Introduction to Machine Learning

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Probability - Basics

- Marginal Prob.
  - Prob. of an event occurring, p(A). It is not conditioned on another event.
    - Prob. that a card drawn from deck is black: 0.5

- Joint Prob.
  - Prob. of event A and B occurring, p(A and B). Its prob. of intersection of two or more events.
    - Prob. of card is black and 5 is: 1/26
- Conditional Probability
  - Prob. of event A occurring, given that event B occurs, p(A|B).
    - Say, you have drawn a black card, what's the prob. that's its 5. p(5|black) = 1/13

Probability - Basics

- Manipulation between conditional, joint, and marginal probabilities

$$P(A \mid B) = \frac{P(A \text{ and } B)}{P(B)}$$

- Event A is independent of B, if P(A) = P(A|B)
  - Important consequence is multiplication rule

$$P(A \text{ and } B) = P(A \mid B)P(B) = P(A)P(B)$$

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

Example of Bayes Theorem

- Given:
  - A doctor knows that meningitis causes stiff neck 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?

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

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)
  - 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?

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

- Can we 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

Using Bayes Theorem for Classification

- Approach:
  - compute posterior probability P(Y | X_1, X_2, …, X_d) using the Bayes theorem

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

  - *Maximum a-posteriori*: Choose Y that maximizes P(Y | X_1, X_2, …, X_d)
  - Equivalent to choosing value of Y that maximizes P(X_1, X_2, …, X_d|Y) P(Y)
- How to estimate P(X_1, X_2, …, X_d | Y)?

Example Data

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

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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:

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

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.

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 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
2	No	Married	100K	No
3	No	Single	70K	No
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8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Class: $P(Y) = N_c/N$
  - e.g., P(No) = 7/10, P(Yes) = 3/10
- For categorical attributes:

  $P(X_i \mid Y_k) = |X_{ik}|/N_{c_k}$
  - where $|X_{ik}|$ is number of instances having attribute value X_i and belonging to class Y_k
  - Examples:

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

Estimate Probabilities from Data

- For continuous attributes:
  - Discretization: Partition the range into K 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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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

- 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

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(Yes) = 3/10
  P(No) = 7/10
- P(Yes | Divorced) = 1/3 x 3/10 / P(Divorced)
  P(No | Divorced) = 1/7 x 7/10 / P(Divorced)
- 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)

Issues with Naïve Bayes Classifier

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
7	Yes	Divorced	220K	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:

$$\text{Original}: P(A_i \mid C) = \frac{N_{ic}}{N_c}$$

$$\text{Laplace}: P(A_i \mid C) = \frac{N_{ic} + 1}{N_c + c}$$

$$\text{m-estimate}: P(A_i \mid C) = \frac{N_{ic} + mp}{N_c + m}$$

c: number of classes

p: prior probability of the class

m: parameter

N_c: number of instances in the class

N_{ic}: number of instances having attribute value A_i in class c

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)

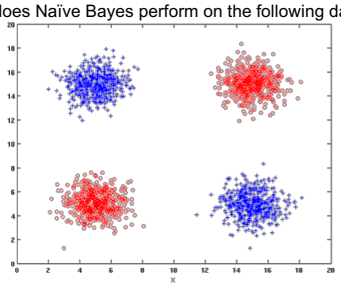
=> Mammals

Naïve Bayes (Summary)

- Robust to isolated noise points
- Handle missing values by ignoring the instance during probability estimate calculations
- Robust to irrelevant attributes
- Independence assumption may not hold for some attributes
  - Use other techniques such as Bayesian Belief Networks (BBN)

Naïve Bayes

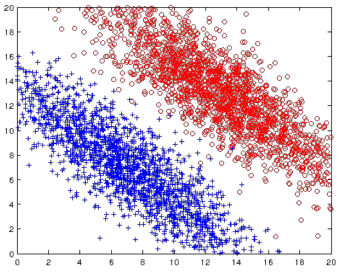
- How does Naïve Bayes perform on the following dataset?



Conditional independence of attributes is violated

Naïve Bayes

- How does Naïve Bayes perform on the following dataset?



Naïve Bayes can construct oblique decision boundaries

Maximum Likelihood Classification

- Uses Bayes decision rule:

$$x \in c_i \quad iff \quad p(c_i \mid x) > p(c_j \mid x) \forall j \neq i$$

How to compute $p(c_i \mid x)$?

Bayes' Theorem:

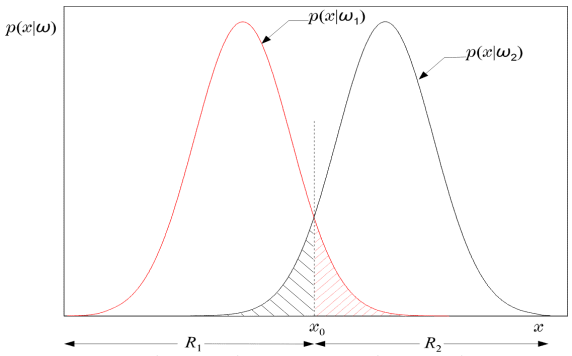
$$p(c_i \mid x) = \frac{p(x \mid c_i).p(c_i)}{p(x)}$$

Where $p(x)$ = prob. of finding a pixel from any class at location x

$$= \sum_{i=1}^{M} p(x \mid c_i).p(c_i).$$

Note: ω, y, c are used interchangeably for "class"

Decision Rule



$R_1(\rightarrow \omega_1)$ *and* $R_2(\rightarrow \omega_2)$

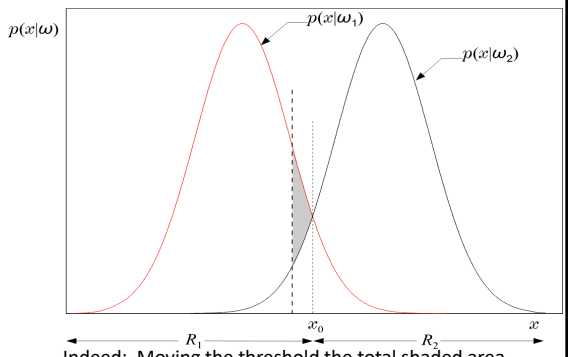
Error and Optimality

- Probability of error
  - Total shaded area

$$P_e = \int_{-\infty}^{x_0} p(x|\omega_2)dx + \int_{x_0}^{+\infty} p(x|\omega_1)dx$$

- Bayesian classifier is optimal with respect to minimizing the classification error probability

Optimality



Indeed: Moving the threshold the total shaded area INCREASES by the extra "grey" area.

MLC

$p(x \mid \omega_i)$: is the class conditional distribution and can be estimated from the training data (e.g., Gaussian)

$p(\omega_i)$: prior probability

Modeling both of these terms is very important for accurate classification

Decision Rule:

$$x \in \omega_i \text{ if } p(x \mid \omega_i)p(\omega_i) > p(x \mid \omega_j)p(\omega_j) \forall i \neq j$$

Simplified:

$$g_i(x) = \ln p(x \mid \omega_i) + \ln p(\omega_i)$$

$$x \in \omega_i \text{ if } g_i(x) > g_j(x) \forall i \neq j$$

MLC

- Model Assumption
  - Training samples were generated by multivariate Gaussian

$$p(x \mid \omega_i) = \frac{1}{\sqrt{(2\pi)^d |\Sigma_i|}} \exp\left[-\frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i)\right]$$

  - MLE $\hat{\mu}_i = \frac{1}{n}\sum_{k=1}^{n} x_k; \hat{\Sigma}_i = \frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu}_1)(x_k - \hat{\mu}_1)'$
- For each feature vector x $p(\omega_i \mid x) = \frac{p(x \mid \omega_i).p(\omega_i)}{p(x)}$
- Apply, ML Decision

$$x \in \omega_i \text{ if } p(x \mid \omega_i)p(\omega_i) > p(x \mid \omega_j)p(\omega_j) \forall i \neq j$$

Discriminant function

- Ln(.) is monotonic. Define:

$$g_i(\underline{x}) = \ln(p(\underline{x}|\omega_i)P(\omega_i)) =$$

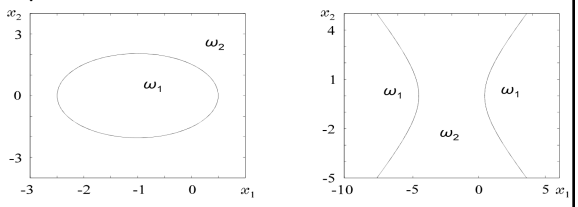
$$\ln p(\underline{x}|\omega_i) + \ln P(\omega_i)$$

$$g_i(\underline{x}) = -\frac{1}{2}(\underline{x}-\underline{\mu}_i)^T \Sigma_i^{-1}(\underline{x}-\underline{\mu}_i) + \ln P(\omega_i) + -(\frac{d}{2})\ln 2\pi - (\frac{1}{2})\ln|\Sigma_i|$$

Note: ω, y, c are used interchangeably for "class"

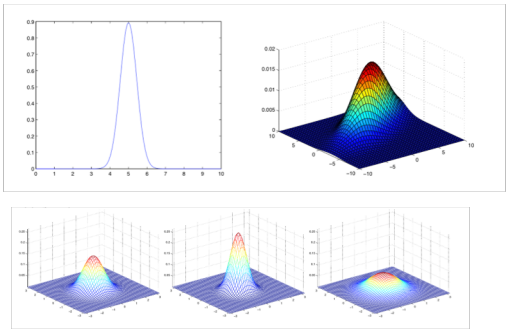
Discriminant function

- Note that $g_i(x)$ is quadratic, and produces quadrics, ellipsoids, parabolas, hyperbolas, and pairs of lines as decision boundaries

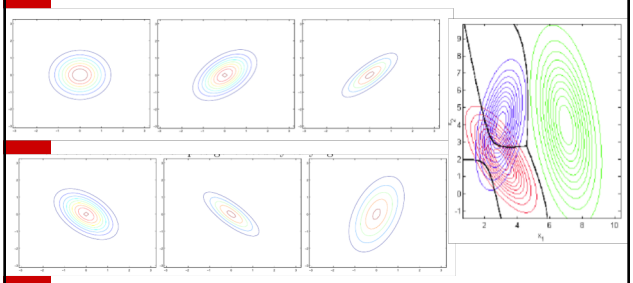


Accurate Assessment of Covariance is important, as it influences decision boundaries

Covariance Matrix



Covariance Matrix



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as it influences decision boundaries

Any Questions?