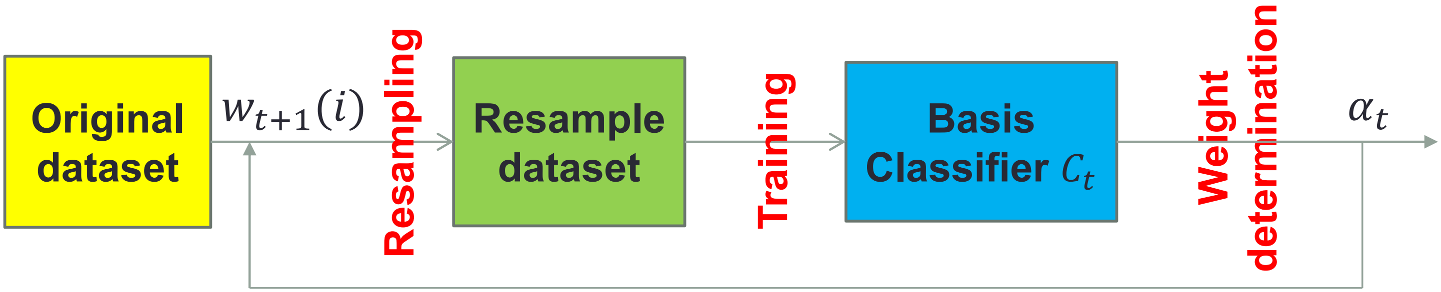
Adaptive Boosting (AdaBoost) Classifier

- Suppose there exists T "basis" classifiers C_t, $t = 1 \dots T$
- Each classifier is associated with a weight α_t
- For a query input $\boldsymbol{x}$, the output y is determined by weighted majority voting:



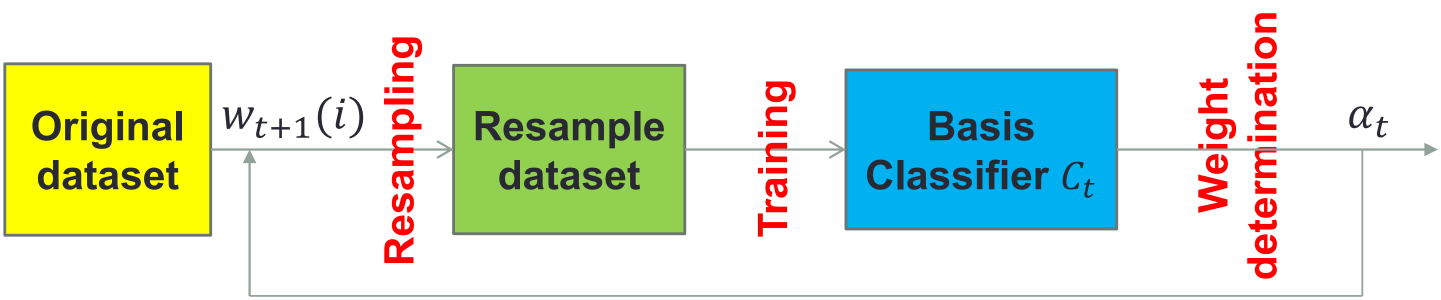
Basis Classifier Training

- Let $\{(\boldsymbol{x}_i, y_i) | i = 1 \dots N\}$ denote a set of samples, $y_i = \{+1, -1\}$
- Objective: generate basis classifiers $C_t, t = 1 \dots T$
- The basis classifiers are developed iteratively
- In each iteration, data points are sampled with replacement using weight $w_t(i)$
- The initial sample weights $w_1(i) = \frac{1}{N}, i = 1 \dots N$



Basis Classifier Training Steps

- Determine the follows in each iteration
    1. The error rate ε_t for the basis classifier C_t
    2. The weights α_t for the basis classifier C_t
    3. The resampling weights w_{t+1} for the next iteration



Basis Classifier Error Rate ε_t

- The (misclassification) error rate of a base classifier C_t is:

$$\varepsilon_t = \frac{1}{N}\sum_{i=1}^{N} w_t(i) I(C_t(\boldsymbol{x}_i) \neq y_i)$$

where $w_t(i) \in \Re$ is the weight assigned to sample $(\boldsymbol{x}_i, y_i)$,

$$\begin{cases} I(p) = 1 & \text{when } p \text{ is true} \\ I(p) = 0 & \text{otherwise} \end{cases},$$

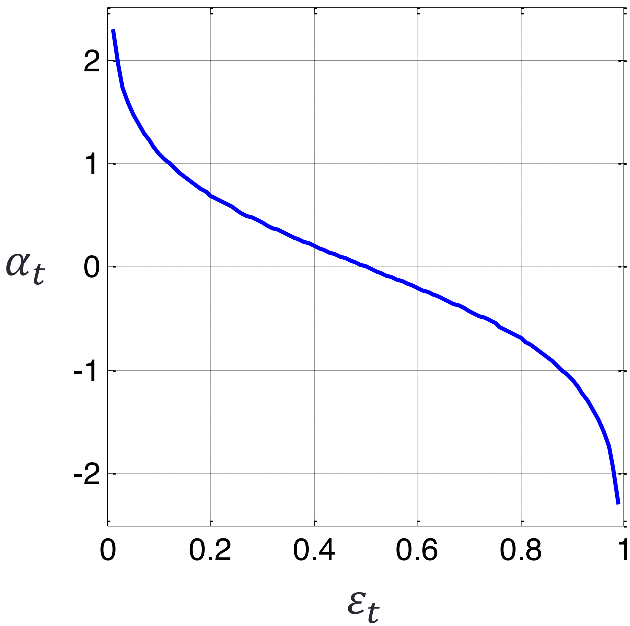
- Note that $0 \leq \varepsilon_t \leq 1$

Basis Classifier Weight α_t

- The weight $\alpha_t \in \Re$ of a basis classifier C_t is defined as

$$\alpha_t = \frac{1}{2}\ln\left(\frac{1-\varepsilon_t}{\varepsilon_t}\right)$$

- The lower a base classifier's error rate ε_t, the higher its weight α_t for voting



Resampling Sample Weights $w_{t+1}(i)$

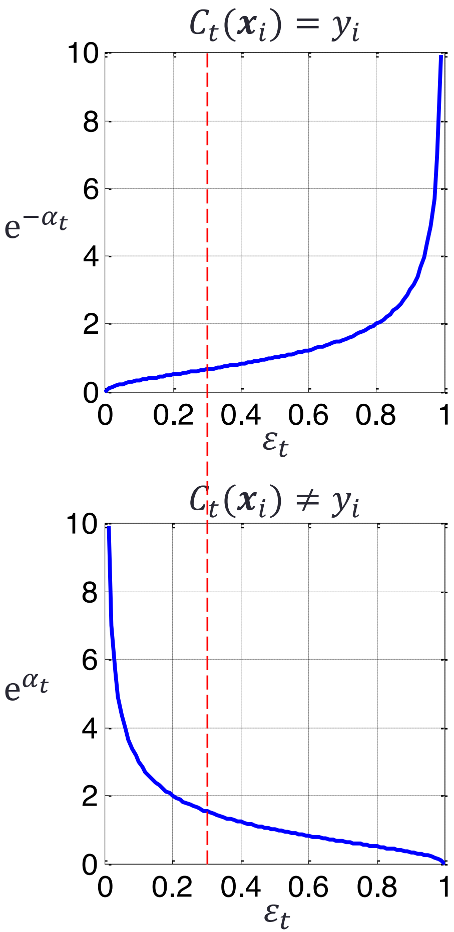
- The weights of sample $(\boldsymbol{x}_i, y_i)$ for next iteration is

$$w_{t+1}(\mathrm{i}) = \frac{w_t(i)}{z_t}\begin{cases} \mathrm{e}^{-\alpha_t} & \text{if } C_t(\boldsymbol{x}_i) = y_i \\ \mathrm{e}^{\alpha_t} & \text{if } C_t(\boldsymbol{x}_i) \neq y_i \end{cases}$$

where z_t is a normalization factor that ensures

$$\sum_i w_{t+1}(i) = 1$$

- The weights of incorrectly classified samples is increased

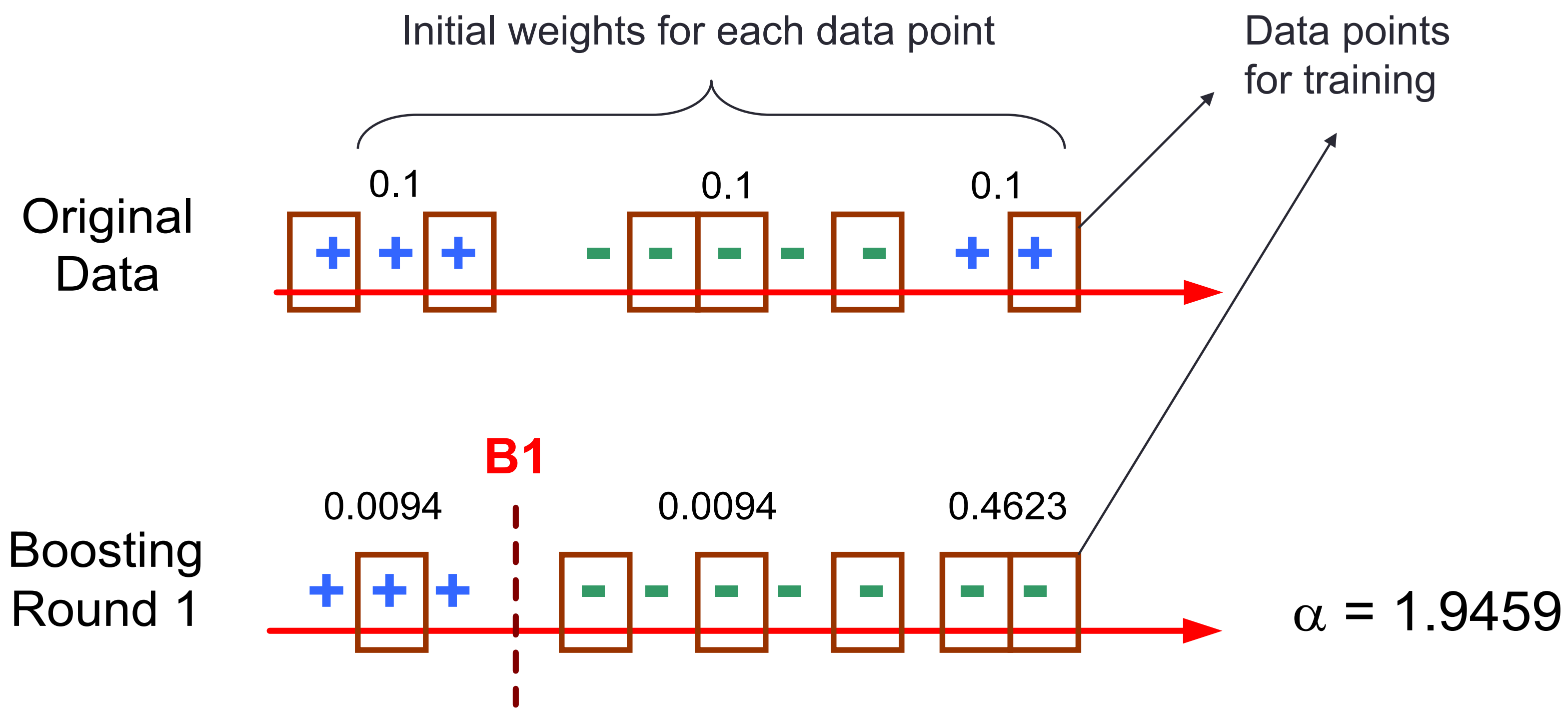


AdaBoost Classifier

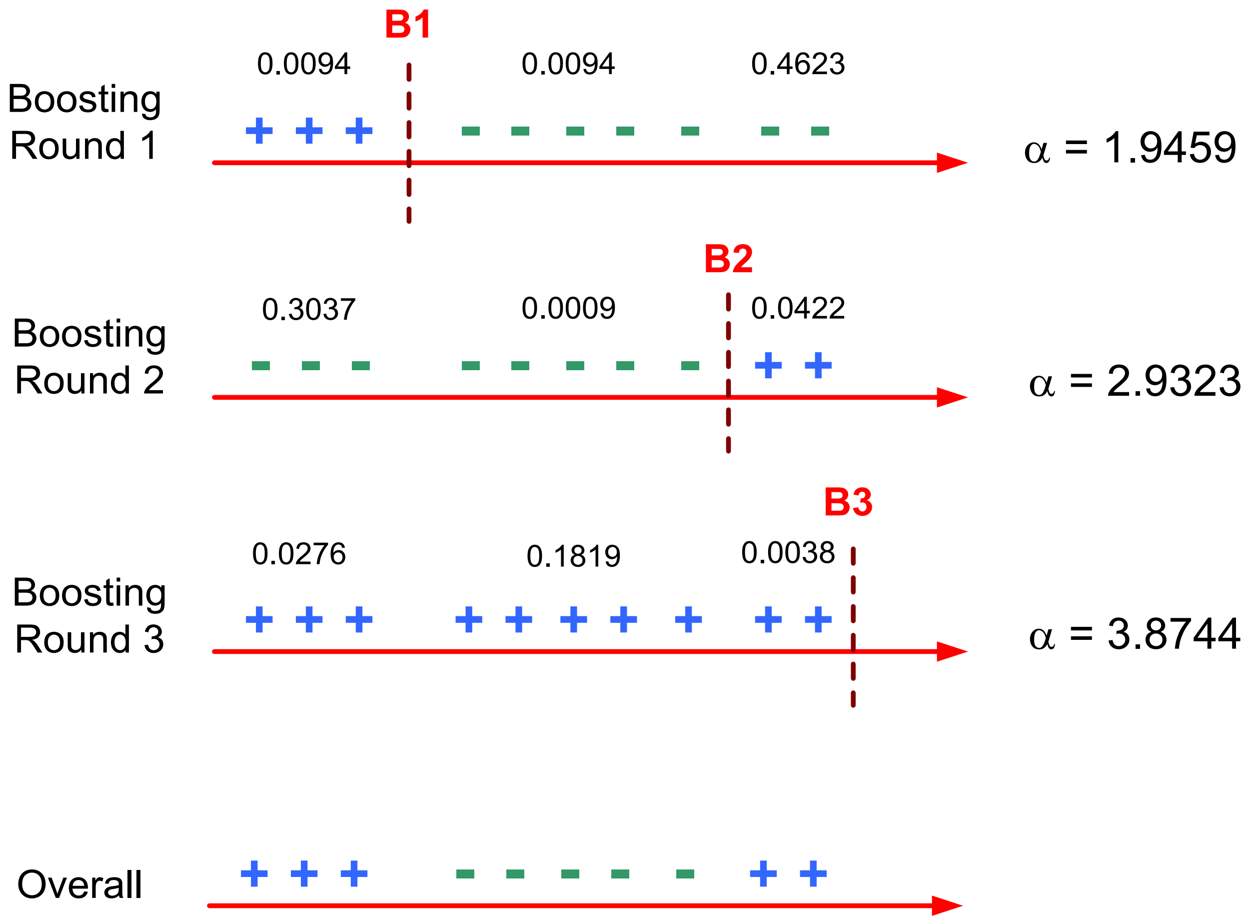
- Output is determined by weighted majority voting:

$$C^*(\boldsymbol{x}) = \arg\max_y \sum_{t=1}^{T} \alpha_t I(C_t(\boldsymbol{x}) = y)$$

Illustrating AdaBoost



Illustrating AdaBoost



Ensemble Method Summary

- Ensemble methods use multiple models to obtain better predictive performance
- Bagging increases prediction accuracy because it reduces the variance of the individual classifier

Acknowledgement

- Especially thank Dr. Tom Mitchell for sharing his valuable teaching material in this course

References

- P. Tan, M. Steinbach, and V. Kumar, *Introduction to Data Mining*