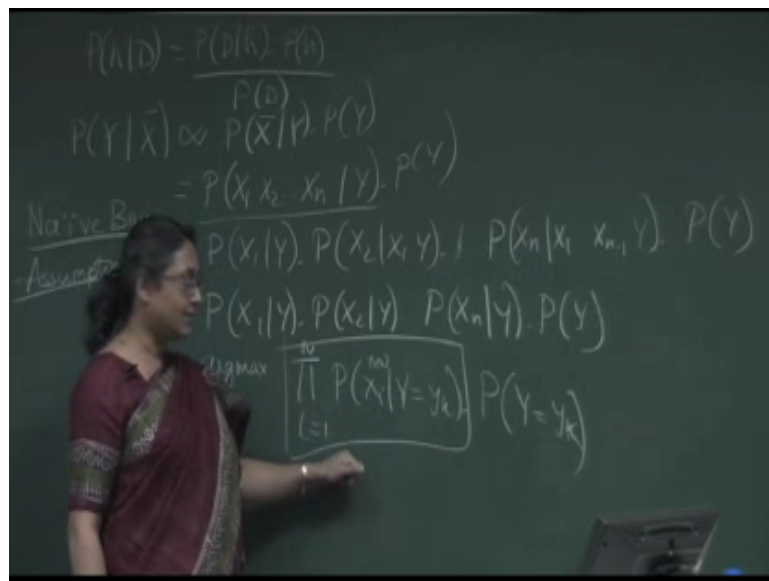


Introduction to Machine Learning
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Lecture – 17
Naive Bayes

Good morning. Today, we will talk about part c of the module on Bayesian learning. Today's topic is Naive Bayes. In the last class, we looked at the Bayes theorem.

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To recapitulate, it says the posterior probability of a hypothesis given the data is given by probability of D given h times prior probability of the hypothesis divided by the likelihood of the data. So, if you are trying to find out, let us apply Bayes theorem to classification. You want to find out the classification Y given the input X. So, if you apply Bayes theorem, probability Y by X is proportional to – as we have seen that, for different hypothesis, the likelihood of the data is identical. So, we need not consider it. So, we can consider the probability Y by Y given X. So, it is proportional to probability of X given Y times probability of Y; that is now X is the input instance and it can be a vector of features.

So, we can write it as probability X_1, X_2, \dots, X_n ; if small n is the number of features by Y times P Y. Now, this probability X_1, X_2, \dots, X_n given Y is a joint probability. And, joint probability is difficult to learn and represent, because if there are n features; even if

the features are Boolean, there are 2^n possible combinations of the features. And, you have to store the probability values corresponding to all of them. And, this is an intractable problem.

Now, in Naive Bayes, which we will talk about today, we make a simplifying assumption. The assumption that we make is that, individual X_i 's are independent given Y . In general, we can write this part as probability X_1 given Y times probability X_2 given X_1, Y times probability X_n given $X_1, X_2, \dots, X_{n-1}, Y$ times probability of Y .

Now, in the Naive Bayes assumption, we say that, probability of X_i given X_j, Y is equal to probability X_i given Y ; or X_i and X_j are independent given Y . And, based on that assumption, we can rewrite this as probability of X_1 given Y times probability X_2 given Y times probability of X_n given Y times probability of Y . This is based on the Naive Bayes assumption. So, we are assuming conditional independence among the individual attributes X_1, X_2, \dots, X_n . And based on this, we can do the classification. So, we are assuming all the input features are conditionally independent; and this can be computed as probability X_1 given Y , X_2 given Y , X_n given Y , etcetera.

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Naïve Bayes

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, classification rule for $X^{new} = \langle X_1, \dots, X_n \rangle$ is:

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

So, if you look at the slide, from Bayes rule, if the probability of Y taking a particular value y_k given the value of the input features X_1, X_2, \dots, X_n is given by probability Y equal to y_k times probability X_1, X_2, \dots, X_n given Y equal to y_k divided by – this is the denominator, which is independent of Y equal to y_k .

Assuming conditional independence, we get it as probability $Y = y_k$ times product of probability X_i given $Y = y_k$. And, there is a denominator. And based on this, we can get a classifier. The classifier says that, given a new example, the classification Y_{new} is that y_k for which this quantity is maximized; that is, the product over all the training, all the attributes, probability X_i given Y of the training example of the new instance probability X_i^{new} given Y , given $Y = y_k$ times probability of the prior probability $Y = y_k$. So, these times this is maximum. So, you want to take that classification for which the prior probability of $Y = y_k$ times this product is maximum.

Now, if we look at the individual probabilities that we require to compute this, what do we notice is that, for each value of suppose Y takes two values: plus and minus; we need to know for all such cases, we need to know a probability of $Y = \text{true}$, probability of $Y = \text{false}$. And, for each feature X_i , we need to know probability of X_i given $Y = \text{plus}$; probability of X_i given $Y = \text{minus}$. And, X_i can have different values.

Suppose X_i has 3 values, for each of the values of X_i , we have to estimate probability $X_i = \text{value 1}$ given $Y = \text{plus}$; probability $X_i = \text{value 2}$ given $Y = \text{plus}$; probability $X_i = \text{value 3}$ given $Y = \text{plus}$. Similarly, probability $X_i = \text{value 1}$ given $Y = \text{minus}$ and so on. So, what we have is that are the number of probabilities that we required to calculate.

Let us assume that, X_1, X_2, X_n and Y are binary attributes. For a Y , we require two values; actually, one of them will suffice that; then we can get for if each X_i has two values; so, for each X_i will require $X_i = \text{true}$ for each value of Y . If we know $X_i = \text{true}$, we can also get $X_i = \text{false}$. So, we have $X_i = \text{true}$ given $Y = \text{true}$; $X_i = \text{true}$ given $Y = \text{false}$. So, two values for each X_i . So, total $2n$ plus two values – $2n$ plus 1 value will suffice to represent these probabilities, which is very much possible. And, this is a simple; this gives us a simple algorithm for classification called Naive Bayes.

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Naïve Bayes Algorithm – discrete X_i

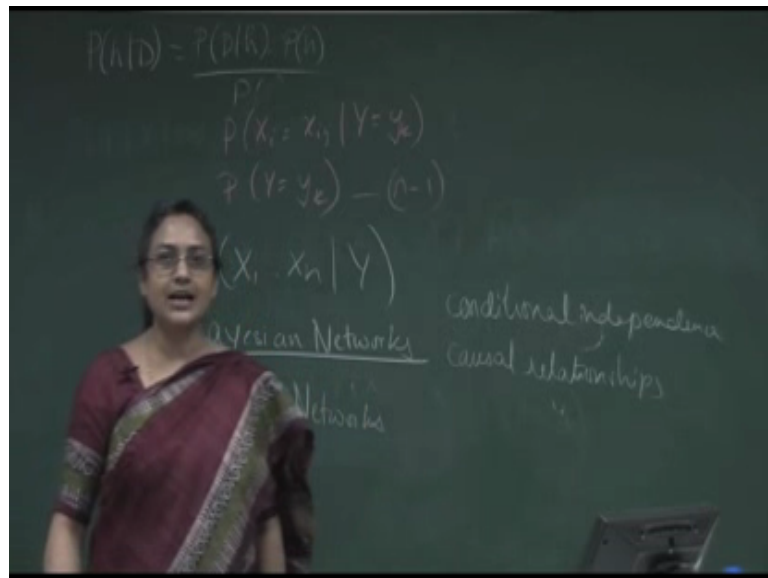
- Train Naïve Bayes (examples)
 - for each* value y_k
 - estimate $\pi_k \equiv P(Y = y_k)$
 - for each* value x_{ij} of each attribute X_i
 - estimate $\theta_{ijk} \equiv P(X_i = x_{ij} | Y = y_k)$
- Classify (X^{new})
 - $$Y^{new} \leftarrow \arg \max_{y_k} P(Y = y_k) \prod_i P(X_i^{new} | Y = y_k)$$
 - $$Y^{new} \leftarrow \arg \max_{y_k} \pi_k \prod_i \theta_{ijk}$$

* probabilities must sum to 1, so need estimate only n-1 parameters...

Now, let us see what is the resulting Naive Bayes algorithm? When you have discrete values of X ; for which you can look at the slide, which gives the outline of the Naive Bayes algorithm. This is a very simple algorithm. So, when we train Naive Bayes, we take the training set; and for each value y_k ; suppose there are n values of y_k , we need to estimate only n minus 1 parameters, because y_k equal to 1, y_k equal to 2 from y_k equal to 3, you know the probabilities of some of the probabilities is 1.

So, you need to estimate only n minus 1 of the values. Anyway for each value y_k , we will estimate π_k as the probability of Y equal to y_k . This is the prior probability. How do we estimate that? Suppose we are given 100 training examples, and y_k has three values: v_1, v_2, v_3 , y_k equal to v_1 for 70 of the examples; v_2 for 20 of the examples; v_3 for 10 of the examples; then, probability of Y equal to y_k could be estimated to be 70 by 100; for value 2, 20 by 100; for value 3, 10 by 100 or some other estimate measure which we will again talk about.

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Now, for each value x_{ij} of each attribute X_i for the j -th instance for each attribute X_i for each x_{ij} , we will estimate θ_{ijk} as the parameter that, probability that X equal to x_{ij} given Y equal to y_k . So, if y_k takes n different values; then, this will require n minus 1 estimate. If each x takes k values, we require how many estimates? We require 2 into n estimates, so 3 minus 1 into n . So, small x_{ij} is the different values that attribute x_i can take. So, these probabilities we need to estimate. Now, based on this estimate, we can have the class.

So, in the training phase, we learnt this estimates from the training examples. And after we have learnt the estimate, you look at the slide again; we can classify a new instance X_{new} as its class Y_{new} is that y_k for which this expression is maximized; probability Y equal to y_k times product over i ; probability X_i new given Y equal to y_k as we have seen. In terms of simplified values of the parameters that we have written, this is given by this. So this is the Naive Bayes algorithm for the case, where all the attributes are discrete valued or nominal valued.

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Estimating Parameters: Y, X_i discrete-valued

Maximum likelihood estimates (MLE's):

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

Number of items in set D for which $Y=y_k$

Before we proceed, let us look at an example and one more thing that I forgot to tell you is that, when we estimate these parameters – probability of X_i given Y or probability Y , we may sometimes come across a situation, where in the training example, the count for computing the probability is 0. Then, we have a problem. You see in the classification, we have a product that we are computing. We are taking the product of this probability and the product of these probabilities.

Now, if we have insufficient training instances, there may be a case, where probability X_i equal to X_{ij} given Y equal to y_k ; you know there is no training example for a particular y_k for which X_i is a particular value of X_{ij} . So, this value if we do Naive estimation of the probabilities by frequency counting, this probability will become 0. And, if one probability term becomes 0, the entire product becomes 0. In order to avoid that, we need to do something called smoothing in order to avoid such situations. And so, what we do is that, when we do the estimating of the different parameters; for example, when we try to estimate π_k ; for π_k , we look at the number of times y equal to y_k divided by total number of data instances.

For θ_{ijk} estimate, which is probability X_i equal to small x_{ij} given Y equal to y_k , we count the number of instances for which capital X_i equal to small x_{ij} and Y equal to y_k divided by number of instances for which Y equal to y_k . This is the simple formula for maximum likelihood estimation. And in this case there it is possible that, especially

in computing θ_{ijk} , sometimes we will get the numerator as 0. In order to avoid that, we introduce smoothing, where we initialize some small probability to each of these values. And we will see in a later slide that, we can add plus 1 to each of the numerator and compensate it by some value added to the denominator.

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Example

- Example: Play Tennis

PlayTennis: training examples

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

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But, before that, let us look at an example. This is an example taken from a Mitchell's book on Machine Learning; where, we have a description of different days. And the attributes are outlook, temperature, humidity and wind. These are the climate attributes of different days. And, the target attribute is whether it is a good day for playing tennis.

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Example					
Learning Phase					
Outlook	Play=Yes	Play=No	Temperature	Play=Yes	Play=No
Sunny	2/9	3/5	Hot	2/9	2/5
Overcast	4/9	0/5	Mild	4/9	2/5
Rain	3/9	2/5	Cool	3/9	1/5

Humidity	Play=Yes	Play=No	Wind	Play=Yes	Play=No
High	3/9	4/5	Strong	3/9	3/5
Normal	6/9	1/5	Weak	6/9	2/5

$$P(\text{Play=Yes}) = 9/14 \quad P(\text{Play=No}) = 5/14$$

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Given this training example, if you apply Naive Bayes to it, in the training phase, you will output the probabilities. So, if outlook is sunny, play equal to yes – given outlook is sunny is 2 by 9; play equal to - given outlook is sunny is 3 by 5; play equal to yes – given outlook is overcast is 4 by 9; play equal to no - given outlook over cast is 0 by 5 and so on. These are the values that we get by doing the maximum likelihood instance; estimation from the data.

These are the prior probabilities for playing tennis and for not playing tennis. And, these are the values of θ_{ijk} . So, these can be estimated using the previous maximum likelihood estimate formula that we have seen. And this is how we get these values. Now, this is what happens in the training phase.

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Example

Test Phase

- Given a new instance, predict its label
 $\mathbf{x}' = (\text{Outlook}=\text{Sunny}, \text{Temperature}=\text{Cool}, \text{Humidity}=\text{High}, \text{Wind}=\text{Strong})$
- Look up tables achieved in the learning phase

$P(\text{Outlook}=\text{Sunny} \text{Play}=\text{Yes}) = 2/9$	$P(\text{Outlook}=\text{Sunny} \text{Play}=\text{No}) = 3/5$
$P(\text{Temperature}=\text{Cool} \text{Play}=\text{Yes}) = 3/9$	$P(\text{Temperature}=\text{Cool} \text{Play}=\text{No}) = 1/5$
$P(\text{Humidity}=\text{High} \text{Play}=\text{Yes}) = 3/9$	$P(\text{Humidity}=\text{High} \text{Play}=\text{No}) = 4/5$
$P(\text{Wind}=\text{Strong} \text{Play}=\text{Yes}) = 3/9$	$P(\text{Wind}=\text{Strong} \text{Play}=\text{No}) = 3/5$
$P(\text{Play}=\text{Yes}) = 9/14$	$P(\text{Play}=\text{No}) = 5/14$

- Decision making with the MAP rule

$P(\text{Yes} | \mathbf{x}') = [P(\text{Sunny} | \text{Yes})P(\text{Cool} | \text{Yes})P(\text{High} | \text{Yes})P(\text{Strong} | \text{Yes})]P(\text{Play}=\text{Yes}) = 0.0053$
 $P(\text{No} | \mathbf{x}') = [P(\text{Sunny} | \text{No})P(\text{Cool} | \text{No})P(\text{High} | \text{No})P(\text{Strong} | \text{No})]P(\text{Play}=\text{No}) = 0.0206$

Given the fact $P(\text{Yes} | \mathbf{x}') < P(\text{No} | \mathbf{x}')$, we label \mathbf{x}' to be "No".

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In the test phase, you have given a new instance and you have to predict its (Refer Time: 16:52) For example, suppose the new instance is outlook is sunny, temperature equal to cool, humidity is high and wind is strong. And based on this probability values that we have seen in the previous page, we can do the decision with the MAP rule.

And we find out that, probability yes given \mathbf{x}' turns out to be 0.0053; probability no given \mathbf{x}' is 0.0206. And, because probability of yes given \mathbf{x}' is less than probability no given \mathbf{x}' , we label \mathbf{x}' to be no. So this is a simple application of Naive Bayes; it is an extremely simple algorithm. We look at the training set. You estimate; do a MLE estimate of the different parameters; then given the test set, we apply that formula.

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Estimating Parameters: Y, X_i discrete-valued


If unlucky, our MLE estimate for $P(X_i / Y)$ may be zero.

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

MAP estimates:

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

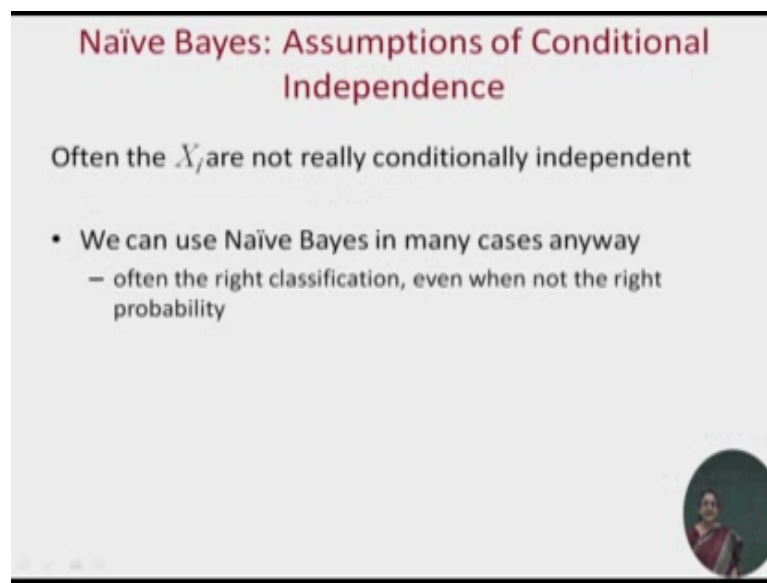
Only difference: "imaginary" examples

$$\hat{\theta}_{ijk} = P(X_i = x_{ij} | Y = y_k) = \frac{\#D\{X_i = x_{ij} \wedge Y = y_k\} + l}{\#D\{Y = y_k\} + lM}$$


Now, as I mentioned that, if you are unlucky, the estimate for probability X_i given Y may be zero, because there may be that, some particular attribute value is not represented for a particular class, because we do not have sufficient training example. To alleviate the fact, we can use smoothing. There are many approaches for smoothing including many sophisticated approaches, but we will introduce only a simplest approach for smoothing.

What we do is that, for every probability estimates that we do, we add some number; that number could be 1 or could be a fraction 1, which corresponds to some imaginary instances, because we are adding a small positive value to the numerator. We must compensate by adding 1 into R to the denominator, where R is the number of possible values of y_k , so that the sum of the π_k 's become remain 1. Similarly, to estimate θ_{ijk} , we can add 1 here. And in the denominator we must compensate by adding lM , so that the sum of θ_{ijk} over a particular value of ij will be equal to 1. So this is smoothing, which we can apply in order to alleviate the problem due to zero probability.

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The slide has a light blue background with a dark blue header. The title 'Naïve Bayes: Assumptions of Conditional Independence' is in a bold, dark blue font. Below the title, the text 'Often the X_i are not really conditionally independent' is in a smaller, dark blue font. A bulleted list follows, with the first item 'We can use Naïve Bayes in many cases anyway' in bold, and a sub-bullet '— often the right classification, even when not the right probability' in a regular font. In the bottom right corner, there is a small circular profile picture of a person with dark hair and a beard, wearing a blue shirt.

Naïve Bayes: Assumptions of Conditional Independence

Often the X_i are not really conditionally independent

- We can use Naïve Bayes in many cases anyway
 - often the right classification, even when not the right probability

Now, one important assumption that we made in Naive Bayes is that, the X i's are conditionally independent given Y , but this is not really a valid assumption. And, it often does not hold. We can often use the right classification but, even if this assumption does not always hold, Naive Bayes is surprisingly quite effective; given its simplicity, it surprisingly quite effective in many number of cases.

And, often it turns out that, even if the assumption is not valid, Naive Bayes gives the correct classification, because Naive Bayes we are not really using this assumption to find the exact probability, but to choose between the different possible classes. And, in that way, Naive Bayes works quite well in many cases. For example, in text classification, Naive Bayes is a very standard algorithm, which is applied and does surprisingly well it is fast; and because even when the assumptions are not right, it gives the right example.

Now, we will look at the case, where the input attributes are continuous value. We have so far seen that, the both the input attribute and the output attribute are discrete value. What if the input attribute is continuous value? If the input attributes are continuous valued, we can assume that, the conditional probability of that attribute can be modeled by a Gaussian. And based on that, we can have Gaussian Naive Bayes.

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Gaussian Naïve Bayes (continuous X)

- Algorithm: Continuous-valued Features
 - Conditional probability often modeled with the normal distribution

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

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)

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For this, I will request you to look at this slide. Suppose you have continuous valued features, then you can model the conditional probability – probability X_i equal to x given Y equal to y_k as a normal distribution or Gaussian distribution, which is given by this standard formula $\frac{1}{\sigma_{ik} \sqrt{2\pi}} e^{-\frac{(x - \mu_{ik})^2}{2\sigma_{ik}^2}}$. Sometimes we may assume that, this variance – the sigma square term here is independent of Y or independent of X_i or both. We can assume that this is same for all X_i or Y or you can assume that they are same for all Y_i and so on. This makes the model have less number of parameters if you wish. But, under this assumption we can have the Gaussian Naive Bayes algorithm.

In the Gaussian Naive Bayes algorithm, in the training phase, we look at the training dataset. And from the training dataset, we estimate π_k as before; π_k is probability Y equal to y_k . The prior probability of the different classes this is estimated as before, but for each attribute X_i we estimate the μ_{ik} and σ_{ik} .

For each X_i for a particular y_k , in order to find probability X_i given Y , we estimate μ and σ from the data. And after we have done this estimate, in the testing phase, we can classify the new instance X_{new} as Y_{new} is that y_k for which this is the standard formula for Naive Bayes. Here probability Y equal to y_k was estimated as π_k . And, for probability X_i new given Y equal to y_k , we use a normal distribution over X_i new μ σ ; where, μ σ were the parameters found in the training phase. So, based on

that, we can apply the Gaussian Naive Bayes algorithm.

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Estimating Parameters: Y discrete, X_j continuous

Maximum likelihood estimates:

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

Annotations for the first equation:

- $\hat{\mu}_{ik}$: ith feature, kth class
- X_i^j : jth training example
- $\delta(z) = 1$ if z true, else 0

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


Now, in the Gaussian Naive Bayes, is used for continuous X and so this is used particularly in case, where X is – X is continuous and Y is discrete. And, the maximum likelihood estimate as we have said, the estimate of μ 1 sigma is given by – μ is given by estimate of the mean of the sample. This is the standard way of doing maximum likelihood estimate. And sigma is also obtained by the standard deviation of the sample as is given by this slide. So, to conclude Naive Bayes, is a very simple algorithm, which makes the Naive as the assumption that the different attributes X_i and X_j are independent given the value of the class.

This assumption is not always realistic, but it simplifies our computations greatly; and in many cases, the resulting algorithm is quite good even though it is so simple. Even though the independence assumption is not always satisfied in practice, as attributes are often correlated, we are get quite good results.

But, we cannot always apply Naive Bayes. And as we have seen, we cannot do the full joint distribution. Probability $X_1 X_n$ given Y , it is not tractable to really do this. And to alleviate this, we study Bayesian networks. In Bayesian networks, we can strike a balance; we need not make full independence assumptions or full dependent assumptions, rather we denote the causal relationships and conditional independence.

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Naïve Bayes

- Example: Continuous-valued Features
 - Temperature is naturally of continuous value.
Yes: 25.2, 19.3, 18.5, 21.7, 20.1, 24.3, 22.8, 23.1, 19.8
No: 27.3, 30.1, 17.4, 29.5, 15.1
 - Estimate mean and variance for each class
$$\mu = \frac{1}{N} \sum_{n=1}^N x_n, \quad \sigma^2 = \frac{1}{N} \sum_{n=1}^N (x_n - \mu)^2$$
$$\mu_{Yes} = 21.64, \quad \sigma_{Yes} = 2.35$$
$$\mu_{No} = 23.88, \quad \sigma_{No} = 7.09$$
 - **Learning Phase:** output two Gaussian models for $P(\text{temp}|C)$
$$\hat{P}(x|Yes) = \frac{1}{2.35\sqrt{2\pi}} \exp\left(-\frac{(x-21.64)^2}{2 \times 2.35^2}\right) = \frac{1}{2.35\sqrt{2\pi}} \exp\left(-\frac{(x-21.64)^2}{11.09}\right)$$
$$\hat{P}(x|No) = \frac{1}{7.09\sqrt{2\pi}} \exp\left(-\frac{(x-23.88)^2}{2 \times 7.09^2}\right) = \frac{1}{7.09\sqrt{2\pi}} \exp\left(-\frac{(x-23.88)^2}{50.25}\right)$$

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The specific conditional independence of the different attributes; and in belief networks, we also denote causal relationships. So, we show the actual relations and actual independences between the attributes. And based on this we can get different learning algorithms, which I have do not make as Naive assumptions as Naive Bayes, but can capture the relationships in the domain.

And it is an advanced topic, and we have different types of the Bayesian networks; we have belief networks also called Directed graphical model. We also have another type of networks – Bayesian networks, which are called Undirected graphical models. And these can capture different relationships. But today we finish this topic.

Thank you very much.