Artificial Intelligence and Machine Learning (IS353IA)

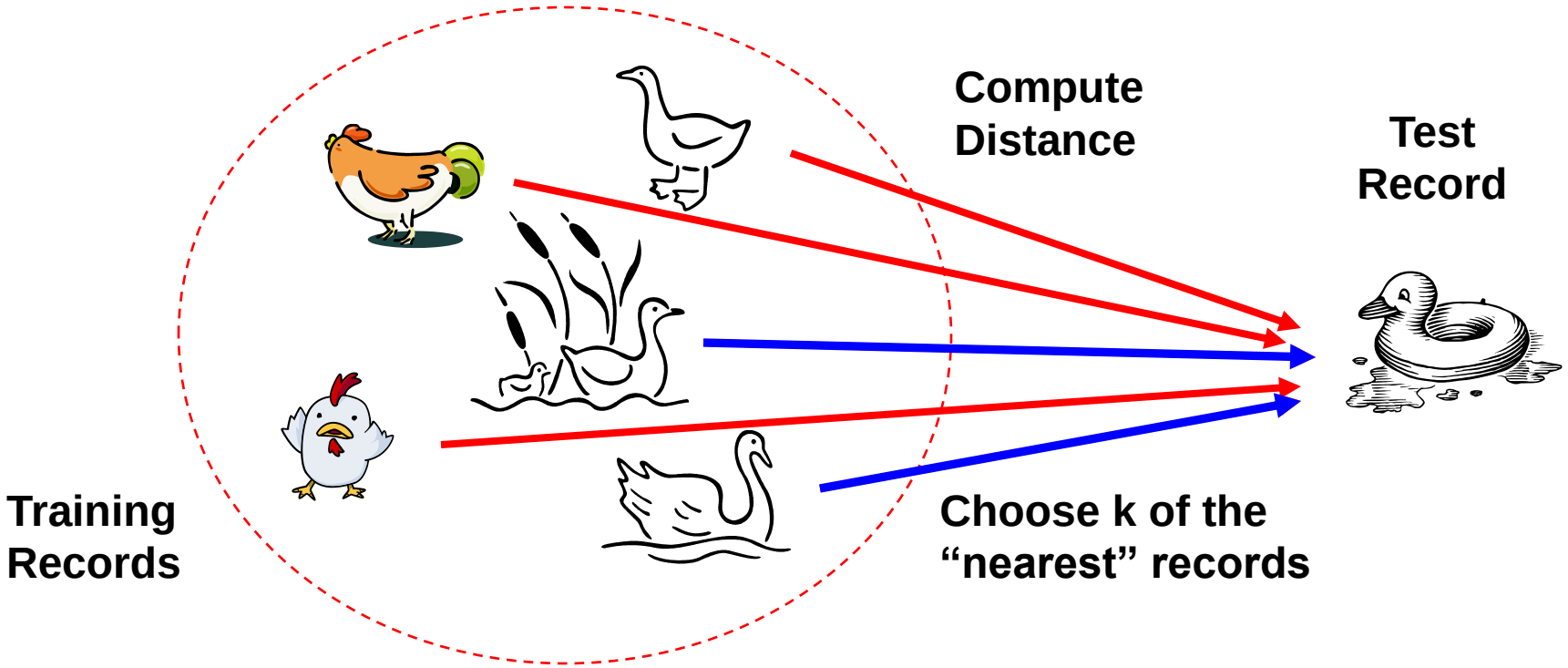
Unit-IV

Contents

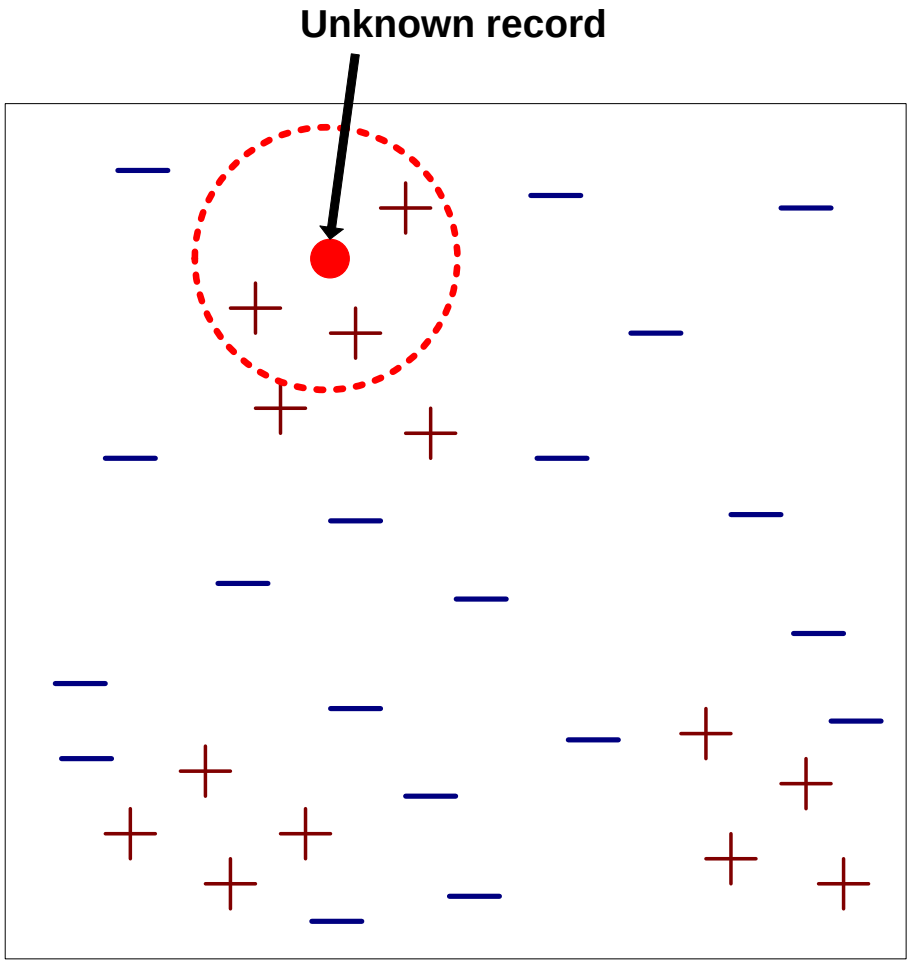
- Nearest Neighbor Classifiers
- Naive Bayes Classifier
- Logistic Regression
- Ensemble Methods

Nearest Neighbor Classifiers

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it's probably a duck



Nearest-Neighbor Classifiers



- Requires the following:
  - A set of labeled records
  - Proximity metric to compute distance/similarity between a pair of records
    - e.g., Euclidean distance
  - The value of *k*, the number of nearest neighbors to retrieve
  - A method for using class labels of K nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

How to Determine the class label of a Test Sample?

- Take the majority vote of class labels among the k-nearest neighbors
- Weight the vote according to distance
  - weight factor, $w = 1/d^2$

Choice of proximity measure matters

- For documents, cosine is better than correlation or Euclidean

1 1 1 1 1 1 1 1 1 1 1 0		0 0 0 0 0 0 0 0 0 0 0 1
	vs	
0 1 1 1 1 1 1 1 1 1 1 1		1 0 0 0 0 0 0 0 0 0 0 0

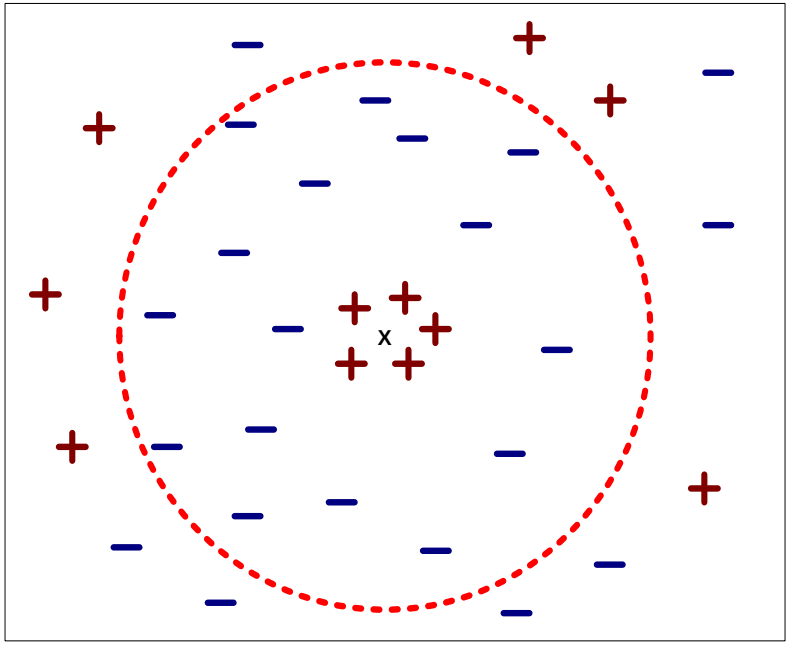
Euclidean distance = 1.4142 for both pairs, but the cosine similarity measure has different values for these pairs.

Nearest Neighbor Classification…

- **Data preprocessing is often required**
  - 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
  - Time series are often standardized to have 0 means a standard deviation of 1

Nearest Neighbor Classification…

- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes

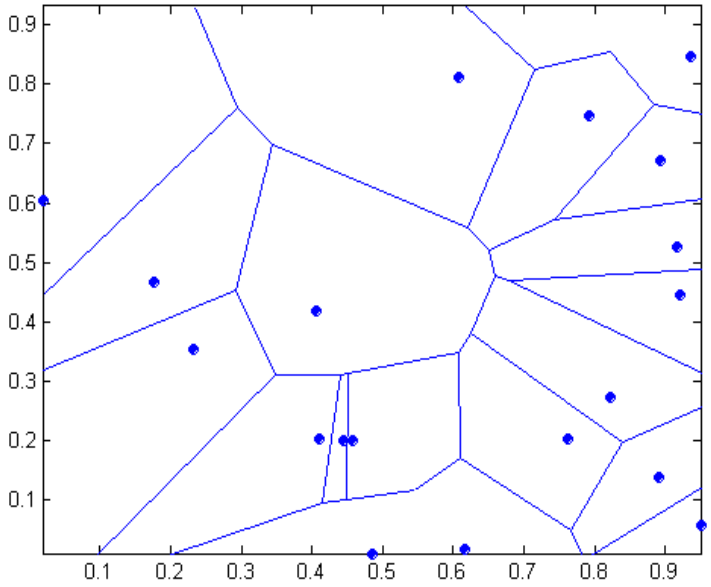


Nearest-neighbor classifiers

- Nearest neighbor classifiers are local classifiers

- They can produce decision boundaries of arbitrary shapes.

1-nn decision boundary is a Voronoi Diagram

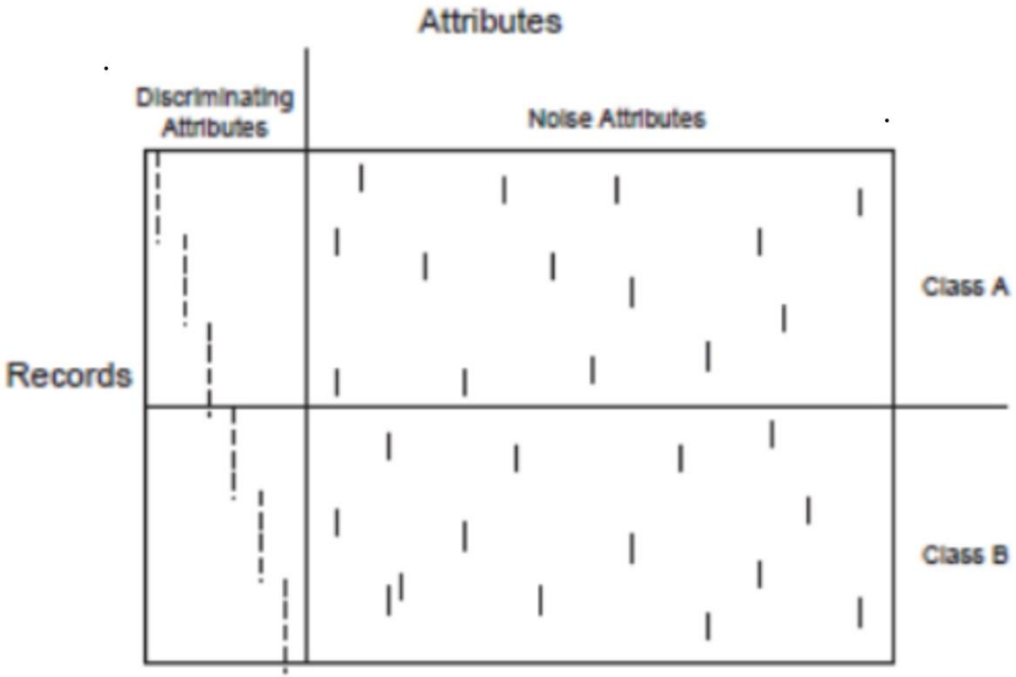


Nearest Neighbor Classification…

- **How to handle missing values in training and test sets?**
  - Proximity computations normally require the presence of all attributes
  - Some approaches use the subset of attributes present in two instances
    - This may not produce good results since it effectively uses different proximity measures for each pair of instances
    - Thus, proximities are not comparable

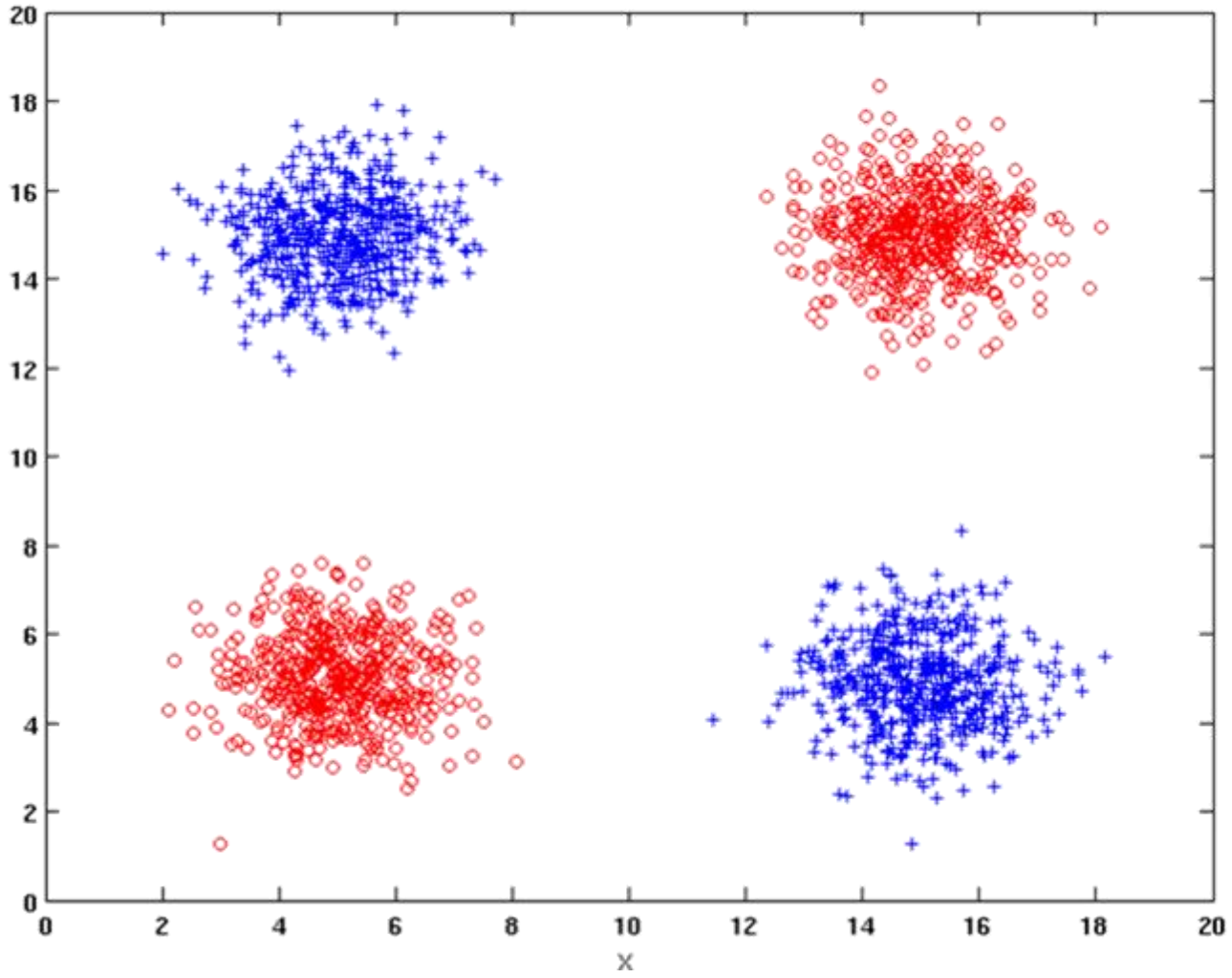
Handling Irrelevant and Redundant Attributes

- Irrelevant attributes add noise to the proximity measure
- Redundant attributes bias the proximity measure towards certain attributes

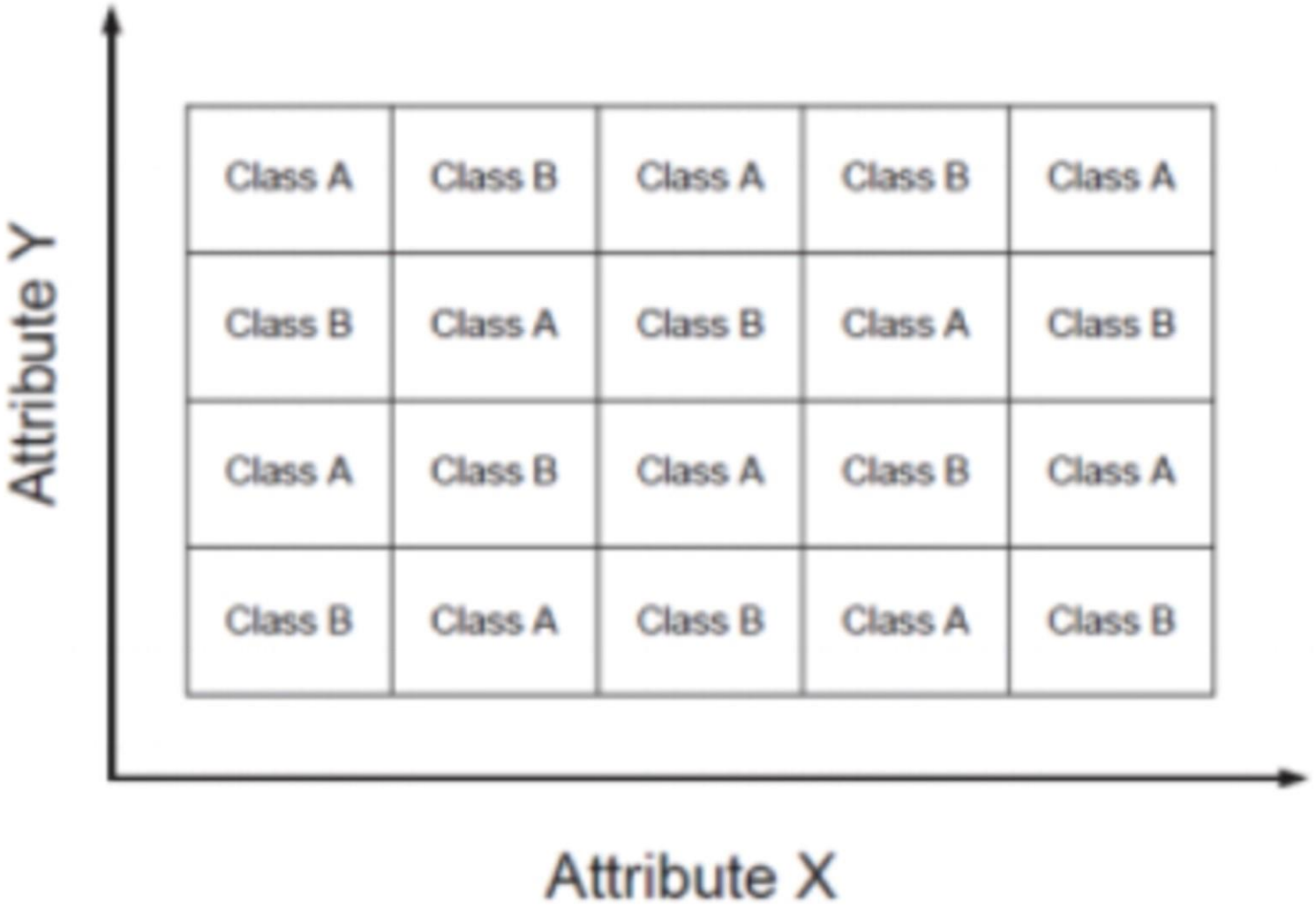


(a) Synthetic data set 1.

K-NN Classifiers: Handling attributes that are interacting



Handling attributes that are interacting



Improving KNN Efficiency

- Avoid having to compute distance to all objects in the training set
  - Multi-dimensional access methods (k-d trees)
  - Fast approximate similarity search
  - Locality Sensitive Hashing (LSH)
- Condensing
  - Determine a smaller set of objects that give the same performance
- Editing
  - Remove objects to improve efficiency

Naive Bayes Classifier

Bayes Classifier

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

$$P(Y \mid X) = \frac{P(X, Y)}{P(X)}$$

$$P(X \mid Y) = \frac{P(X, Y)}{P(Y)}$$

- Bayes theorem:

$$P(Y \mid X) = \frac{P(X \mid Y)P(Y)}{P(X)}$$

Using Bayes Theorem for Classification

- Consider each attribute and class label as random variables
- Given a record with attributes (X_1, X_2,…, X_d), the goal is to predict class Y
  - Specifically, we want to find the value of Y that maximizes $P(Y| X_1, X_2,…, X_d)$
- Can we estimate $P(Y| X_1, X_2,…, X_d)$ directly from data?

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

Using Bayes Theorem for Classification

- Approach:
  - compute posterior probability $P(Y \mid X_1, X_2, \ldots, X_d)$ using the Bayes theorem

$$P(Y \mid X_1 X_2 \ldots X_n) = \frac{P(X_1 X_2 \ldots X_d \mid Y) P(Y)}{P(X_1 X_2 \ldots X_d)}$$

  - *Maximum a-posteriori*: Choose Y that maximizes
    $P(Y \mid X_1, X_2, \ldots, X_d)$
  - Equivalent to choosing value of Y that maximizes
    $P(X_1, X_2, \ldots, X_d \mid Y)\, P(Y)$

- How to estimate $P(X_1, X_2, \ldots, X_d \mid Y)$?

Example Data

Given a Test Record:

$$X = (\text{Refund} = \text{No}, \text{Divorced}, \text{Income} = 120\text{K})$$

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

- We need to estimate

  P(Evade = Yes | X) and P(Evade = No | X)

  In the following we will replace

  Evade = Yes by Yes, and

  Evade = No by No

Example Data

Given a Test Record:

$$X = (\text{Refund} = \text{No}, \text{Divorced}, \text{Income} = 120\text{K})$$

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
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7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Using Bayes Theorem:

- $P(\text{Yes} \mid X) = \dfrac{P(X \mid \text{Yes})P(\text{Yes})}{P(X)}$
- $P(\text{No} \mid X) = \dfrac{P(X \mid \text{No})P(\text{No})}{P(X)}$
- How to estimate $P(X \mid \text{Yes})$ and $P(X \mid \text{No})$?

Conditional Independence

- **X** and **Y** are conditionally independent given **Z** if P(**X**|**YZ**) = P(**X**|**Z**)

- Example: Arm length and reading skills
  - Young child has shorter arm length and limited reading skills, compared to adults
  - If age is fixed, no apparent relationship between arm length and reading skills
  - Arm length and reading skills are conditionally independent given age

Naïve Bayes Classifier

- Assume independence among attributes X_i when class is given:
  - $P(X_1, X_2, \ldots, X_d \mid Y_j) = P(X_1 \mid Y_j)\, P(X_2 \mid Y_j) \ldots P(X_d \mid Y_j)$
  - Now we can estimate $P(X_i \mid Y_j)$ for all X_i and Y_j combinations from the training data
  - New point is classified to Y_j if $P(Y_j) \prod P(X_i \mid Y_j)$ is maximal.

Naïve Bayes on Example Data

Given a Test Record:

$$X = (\text{Refund} = \text{No}, \text{Divorced}, \text{Income} = 120\text{K})$$

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
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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

P(X | Yes) =

P(Refund = No | Yes) x

P(Divorced | Yes) x

P(Income = 120K | Yes)

P(X | No) =

P(Refund = No | No) x

P(Divorced | No) x

P(Income = 120K | No)

Estimate Probabilities from Data

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
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7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- $P(y)$ = fraction of instances of class y
  - e.g., P(No) = 7/10,
    P(Yes) = 3/10
- For categorical attributes:

$$P(X_i = c | y) = n_c / n$$

  - where $|X_i = c|$ is number of instances having attribute value $X_i = c$ and belonging to class y
  - Examples:

P(Status=Married|No) = 4/7
P(Refund=Yes|Yes)=0

Estimate Probabilities from Data

- For continuous attributes:
  - Discretization: Partition the range into bins:
    - Replace continuous value with bin value
      - Attribute changed from continuous to ordinal
  - 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, use it to estimate the conditional probability $P(X_i|Y)$

Estimate Probabilities from Data

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
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7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Normal distribution:

$$P(X_i \mid Y_j) = \frac{1}{\sqrt{2\pi\sigma_{ij}^2}} e^{-\frac{(X_i - \mu_{ij})^2}{2\sigma_{ij}^2}}$$

  - One for each (X_i, Y_i) pair

- For (Income, Class=No):
  - If Class=No
    - sample mean = 110
    - sample variance = 2975

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

Example of Naïve Bayes Classifier

Given a Test Record:

$$X = (\text{Refund} = \text{No}, \text{Divorced}, \text{Income} = 120\text{K})$$

Naïve Bayes Classifier:

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

For Taxable Income:
If class = No: sample mean = 110
sample variance = 2975
If class = Yes: sample mean = 90
sample variance = 25

- P(X | No) = P(Refund=No | No)
  × P(Divorced | No)
  × P(Income=120K | No)
  = 4/7 × 1/7 × 0.0072 = 0.0006

- P(X | Yes) = P(Refund=No | Yes)
  × P(Divorced | Yes)
  × P(Income=120K | Yes)
  = 1 × 1/3 × 1.2 × 10^{-9} = 4 × 10^{-10}

Since P(X|No)P(No) > P(X|Yes)P(Yes)

Therefore P(No|X) > P(Yes|X)

=> Class = No

Naïve Bayes Classifier can make decisions with partial information about attributes in the test record

Even in absence of information about any attributes, we can use Apriori Probabilities of Class Variable:

Naïve Bayes Classifier:

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

For Taxable Income:
If class = No: sample mean = 110
sample variance = 2975
If class = Yes: sample mean = 90
sample variance = 25

P(Yes) = 3/10

P(No) = 7/10

If we only know that marital status is Divorced, then:

P(Yes | Divorced) = 1/3 x 3/10 / P(Divorced)

P(No | Divorced) = 1/7 x 7/10 / P(Divorced)

If we also know that Refund = No, then

P(Yes | Refund = No, Divorced) = 1 x 1/3 x 3/10 / P(Divorced, Refund = No)

P(No | Refund = No, Divorced) = 4/7 x 1/7 x 7/10 / P(Divorced, Refund = No)

If we also know that Taxable Income = 120, then

P(Yes | Refund = No, Divorced, Income = 120) = 1.2×10^{-9} x 1 x 1/3 x 3/10 / P(Divorced, Refund = No, Income = 120)

P(No | Refund = No, Divorced Income = 120) = 0.0072 x 4/7 x 1/7 x 7/10 / P(Divorced, Refund = No, Income = 120)

Issues with Naïve Bayes Classifier

Given a Test Record:

X = (Married)

Naïve Bayes Classifier:

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

For Taxable Income:
If class = No: sample mean = 110
sample variance = 2975
If class = Yes: sample mean = 90
sample variance = 25

P(Yes) = 3/10

P(No) = 7/10

P(Yes | Married) = 0 x 3/10 / P(Married)

P(No | Married) = 4/7 x 7/10 / P(Married)

Issues with Naïve Bayes Classifier

Consider the table with Tid = 7 deleted

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
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Naïve Bayes Classifier:

P(Refund = Yes | No) = 2/6
P(Refund = No | No) = 4/6
P(Refund = Yes | Yes) = 0
P(Refund = No | Yes) = 1
P(Marital Status = Single | No) = 2/6
P(Marital Status = Divorced | No) = 0
P(Marital Status = Married | No) = 4/6
P(Marital Status = Single | Yes) = 2/3
P(Marital Status = Divorced | Yes) = 1/3
P(Marital Status = Married | Yes) = 0/3
For Taxable Income:
If class = No: sample mean = 91
sample variance = 685
If class = No: sample mean = 90
sample variance = 25

Given X = (Refund = Yes, Divorced, 120K)

P(X | No) = 2/6 X 0 X 0.0083 = 0

P(X | Yes) = 0 X 1/3 X 1.2 X 10^{-9} = 0

Naïve Bayes will not be able to classify X as Yes or No!

Issues with Naïve Bayes Classifier

- If one of the conditional probabilities is zero, then the entire expression becomes zero
- Need to use other estimates of conditional probabilities than simple fractions
- Probability estimation:

original: $P(X_i = c|y) = \frac{n_c}{n}$

Laplace Estimate: $P(X_i = c|y) = \frac{n_c + 1}{n + v}$

m − estimate: $P(X_i = c|y) = \frac{n_c + mp}{n + m}$

n: number of training instances belonging to class y

n_c: number of instances with $X_i = c$ and $Y = y$

v: total number of attribute values that X_i can take

p: initial estimate of ($P(X_i = c|y)$ known apriori

m: hyper-parameter for our confidence in p

Example of Naïve Bayes Classifier

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

A: attributes

M: mammals

N: non-mammals

$$P(A \mid M) = \frac{6}{7} \times \frac{6}{7} \times \frac{2}{7} \times \frac{2}{7} = 0.06$$

$$P(A \mid N) = \frac{1}{13} \times \frac{10}{13} \times \frac{3}{13} \times \frac{4}{13} = 0.0042$$

$$P(A \mid M)P(M) = 0.06 \times \frac{7}{20} = 0.021$$

$$P(A \mid N)P(N) = 0.004 \times \frac{13}{20} = 0.0027$$

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

P(A|M)P(M) > P(A|N)P(N)

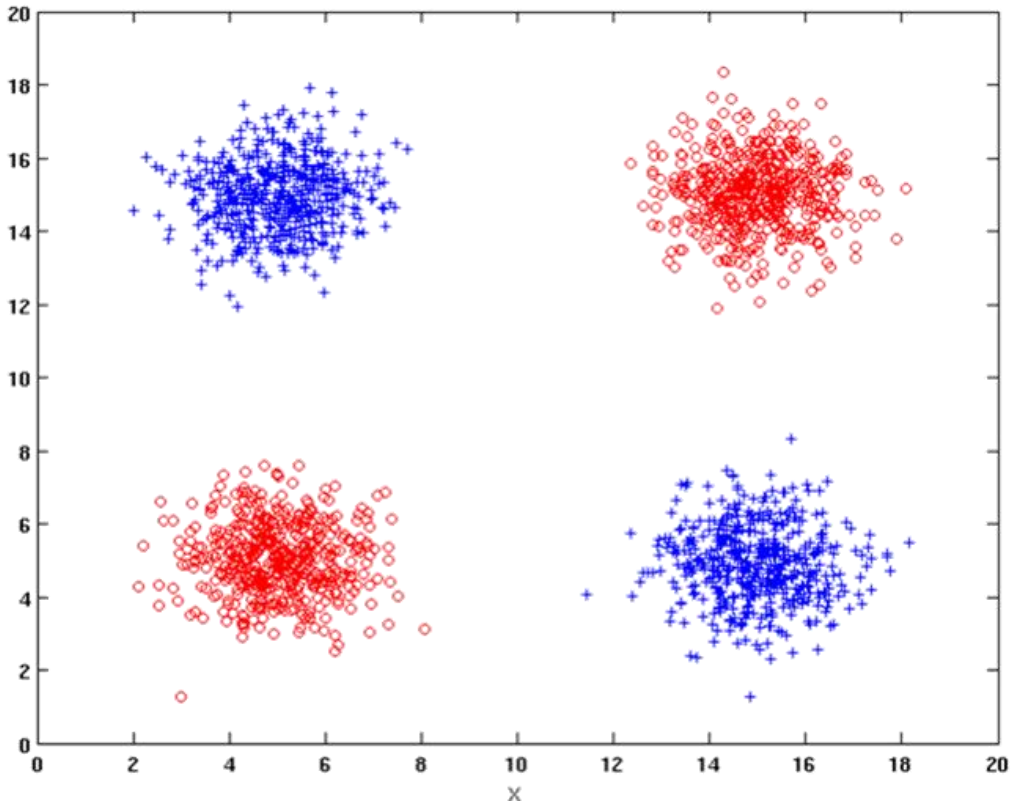
=> Mammals

Naïve Bayes (Summary)

- Robust to isolated noise points
- Handle missing values by ignoring the instance during probability estimate calculations
- Robust to irrelevant attributes
- Redundant and correlated attributes will violate class conditional assumption
  - Use other techniques such as Bayesian Belief Networks (BBN)

Naïve Bayes

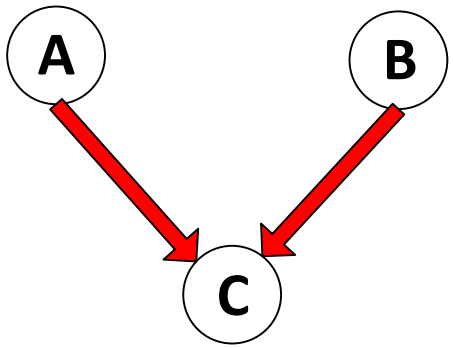
- How does Naïve Bayes perform on the following dataset?



Conditional independence of attributes is violated

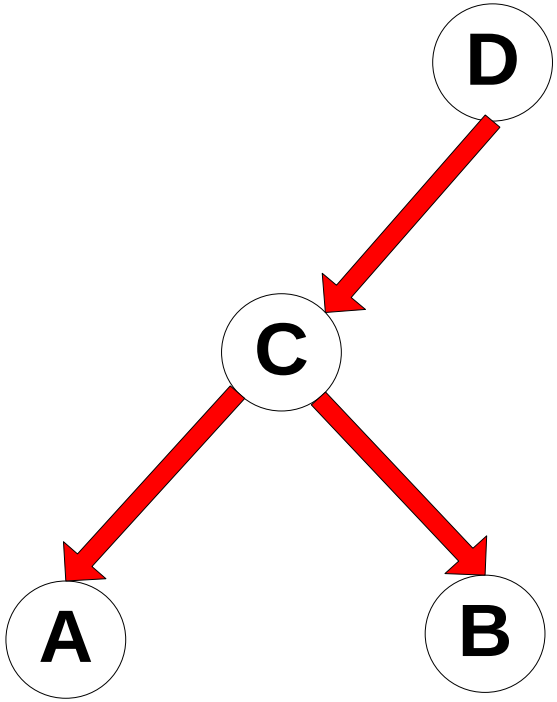
Bayesian Belief Networks

- Provides graphical representation of probabilistic relationships among a set of random variables
- Consists of:
  - A directed acyclic graph (dag)
    - Node corresponds to a variable
    - Arc corresponds to dependence relationship between a pair of variables



  - A probability table associating each node to its immediate parent

Conditional Independence



D is parent of C

A is child of C

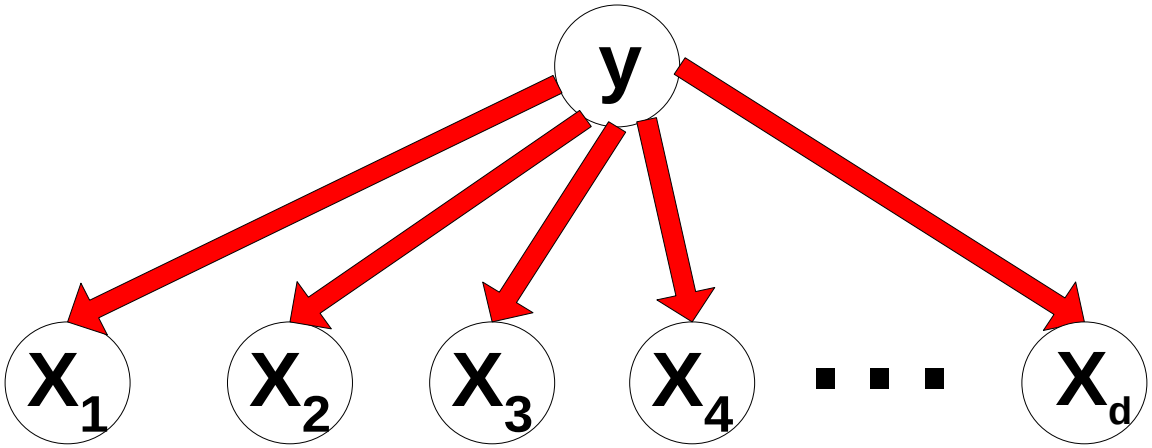
B is descendant of D

D is ancestor of A

- A node in a Bayesian network is conditionally independent of all of its nondescendants, if its parents are known

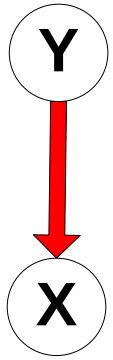
Conditional Independence

- Naïve Bayes assumption:



Probability Tables

- If X does not have any parents, table contains prior probability P(X)



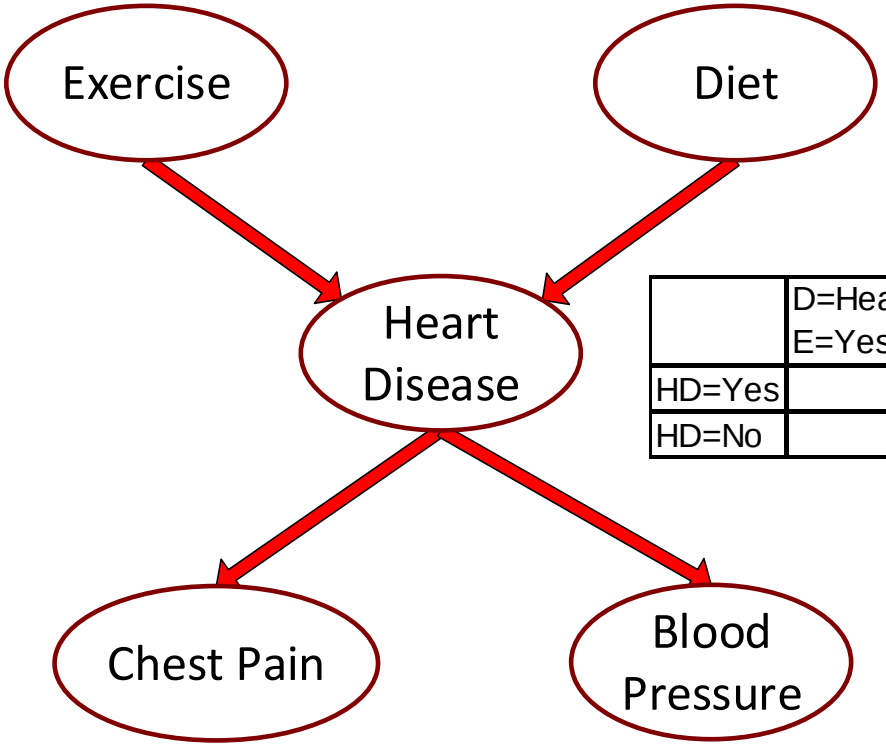
- If X has only one parent (Y), table contains conditional probability P(X|Y)

- If X has multiple parents (Y_1, Y_2,…, Y_k), table contains conditional probability P(X|Y_1, Y_2,…, Y_k)

Example of Bayesian Belief Network

Exercise=Yes	0.7
Exercise=No	0.3

Diet=Healthy	0.25
Diet=Unhealthy	0.75



	D=Healthy E=Yes	D=Healthy E=No	D=Unhealthy E=Yes	D=Unhealthy E=No
HD=Yes	0.25	0.45	0.55	0.75
HD=No	0.75	0.55	0.45	0.25

	HD=Yes	HD=No
CP=Yes	0.8	0.01
CP=No	0.2	0.99

	HD=Yes	HD=No
BP=High	0.85	0.2
BP=Low	0.15	0.8

Example of Inferencing using BBN

- Given: X = (E=No, D=Yes, CP=Yes, BP=High)
  - Compute P(HD|E,D,CP,BP)?

- P(HD=Yes| E=No,D=Yes) = 0.55
  P(CP=Yes| HD=Yes) = 0.8
  P(BP=High| HD=Yes) = 0.85
  - P(HD=Yes|E=No,D=Yes,CP=Yes,BP=High)
    $\propto 0.55 \times 0.8 \times 0.85 = 0.374$

- P(HD=No| E=No,D=Yes) = 0.45
  P(CP=Yes| HD=No) = 0.01
  P(BP=High| HD=No) = 0.2
  - P(HD=No|E=No,D=Yes,CP=Yes,BP=High)
    $\propto 0.45 \times 0.01 \times 0.2 = 0.0009$

Classify X as Yes

Logistic Regression

Logistic Model

Logistic model (or **logit model**) is a statistical model that models the probability of an event taking place by having the log-odds for the event be a linear combination of one or more independent variables.

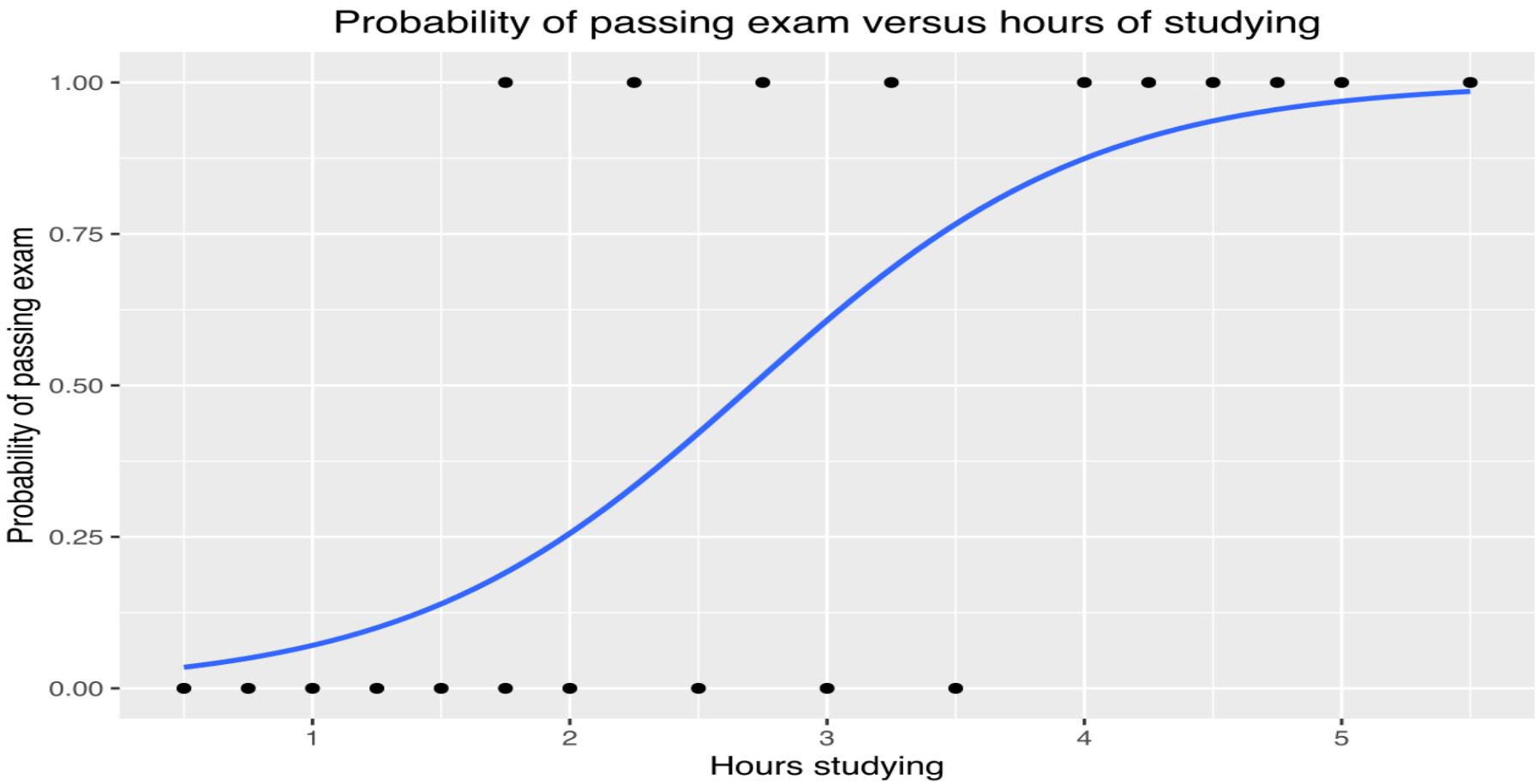
The logistic function is of the form:

$$p(x) = \frac{1}{1 + e^{-(x-\mu)/s}}$$

where μ is a location parameter (the midpoint of the curve, where $p(\mu) = 1/2$) and s is a scale parameter. This expression may be rewritten as:

$$p(x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$

An example curve



Example graph of a logistic regression curve fitted to data. The curve shows the probability of passing an exam (binary dependent variable) versus hours studying (scalar independent variable).

Logistic Regression

- Logistic regression is a probabilistic discriminative model that directly estimates the odds of a data instance a using its attribute values.
- Basic idea is to use linear predictor, z = wT x + b, for representing the odds of x as follows:

$$\frac{P(y=1|\mathbf{x})}{P(y=0|\mathbf{x})} = e^{z} = e^{\mathbf{w}^T\mathbf{x}+b},$$

where w and b are the parameters of the model and aT denotes the transpose of a vector a. Note that if wT x + b > 0, then x belongs to class 1 since its odds is greater than 1. Otherwise, x belongs to class 0.

Cont…

Since P(y = 0|x) + P(y = 1|x) = 1, we can re-write

$$\frac{P(y=1|\mathbf{x})}{1-P(y=1|\mathbf{x})} = e^{z}.$$

This can be further simplified to express P(y = 1|x) as a function of z.

$$P(y=1|\mathbf{x}) = \frac{1}{1+e^{-z}} = \sigma(z),$$

where the function σ(.) is known as the logistic or sigmoid function

Logistic Regression as a Generalized Linear Model

- Logistic regression belongs to a broader family of statistical regression models, known as generalized linear models (GLM).

$$g(\mu) = z = \mathbf{w}^T \mathbf{x} + b.$$

$$g(\mu) = \log\left(\frac{\mu}{1-\mu}\right).$$

- Even though logistic regression has relationships with regression models, it is a classification model since the computed posterior probabilities are eventually used to determine the class label of a data instance.

Learning Model Parameters

- The parameters of logistic regression, (w, b), are estimated during training using a statistical approach known as the maximum likelihood estimation (MLE) method.

$$\mathcal{L}(\mathbf{w}, b) = \prod_{i=1}^{n} P(y_i|\mathbf{x_i}, \mathbf{w}, b) = \prod_{i=1}^{n} P(y = 1|\mathbf{x_i})^{y_i} \times P(y = 0|\mathbf{x_i})^{1-y_i}.$$

Characteristics of Logistic Regression

- Discriminative model for classification.
- The learned parameters of logistic regression can be analyzed to understand the relationships between attributes and class labels.
- Can work more robustly even in high-dimensional settings
- Can handle irrelevant attributes
- Cannot handle data instances with missing values

Ensemble Techniques

Ensemble Methods

- There are techniques for improving classification accuracy by aggregating the predictions of multiple classifiers.
  - known as ***ensemble*** *or* ***classifier combination*** methods.
- An ensemble method constructs a set of **base classifiers** from training data and performs classification
  - by taking a vote on the predictions made by each base classifier.

Ensemble Methods

- Construct a set of base classifiers learned from the training data

- Predict class label of test records by combining the predictions made by multiple classifiers (e.g., by taking majority vote)

Example: Why Do Ensemble Methods Work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\epsilon = 0.35$
  - Majority vote of classifiers used for classification
  - If all classifiers are identical:
    - Error rate of ensemble = ϵ (0.35)
  - If all classifiers are independent (errors are uncorrelated):
    - Error rate of ensemble = probability of having more than half of base classifiers being wrong

$$e_{\text{ensemble}} = \sum_{i=13}^{25} \binom{25}{i} \epsilon^i (1-\epsilon)^{25-i} = 0.06$$

Necessary Conditions for Ensemble Methods

- Ensemble Methods work better than a single base classifier if:
  1. All base classifiers are independent of each other
  2. All base classifiers perform better than random guessing (error rate < 0.5 for binary classification)

Classification error for an ensemble of 25 base classifiers, assuming their errors are uncorrelated.

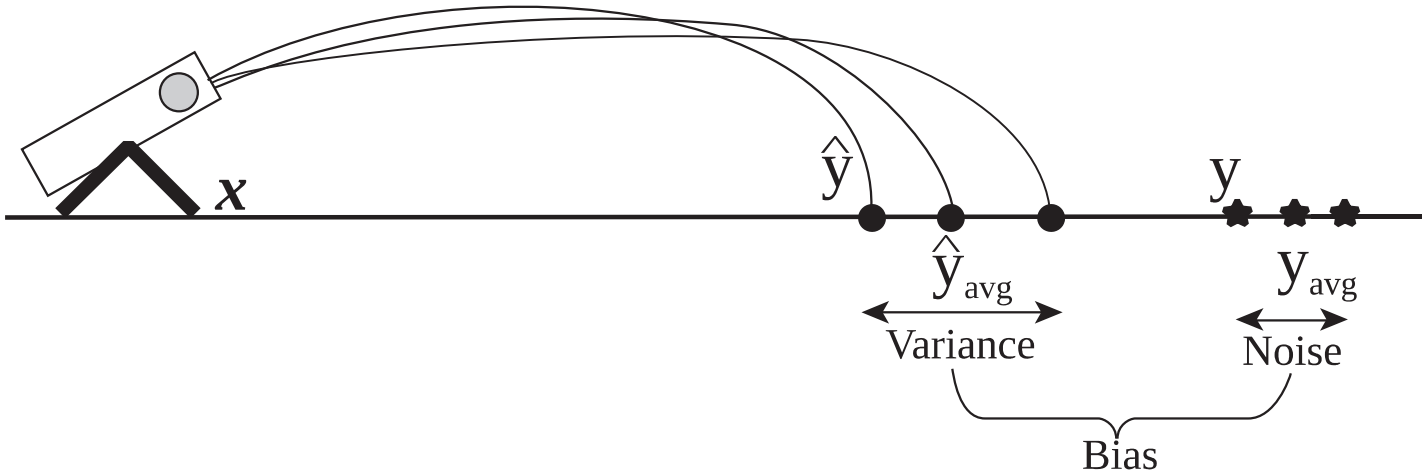
Comparison between errors of base classifiers and errors of the ensemble classifier

Rationale for Ensemble Learning

- Ensemble Methods work best with **unstable base classifiers**
  - Classifiers that are sensitive to minor perturbations in training set, due to *high model complexity*
  - Examples: Unpruned decision trees, ANNs, …

Bias-Variance Decomposition

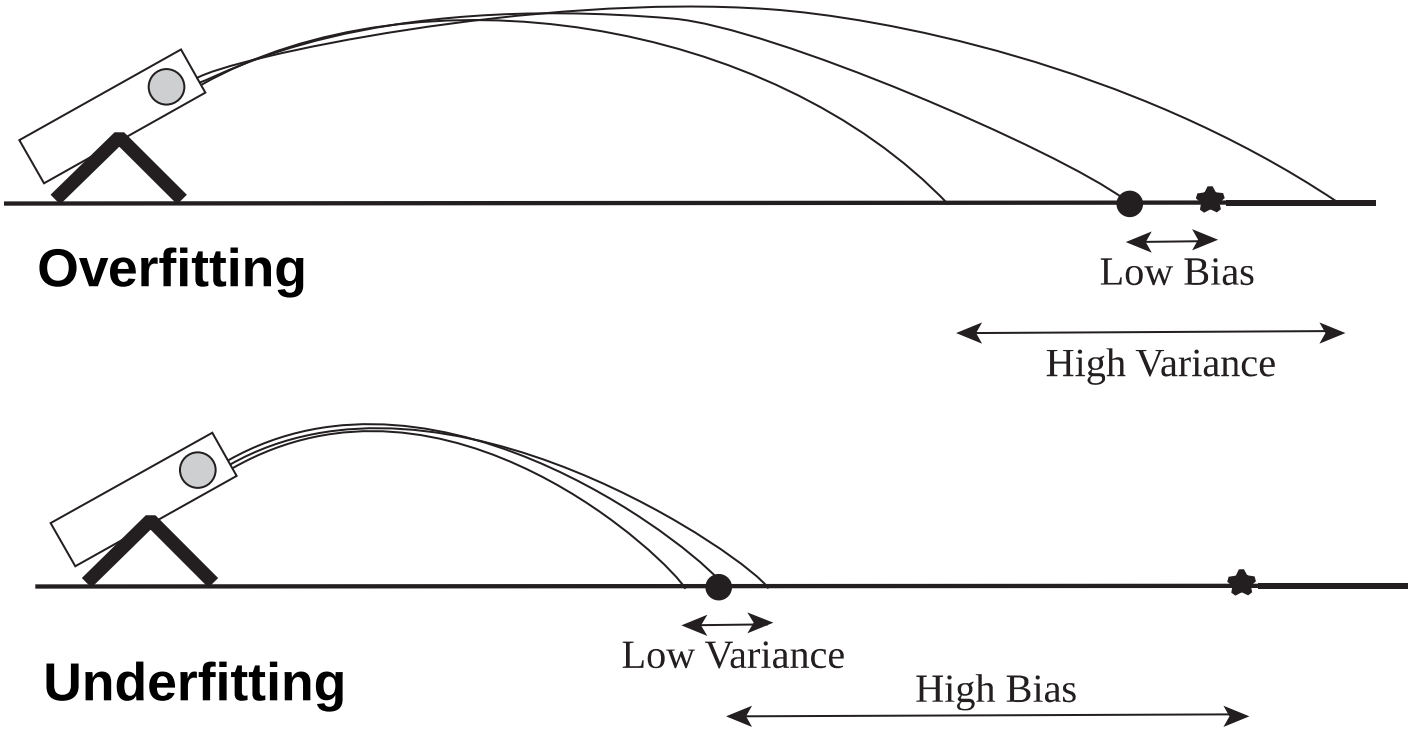
- Analogous problem of reaching a target y by firing projectiles from x (regression problem)



- For classification, the generalization error of model m can be given by:

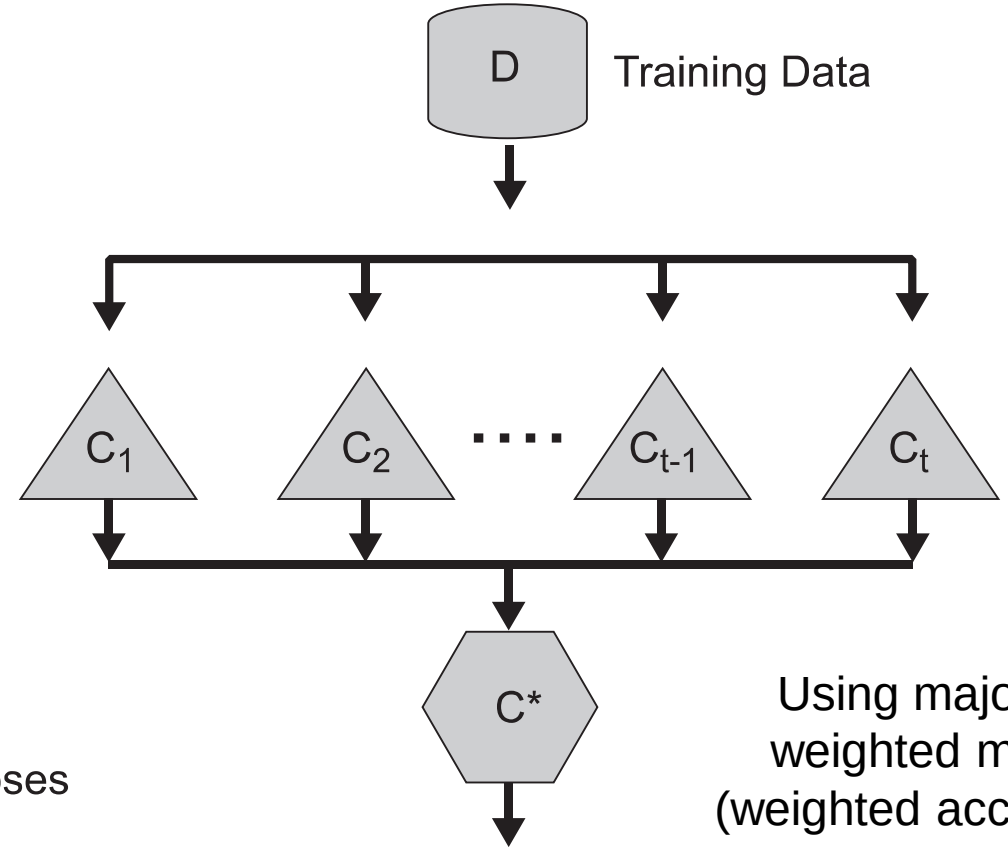
$$gen.error(m) = c_1 + bias(m) + c_2 \times variance(m)$$

Bias-Variance Trade-off and Overfitting



- Ensemble methods try to reduce the variance of complex models (with low bias) by *aggregating* responses of multiple base classifiers

General Approach of Ensemble Learning



A logical view of the ensemble learning method.

Constructing Ensemble Classifiers

- By manipulating training set
  - Example: bagging, boosting
- By manipulating input features
  - Example: random forests
- By manipulating class labels
  - Example: error-correcting output coding
- By manipulating learning algorithm
  - Example: injecting randomness in the initial weights of ANN

Constructing Ensemble Classifiers

- By manipulating training set
  - multiple training sets are created by resampling the original data according to some sampling distribution and constructing a classifier from each training set.
  - The sampling distribution determines how likely it is that an example will be selected for training, and it may vary from one trial to another.
    - Example: bagging, boosting

- By manipulating input features
  - a subset of input features is chosen to form each training set. The subset can be either chosen randomly or based on the recommendation of domain experts.
  - this approach works very well with data sets that contain highly redundant features
  - Example: random forests --ensemble method that manipulates its input features and uses decision trees as its base classifiers

Constructing Ensemble Classifiers

- By manipulating class labels
  - Example: error-correcting output coding
- can be used when the number of classes is sufficiently large.
- The training data is transformed into a binary class problem by randomly partitioning the class labels into two disjoint subsets, *A*0 and *A*1.
- Training examples whose class label belongs to the subset *A*0 are assigned to class 0, while those that belong to the subset *A*1 are assigned to class 1.
- The relabeled examples are then used to train a base classifier.
- By repeating this process multiple times, an ensemble of base classifiers is obtained. When a test example is presented, each base classifier *Ci* is used to predict its class label.
- If the test example is predicted as class 0, then all the classes that belongto *A*0 will receive a vote. Conversely, if it is predicted to be class 1, then all the classes that belong to *A*1 will receive a vote.
- The votes are tallied and the class that receives the highest vote is assigned to the test

Constructing Ensemble Classifiers

- By manipulating learning algorithm
  - Example: injecting randomness in the initial weights of ANN
- Many learning algorithms can be manipulated in such a way that applying the algorithm several times on the same training data will result in the construction of different classifiers.
- For example, an artificial neural network can change its network topology or the initial weights of the links between neurons.
- Similarly, an ensemble of decision trees can be constructed by injecting randomness into the tree-growing procedure. For example, instead of choosing the best splitting attribute at each node, we can randomly choose one of the top *k* attributes for splitting.

- The **first three approaches are generic methods** that are applicable to any classifier, whereas the fourth approach depends on the type of classifier used.
- The **base classifiers** for most of these approaches can be generated sequentially (one after another) or in **parallel** (all at once).

Bagging (Bootstrap AGGregatING)

- Bootstrap sampling: sampling with replacement

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 bootstrap sample
- Probability of a training instance being selected in a bootstrap sample is:
  - $1 - (1 - 1/n)^n$ (n: number of training instances)
  - ~0.632 when n is large

Bagging Algorithm

Algorithm 4.5 Bagging algorithm.

1: Let k be the number of bootstrap samples.
2: **for** $i = 1$ to k **do**
3: Create a bootstrap sample of size N, D_i.
4: Train a base classifier C_i on the bootstrap sample D_i.
5: **end for**
6: $C^*(x) = \underset{y}{\operatorname{argmax}} \sum_i \delta\big(C_i(x) = y\big)$.

$\{\delta(\cdot) = 1$ if its argument is true and 0 otherwise.$\}$

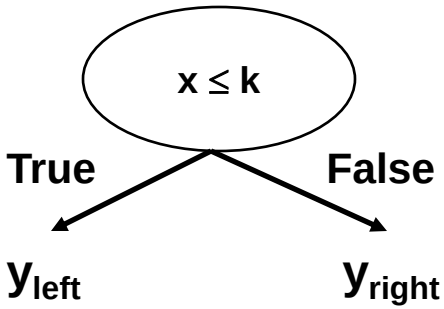
Bagging Example

- Consider 1-dimensional data set:

Original Data:

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
y	1	1	1	-1	-1	-1	-1	1	1	1

- Classifier is a decision stump (decision tree of size 1)
  - Decision rule: $x \leq k$ versus $x > k$
  - Split point k is chosen based on entropy



Bagging Example

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 ➔ y = 1
x > 0.35 ➔ y = -1

Bagging Example

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 ➔ y = 1
x > 0.35 ➔ y = -1

Bagging Round 2:

x	0.1	0.2	0.3	0.4	0.5	0.5	0.9	1	1	1
y	1	1	1	-1	-1	-1	1	1	1	1

x <= 0.7 ➔ y = 1
x > 0.7 ➔ y = 1

Bagging Round 3:

x	0.1	0.2	0.3	0.4	0.4	0.5	0.7	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.35 ➔ y = 1
x > 0.35 ➔ y = -1

Bagging Round 4:

x	0.1	0.1	0.2	0.4	0.4	0.5	0.5	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.3 ➔ y = 1
x > 0.3 ➔ y = -1

Bagging Round 5:

x	0.1	0.1	0.2	0.5	0.6	0.6	0.6	1	1	1
y	1	1	1	-1	-1	-1	-1	1	1	1

x <= 0.35 ➔ y = 1
x > 0.35 ➔ y = -1

Bagging Example

Bagging Round 6:

x	0.2	0.4	0.5	0.6	0.7	0.7	0.7	0.8	0.9	1
y	1	-1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 7:

x	0.1	0.4	0.4	0.6	0.7	0.8	0.9	0.9	0.9	1
y	1	-1	-1	-1	-1	1	1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 8:

x	0.1	0.2	0.5	0.5	0.5	0.7	0.7	0.8	0.9	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 9:

x	0.1	0.3	0.4	0.4	0.6	0.7	0.7	0.8	1	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ➔ y = -1
x > 0.75 ➔ y = 1

Bagging Round 10:

x	0.1	0.1	0.1	0.1	0.3	0.3	0.8	0.8	0.9	0.9
y	1	1	1	1	1	1	1	1	1	1

x <= 0.05 ➔ y = 1
x > 0.05 ➔ y = 1

Bagging Example

- Summary of Trained Decision Stumps:

Round	Split Point	Left Class	Right Class
1	0.35	1	-1
2	0.7	1	1
3	0.35	1	-1
4	0.3	1	-1
5	0.35	1	-1
6	0.75	-1	1
7	0.75	-1	1
8	0.75	-1	1
9	0.75	-1	1
10	0.05	1	1

Bagging Example

- Use majority vote (sign of sum of predictions) to determine class of ensemble classifier

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	1	1	1	-1	-1	-1	-1	-1	-1	-1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
4	1	1	1	-1	-1	-1	-1	-1	-1	-1
5	1	1	1	-1	-1	-1	-1	-1	-1	-1
6	-1	-1	-1	-1	-1	-1	-1	1	1	1
7	-1	-1	-1	-1	-1	-1	-1	1	1	1
8	-1	-1	-1	-1	-1	-1	-1	1	1	1
9	-1	-1	-1	-1	-1	-1	-1	1	1	1
10	1	1	1	1	1	1	1	1	1	1
Sum	2	2	2	-6	-6	-6	-6	2	2	2
Sign	1	1	1	-1	-1	-1	-1	1	1	1

Predicted Class

- Bagging can also increase the complexity (representation capacity) of simple classifiers such as decision stumps

Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records
  - Initially, all N records are assigned equal weights (for being selected for training)
  - Unlike bagging, weights may change at the end of each boosting round

Boosting

- Records that are wrongly classified will have their weights increased in the next round
- Records that are classified correctly will have their weights decreased in the next round

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
- Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

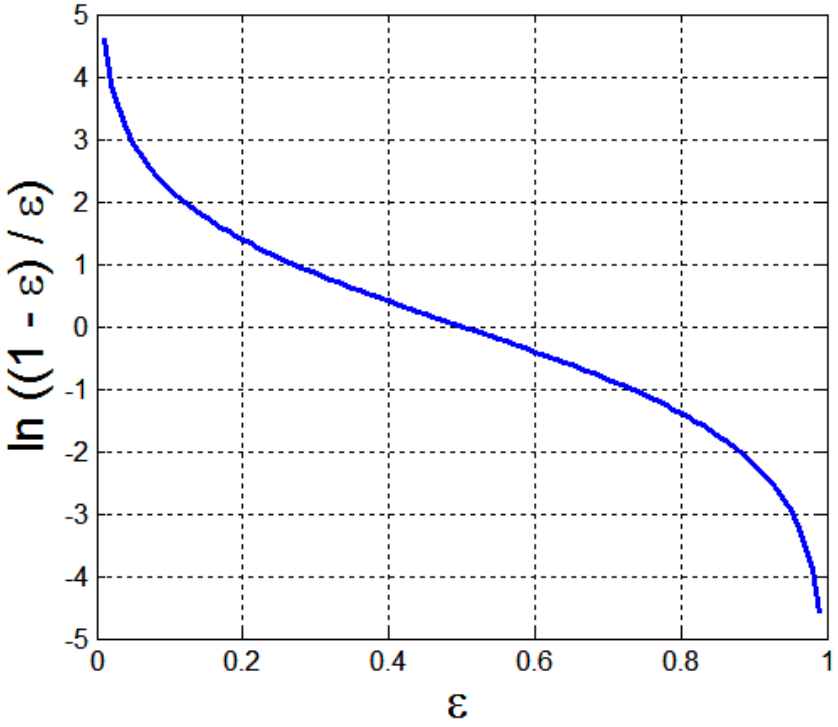
AdaBoost

- Base classifiers: $C_1, C_2, \ldots, C_T$
- Error rate of a base classifier:

$$\epsilon_i = \frac{1}{N}\sum_{j=1}^{N} w_j^{(i)}\, \delta(C_i(x_j) \neq y_j)$$

- Importance of a classifier:

$$\alpha_i = \frac{1}{2}\ln\left(\frac{1-\varepsilon_i}{\varepsilon_i}\right)$$



AdaBoost Algorithm

- Weight update:

$$w_j^{(i+1)} = \frac{w_j^{(i)}}{Z_i} \times \begin{cases} e^{-\alpha_i} & \text{if } C_i(x_j) = y_j \\ e^{\alpha_i} & \text{if } C_i(x_j) \neq y_j \end{cases}$$

Where Z_i is the normalization factor

- If any intermediate rounds produce error rate higher than 50%, the weights are reverted back to 1/n and the resampling procedure is repeated
- Classification:

$$C^*(x) = \arg\max_y \sum_{i=1}^{T} \alpha_i \delta(C_i(x) = y)$$

AdaBoost Algorithm

Algorithm 4.6 AdaBoost algorithm.

1: $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$. {Initialize the weights for all N examples.}
2: Let k be the number of boosting rounds.
3: **for** $i = 1$ to k **do**
4: Create training set D_i by sampling (with replacement) from D according to $\mathbf{w}$.
5: Train a base classifier C_i on D_i.
6: Apply C_i to all examples in the original training set, D.
7: $\epsilon_i = \frac{1}{N}\left[\sum_j w_j \, \delta\big(C_i(x_j) \neq y_j\big)\right]$ {Calculate the weighted error.}
8: **if** $\epsilon_i > 0.5$ **then**
9: $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$. {Reset the weights for all N examples.}
10: Go back to Step 4.
11: **end if**
12: $\alpha_i = \frac{1}{2} \ln \frac{1-\epsilon_i}{\epsilon_i}$.
13: Update the weight of each example according to Equation 4.103.
14: **end for**
15: $C^*(\mathbf{x}) = \underset{y}{\operatorname{argmax}} \sum_{j=1}^{T} \alpha_j \delta(C_j(\mathbf{x}) = y)\big)$.

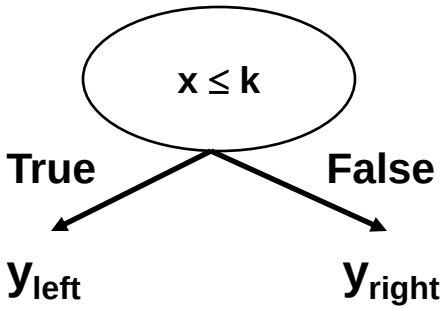
AdaBoost Example

- Consider 1-dimensional data set:

Original Data:

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
y	1	1	1	-1	-1	-1	-1	1	1	1

- Classifier is a decision stump
  - Decision rule: $x \leq k$ versus $x > k$
  - Split point k is chosen based on entropy



AdaBoost Example

- Training sets for the first 3 boosting rounds:

Boosting Round 1:

x	0.1	0.4	0.5	0.6	0.6	0.7	0.7	0.7	0.8	1
y	1	-1	-1	-1	-1	-1	-1	-1	1	1

Boosting Round 2:

x	0.1	0.1	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3
y	1	1	1	1	1	1	1	1	1	1

Boosting Round 3:

x	0.2	0.2	0.4	0.4	0.4	0.4	0.5	0.6	0.6	0.7
y	1	1	-1	-1	-1	-1	-1	-1	-1	-1

- Summary:

Round	Split Point	Left Class	Right Class	alpha
1	0.75	-1	1	1.738
2	0.05	1	1	2.7784
3	0.3	1	-1	4.1195

AdaBoost Example

- Weights

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
2	0.311	0.311	0.311	0.01	0.01	0.01	0.01	0.01	0.01	0.01
3	0.029	0.029	0.029	0.228	0.228	0.228	0.228	0.009	0.009	0.009

- Classification

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	-1	-1	-1	-1	-1	-1	-1	1	1	1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
Sum	5.16	5.16	5.16	-3.08	-3.08	-3.08	-3.08	0.397	0.397	0.397
Sign	1	1	1	-1	-1	-1	-1	1	1	1

Predicted Class

Random Forest Algorithm

- Construct an ensemble of decision trees by manipulating training set as well as features
  - Use bootstrap sample to train every decision tree (similar to Bagging)
  - Use the following tree induction algorithm:
    - At every internal node of decision tree, randomly sample p attributes for selecting split criterion
    - Repeat this procedure until all leaves are pure (unpruned tree)

Random Forest Algorithm

Given a training set D consisting of n instances and d attributes, the basic procedure of training a random forest classifier can be summarized using the following steps:

1. Construct a bootstrap sample D_i of the training set by randomly sampling n instances (with replacement) from D.

2. Use D_i to learn a decision tree T_i as follows. At every internal node of T_i, randomly sample a set of p attributes and choose an attribute from this subset that shows the maximum reduction in an impurity measure for splitting. Repeat this procedure till every leaf is pure, i.e., containing instances from the same class.

Characteristics of Random Forest

- Base classifiers are unpruned trees and hence are *unstable classifiers*
- Base classifiers are *decorrelated* (due to randomization in training set as well as features)
- Random forests reduce variance of unstable classifiers without negatively impacting the bias
- Selection of hyper-parameter p
  - Small value ensures lack of correlation
  - High value promotes strong base classifiers
  - Common default choices: $\sqrt{d}$, $\log_2(d+1)$

Gradient Boosting

- Constructs a series of models
  - Models can be any predictive model that has a differentiable loss function
  - Commonly, trees are the chosen model
    - XGboost (extreme gradient boosting) is a popular package because of its impressive performance
- Boosting can be viewed as optimizing the loss function by iterative functional gradient descent.
- Implementations of various boosted algorithms are available in Python, R, Matlab, and more.

References:

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