

THEORY OF NAIVE BAYES

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Learning classifiers by learning $P(Y|X)$

Simple example:

Joint Distributions

X_1	X_2	X_1 Y	Prob.
0	0	0	p_1
0	0	1	p_2
0	1	0	p_3
0	1	1	p_4
1	0	0	p_5
1	0	1	p_6
1	1	0	p_7
1	1	1	p_8
			$\sum_{i=1}^8 p_i = 1$

X_1	X_2	$P(Y X_1, X_2)$
0	0	p_1
0	1	p_2
1	0	p_3
1	1	p_4

Only 4 parameters!

In general, $X = \langle x_1, \dots, x_n \rangle$ $x_i \in \{0, 1\}$ and $Y \in \{0, 1\}$

Q.1. To estimate $P(Y|X_1, X_2, \dots, X_n)$, how many parameters? 2^n

How can we design a learning algorithm that is practical?

Let's go back to Bayes Rule and see if it helps

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

which is shorthand for

$$(\forall i, j) \quad P(Y = y_i | X = x_j) = \frac{P(X = x_j | Y = y_i) P(Y = y_i)}{P(X = x_j)}$$

equivalently,

$$(\forall i, j) \quad P(Y = y_i | X = x_j) = \frac{P(X = x_j | Y = y_i) P(Y = y_i)}{\sum_k P(X = x_j | Y = y_k) P(Y = y_k)}$$

Q.2. To estimate $P(X_1, X_2, \dots, X_n | Y)$, how many parameters?

case 1: $Y = 1$ $P(X_1, X_2, \dots, X_n | Y=1) \rightarrow 2^n - 1$

case 2: $Y = 0$ $P(X_1, X_2, \dots, X_n | Y=0) \rightarrow 2^n - 1$

$$\frac{2(2^n - 1)}{2(2^n - 1)}$$

Q.3. To estimate $P(Y)$, how many parameters? 1

So, if we use Bayes Rule, we need $2(2^n - 1) + 1$ parameters (worse!)

Naïve Bayes

Naïve Bayes assumes:

$$P(X_1, \dots, X_n | Y) = \prod_i P(X_i | Y)$$

i.e. that X_i and X_j are conditionally independent given Y , $\forall i \neq j$

Conditional Independence

Def. X is conditionally independent of Y given Z , if the probability distribution governing X is independent of the value of Y , given the value of Z

$$(\forall i, j, k) \quad P(X = x_i | Y = y_j, Z = z_k) = P(X = x_i | Z = z_k)$$

shorthand:

$$P(X | Y, Z) = P(X | Z)$$

e.g. $P(\text{Thunder} | \text{Rain}, \text{Lightning}) = P(\text{Thunder} | \text{Lightning})$

NOTE: Thunder and Rain are not independent!

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Naive Bayes uses assumption that X_i are conditionally independent, given Y
 e.g. $P(X_1 | X_2, Y) = P(X_1 | Y)$

Given this assumption, then:

$$\begin{aligned} P(X_1, X_2 | Y) &= P(X_1 | X_2, Y) P(X_2 | Y) && \text{chain rule} \\ &= P(X_1 | Y) P(X_2 | Y) && \text{conditional independence} \end{aligned}$$

In general, $P(X_1, \dots, X_n | Y) = \prod_i P(X_i | Y)$

Q.4 How many parameters to estimate $P(X_1, \dots, X_n | Y)$? $P(Y)$?
 - without conditional independence assumption? $2(2^n - 1) + 1$
 - with conditional independence assumption? $2n + 1$

Naive Bayes in a Nutshell

Bayes Rule: $P(Y=y_k | X_1, \dots, X_n) = \frac{P(Y=y_k) P(X_1, \dots, X_n | Y=y_k)}{\sum_j P(Y=y_j) P(X_1, \dots, X_n | Y=y_j)}$

Assuming conditional independence among X_i 's

$$P(Y=y_k | X_1, \dots, X_n) = \frac{P(Y=y_k) \prod_i P(X_i | Y=y_k)}{\sum_j P(Y=y_j) \prod_i P(X_i | Y=y_j)}$$

So, to pick most probable Y for $X^{\text{new}} = \langle X_1, \dots, X_n \rangle$

$$Y^{\text{new}} \leftarrow \arg \max_{y_k} P(Y=y_k) \prod_i P(X_i^{\text{new}} | Y=y_k)$$

Naive Bayes Algorithm for discrete X_i

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- Train Naive Bayes (examples)

for each* value y_k

estimate $\pi_k \equiv P(Y = y_k)$

for each* value x_{ij} of each attribute X_i

estimate $\theta_{ijk} \equiv P(X_i = x_{ij} | Y = y_k)$

* prob. must sum to 1, so we need to estimate only $n-1$ of these...

- classify (X^{new})

$$Y^{\text{new}} \leftarrow \arg \max_{y_k} P(Y = y_k) \prod_i P(X_i^{\text{new}} | Y = y_k)$$

$$Y^{\text{new}} \leftarrow \arg \max_{y_k} \pi_k \prod_i \theta_{ijk}$$

Estimating Parameters: Y, X_i discrete + valued

Maximum likelihood estimates (MLE's)

$$\hat{\pi}_k = \hat{P}(Y = y_k) = \frac{\# D \{ Y = y_k \}}{|D|}$$

$$\hat{\theta}_{ijk} = \hat{P}(X_i = x_{ij} | Y = y_k) = \frac{\# D \{ X_i = x_{ij} \text{ and } Y = y_k \}}{\# D \{ Y = y_k \}}$$

Number of data points for which $Y = y_k$

~~Naive Bayes~~: MAP estimates (Beta, Dirichlet priors):

$$\hat{\pi}_k = \hat{P}(Y = y_k) = \frac{\# D \{ Y = y_k \} + (\beta_k - 1)}{|D| + \sum_m (\beta_m - 1)}$$

$$\hat{\theta}_{ijk} = \hat{P}(X_i = x_{ij} | Y = y_k) = \frac{\# D \{ X_i = x_{ij} \text{ and } Y = y_k \} + (\beta_k - 1)}{\# D \{ Y = y_k \} + \sum_m (\beta_m - 1)}$$

Naïve Bayes : ~~some~~ Issue #1

- Often X_i 's are not really conditionally independent.
 - We use Naïve Bayes anyway, and it works "pretty well"
 - resulting in right classification, but not right prob. [Domingos & Elkan 1996]

- What is the effect on estimated $P(Y|X)$?

- Extreme case : what if we have two copies $X_i = X_j$

$$P(Y=1|X) = P(Y=1) P(X_1|Y=1) P(X_2|Y=1) \dots$$

Naïve Bayes : Issue #2

If unlucky, the MLE estimate for $P(X_i|Y)$ might be zero.

- Why worry about just one parameter out of many?

$$P(Y|X, \dots, X_n) = \frac{P(Y=1) \prod_i P(X_i|Y=1)}{P(X_1 \dots X_n)}$$

- What can be done to address it?

use MAP estimates by using a prior.

Another way to view Naïve Bayes (Boolean Y) : shape of the decision surface

Decision rule: is this quantity greater than or less than 1?

$$1 \gtrless \frac{P(Y=1|X_1 \dots X_n)}{P(Y=0|X_1 \dots X_n)} = \frac{P(Y=1) \prod_i P(X_i|Y=1)}{P(Y=0) \prod_i P(X_i|Y=0)} \quad P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

$$0 \gtrless \ln \frac{P(Y=1|X_1 \dots X_n)}{P(Y=0|X_1 \dots X_n)} = \ln \frac{P(Y=1)}{P(Y=0)} + \sum_i \ln \frac{P(X_i|Y=1)}{P(X_i|Y=0)}$$

- linear sum of a prior term and conditional prob. terms
- if $X_i \in \{0, 1\}$, then decision is a linear function of X_i 's

What if we have continuous X_i ?

e.g. image classification: X_i is real-valued i th pixel

Naive Bayes requires $P(X_i | Y=y_k)$, but X_i is real-valued (continuous)

$$P(Y=y_k | X_1, \dots, X_n) = \frac{P(Y=y_k) \prod_i P(X_i | Y=y_k)}{\sum_j P(Y=y_j) \prod_i P(X_i | Y=y_j)}$$

Let's assume $P(X_i | Y=y_k)$ follows a Normal (Gaussian) distribution

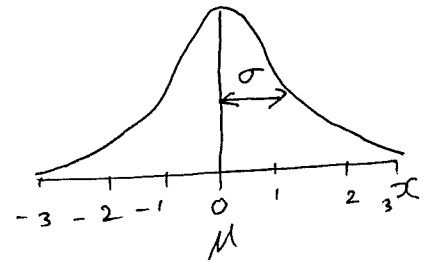
Gaussian Distribution (a.k.a. Normal distribution)

$p(x)$ is a probability density function (pdf)

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2}$$

integral of $p(x)$ is 1.

μ = Mean ; σ^2 = variance



Gaussian Naive Bayes (GNB)

$$P(X_i=x | Y=y_k) = \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} e^{-\frac{1}{2} \left(\frac{x-\mu_{ik}}{\sigma_{ik}} \right)^2}$$

Sometimes assume variance

- is independent of Y (i.e. σ_i)
- or independent of X_i (i.e. σ_k)
- or both (i.e. σ)

Gaussian Naïve Bayes Algorithm : continuous X_i , but discrete Y

- Train Naïve Bayes (examples)

for each value y_k

estimate $\pi_k \equiv P(Y = y_k)$

for each attribute X_i , estimate $P(X_i | Y = y_k)$

class conditional mean μ_{ik} , variance σ_{ik}

- Classify (X^{new})

$$Y^{\text{new}} \leftarrow \arg \max_{y_k} P(Y = y_k) \prod_i P(X_i^{\text{new}} | Y = y_k)$$

$$Y^{\text{new}} \leftarrow \arg \max_{y_k} \pi_k \prod_i \mathcal{N}(X_i^{\text{new}}; \mu_{ik}, \sigma_{ik})$$

Estimating Parameters : continuous X_i , but discrete Y

MLE :

$$\hat{\mu}_{ik} = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j X_i^j \delta(Y^j = y_k)$$

\uparrow i^{th} feature \uparrow k^{th} class \nwarrow j^{th} training example

$\delta() = 1$ if $(Y^j = y_k)$
 else \emptyset

$$\hat{\sigma}_{ik}^2 = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j (X_i^j - \hat{\mu}_{ik})^2 \delta(Y^j = y_k)$$

MAP :