Probabilistic ML algorithms

MLE, MAP and Naïve Bayes Model

Basic probability
notions you
need


## Axioms of Probability Theory

- All probabilities are between 0 and 1

$$
0 \leq P(A) \leq 1
$$

- The true proposition has probability 1 , false has probability 0.

$$
\begin{gathered}
P(\text { true })=1 \quad P(\text { false })=0 \\
P(A O R B)=P(A \cup B)=P(A)+P(B)-P(A \cap B)
\end{gathered}
$$

- Disjunctive probabilities:



## Conditional Probability

- $\mathrm{P}(A \mid B)$ is the probability of $A$ given $B$
- Assumes that $B$ is all and only information known.
- Defined by:

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



## Statistical Independence

- Random variables $A$ and $B$ are independent if and only if:

$$
P(A \mid B)=P(A) \quad P(B \mid A)=P(B)
$$

- Therefore, if $A$ and $B$ are independent:

$$
\begin{gathered}
P(A \mid B)=\frac{P(A \cap B)}{P(B)}=P(A) \\
P(A \cap B)=P(A, B)=P(A) P(B)
\end{gathered}
$$

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. Philosophical Transactions of the Royal Society of London, 53:370-418

Bayes
Formula


## Univariate and Multivariate distributions

- Univariate distribution is when there is only one random variable (e.g. if instance vectors $\boldsymbol{x}$ in $X$ are described by just one feature, or when there is one classification function $C(x)=Y$ )
- The feature or classification space is one-dimensional (for example real numbers, list of labels, ordered labels or binary)
- Multivariate if many random variables are involved (e.g. $\boldsymbol{x}:\left(X_{1}, \ldots, X_{d}\right)$ or $\mathrm{C}(\mathbf{x}):\left(Y_{1}, Y_{2} \ldots . \mathrm{Y}_{\mathrm{N}}\right)$ - multiple features and multiple classes. Now, any feature $j$ (or any class i) can be described by a random variable $X j$ (or Yi).
- If a random variable $X j$ is discrete, we can estimate $P\left(X_{j}=x_{j k}\right)$, the probability mass function PMF, where $x_{j k}$ with $\mathrm{k}=1, \ldots, d_{j}$ are the $\mathrm{d}_{\mathrm{j}}$ possible values for feature $j$. (e.g., binomial multinomial)
- If $X j$ is continuos, then we can estimate $\mathrm{p}(\mathrm{Xj})$, the Probability Density Function PDF of its values (e.g., a Gaussian).


## Probability mass and probability density



## Probabilistic ML

- We reformulate the learning/predictions problems in probabilistic terms
- Input instances $x$ are treated as (univariate or multivariate) random variables, output y is a (univariate or multivariate) random variable, the model to be learned can be described in probabilistic terms, e.g., $P(Y=y \mid X=x)$ the conditional probability of $y$ given the observation of $x$.


## Mapping the terminology

| Symbolic <br> (table) | Geometric (vectors) | Probabilistic <br> interpretation | Variables or values? |
| :--- | :--- | :--- | :--- |
| X : feature <br> space | feature space | (multivariate) random <br> variables | Set of variables |
| x : record, <br> instance | feature vector | Observation, trial, <br> sample, random vector | Set of values |
| D : dataset | Set of feature vectors | A sample of X | Set of valued random <br> vectors |
| Xi: i-th feature | i-th dimension of feature <br> space | i-th random variable of <br> the multivariate <br> distribution | variable |
| xi: a value for | value of i -th coordinate of a <br> feature vector | A value that can be <br> assumed by the <br> fandom variable Xi (a <br> sample/observation of <br> Xi) | value |

In general, in statistics, lowercase indicate observations (values) and uppercase random variables

## Probabilistic formulation of

 ML
## Many machine learning problems can be formulated in probabilistic terms.

- The target of a ML classifier is to learn a classification function (a model M) from data D $f(\boldsymbol{x}): \boldsymbol{x} \rightarrow \boldsymbol{y}$ (or $\boldsymbol{y}$ if output is also a vector)
$>$ Given an unseen instance $\boldsymbol{x}$, assign a category label $y$ to this instance using the learned function $f(\boldsymbol{x})$.
$>$ In a probabilistic formulation, $f(x)$ is a probability function, e.g., $P(y \mid x)$. What is the probability to observe $Y=y$ for the output random variable, given that $X=x$ ?


## Probabilistic formulation

## Two alternative probabilistic formulations of a ML classifier are:

GENERATIVE models: define a function $L(D ; \boldsymbol{\theta})$, where $\boldsymbol{\theta}$ are the parameters of a model $M_{\boldsymbol{\theta}}$ and «;» stands for a joint probability.

- $\mathrm{L}(\mathrm{D} ; \boldsymbol{\theta})$ is the likelyhood of $\boldsymbol{\theta}$ given the observation of $D$. The likelyhood is used to estimate the parameters $\boldsymbol{\theta}$
- Use $\boldsymbol{\theta}$ to specify the model $M_{\boldsymbol{\theta}}$ that explains our data (and predict new ones)
DISCRIMINATIVE models: Use the dataset D to estimate the parameters $\boldsymbol{\theta}$ of a probability function $\mathrm{P}(Y=y \mid \boldsymbol{x})$ which is the conditional probability of class label y given the observation of $\boldsymbol{x}$.



## Understanding the difference

- A generative model implies learning the distribution of the data itself and tells you how likely a given example (instance) is. For example, we can postulate that our data are generated by a Gaussian distribution, $G_{\boldsymbol{\theta}}$ with unknown parameters $\sigma$ and $\mu$. Learning the parameters allows us to predict the probability of observing a particular instance $X=x$.
- A discriminative model ignores the question of whether a given instance x is likely, and just tells you how likely a label (category) is , GIVEN the observation of the instance ( $\mathrm{P}(\mathrm{Y}=\mathrm{yi} \mid \mathrm{X}=\mathrm{x}$ ).
- Here is a nice paper that explains in detail the difference


## Discriminative/generative

$\operatorname{Argmax}(P(Y=\operatorname{dog} / X=x), P(Y=c a t / X=x)$


The model just predicts the probability that a new instance is a cat or dog, only based on whether it is placed wrt the decision boundary

The model «interprets» the input data (provides a probabilistic model that may have generated the observed data) and it is able to say how likely a new instance is to belong to the probability distribution - e.g., of of «cats» or of «dogs» -

## What is this «model» of the data?

An additional dimension is added, a PMF (or PDF) - the «Model» - that «interprets» the data in probabilistic terms (e.g, in this two-dimensional space:
$P\left(X_{1}, X_{2} ;\right.$ Positive $)$ and $P\left(X_{1}, X_{2}\right.$; negative ) )


For example: $x$ and $y$ are the body-mass-index and
cholesterol value of a sample population $D$ of diabetic (positive, D+) and non-diabetic (negative. D-) patients.
We are assuming a gaussian distribution of these values, with unknown $\sigma, \mu$


Generative: find parameters that "explain" all data

For example, if we assume that the values of a continuous random variable X follow a Gaussian distribution, we can estimate the parameters of this distribution for the positive and negative examples ( $\sigma_{+} \mu_{+}, \sigma_{-} \mu_{-}$) in D


## Discriminative:

finds parameters that help to predict relevant data.

Note the analogy between the difference between classifiers and regressors, and discriminative and generative models.

## Generative models formulation

- Let $\boldsymbol{M}$ be a probabilistic formulation (model) of a classification task, our training task is to "fit" the model with respect to our dataset D, like for algebraic models. In probabilistic terms, our task is to model the joint probability $\mathrm{P}\left(D ; M_{\boldsymbol{\theta}}\right)$ where $\boldsymbol{\theta}$ are the model parameters («what is the most likely set of parameters that may have generated D??» The training set $D$ now is seen as an «evidence» generated by some unknown distribution)
- Suppose that we know exactly the "structure" of $\boldsymbol{M}$ (e.g. a softmax function or a gaussian), this means that we can express our model in some precise probabilistic form, but the values of its probabilistic parameters $\boldsymbol{\theta}$ (e.g. the weights of softmax or the $\sigma$ of a Gaussian) are unknown. The problem involves finding

$$
M_{\theta} \text { that "best explains" the training data } D
$$

```
Intuitively: To learn the
parameters of the model we
have to maximize a probability
function of observing the
evidence provided by the
training set D.
```

Goal: After observing several examples $\mathrm{X}_{1} . \mathrm{x}_{\mathrm{N}}$ (a so-called "sufficient statistics") estimate the model parameters, $\boldsymbol{\theta}$, that may have generated the observed data.

## Maximum Likelihood Estimation

In statistics, Maximum Likelihood Estimation (MLE) is a method for estimating the parameters of a statistical model M given observations D , by finding the parameter values that maximize the likelihood of observing D. So, again, it is an optimization problem.

What is the «likelihood»?

# Likelihood Function for Random Variables 

- The likelihood function expresses the joint probability (or probability density) of a sample data D, given a set of model parameters values.
- $L_{D}(\theta)=f(D ; \theta)=f\left(x_{1}, x_{2}, \ldots, x_{|D|} ; \theta\right)$
- $\boldsymbol{f}$ is a function of the parameters, that express:
- Discrete Case: probability mass function (PMF) (e.g. Bernoulli, Geometric, Binomial distributions)
- Continuous Case: a probability density function (PDF) (Gaussian, Poisson, Exponential, Softmax..)
- What does likelihood mean and how is "likelihood" different than "probability"?
- Discrete distributions: likelihood is a synonym for the joint probability of your data D
- Continuous Distribution: likelihood refers to the joint probability density of your data D


## Likelihood Function What are these "parameters"?

- The definition of $\boldsymbol{\theta}$ is quite general.
- A set of parameters $\left\{\Theta_{1}, \Theta_{2}, \ldots, \Theta_{m}\right\}$
> Discrete Case: the parameters are probabilities $\mathrm{P}(\mathrm{Xi}=\mathrm{xi})$, e.g. $P($ Color $=$ red) or conditioned probabilities $P(Y=y \mid X=x)$ (e.g. P(Y=yes/Color=red)
> Continuous Case: the parameters are the coefficients in a probabilistic formulation (e.g., if M is the softmax function (a.k.o. exponential) : $y_{i}=\operatorname{softmax}(\boldsymbol{x}, W)=$ $\frac{e^{x_{i} w_{i}}}{\sum_{j} e^{x_{j} w_{j}}}$ ) parameters $\boldsymbol{\theta}$ are the $\mathrm{w}_{\mathrm{j}}$; if M is a gaussian, $\boldsymbol{\theta}$ are $\sigma$ and $\mu$ )


## Statistical Parameter Fitting (general definition for multivariate case)

- Consider instances in dataset $D:<\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{|\boldsymbol{D}|}>$
- such that:
- The set of values that $\mathrm{y}=Y(\boldsymbol{x})$ can take is known (to simplify, let's $Y$ be univariate and either binomial or multinomial)
- Each $\boldsymbol{x}_{\boldsymbol{i}}$ is sampled from the same distribution
- Each $\boldsymbol{x}_{\boldsymbol{i}}$ is sampled independently of the rest

The task is to find a vector of parameters:
$\Theta$ that have generated the given data $D$. This vector parameter $\Theta$ can be used to (probabilistically) predict the class of future data

## Maximum Likelihood Estimation

## MLE Principle:

Given sufficient statistics, choose parameters that maximize the likelihood function (the likelihood of observing data)

$$
\Theta_{o p t i m a l}=\operatorname{argmax}_{\mathrm{C}}(L(D ; \Theta))=\operatorname{argmax}_{\Theta}(P(D ; \Theta))
$$

- A "sufficient statistics" is a function whose value contains all the information needed to compute any estimate of the parameters
- In MLE we seek the model parameters $\Theta$ that maximize the likelihood ( $\operatorname{argmax}_{\boldsymbol{\theta}}(L)$ ), and the likelihood is expressed as a conditional probability. It is thus an optimization problem (as for all ML algorithms!)


## Maximum Likelihood Estimation

Finding MLE's involves techniques of differential calculus (as usual). To maximize $L_{D}(\boldsymbol{\theta})$ with respect to each $\theta i$ in $\boldsymbol{\theta}$ :

1. First calculate the (partial) derivative of $L_{D}(\boldsymbol{\theta})$ with respect to all $\theta i$,
2. Set the derivative equal to zero, and
3. Solve the resulting equation for $\theta i$.

- These computations can often be simplified by maximizing the log-likelihood function:

$$
\begin{gathered}
l_{D}(\boldsymbol{\theta})=\ln \left(L_{D}(\boldsymbol{\theta})\right) \\
l_{D}(\boldsymbol{\theta})=\sum_{i=1}^{|D|} \ln \left(\boldsymbol{P}\left(\boldsymbol{x}_{\boldsymbol{i}} ; \boldsymbol{\theta}\right)\right) \text { (in the i.i.d.case) }
\end{gathered}
$$

- The natural log is an increasing function, maximizing the log-likelihood is the same as maximizing the likelihood. The loglikelihood often has a much simpler form than the likelihood and is usually easier to differentiate.


## Likelihood Function for discrete variables

- First, we deal with discrete distributions of random variables (so we can directly use the classical probability notation $P$ instead of $f$ ).

$$
L_{D}(\theta)=P(D ; \theta)=P\left(x_{1}, x_{2}, \ldots, x_{|D|} ; \theta\right)
$$

- Note: Categorical distributions like Bernoulli, Binomial and Multinomial are discrete distributions!!!
- For different values of the parameters, the likelihood of our data will be different. For that reason we write likelihood as a function of our parameters ( $\theta$ )
- Furthermore, if the random variables (instances in $X$ ) are identical and independently distributed (i.i.d.), we can apply the independent and identically distributed assumption to the likelihood:

$$
\begin{gathered}
\qquad \boldsymbol{L}_{\boldsymbol{D}}(\boldsymbol{\theta})=\boldsymbol{P}(\boldsymbol{D} ; \boldsymbol{\theta})=\prod_{\boldsymbol{i}=\mathbf{1}}^{|\boldsymbol{D}|} \boldsymbol{P}(\boldsymbol{x i} ; \boldsymbol{\theta}) \\
\text { The joint distribution } P\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{|\boldsymbol{D}|} ; \boldsymbol{\theta}\right)
\end{gathered}
$$

can be expressed as the product of independent joint probabilities of observing each instance!

## MLE for Binomial Distribution (univariate)

- Suppose that $\left(x_{1}, x_{2}, \ldots, x_{|D|}\right)$ represents $n=|D|$ i.i.d. samples of a binary random variable $Y$, that follows a binomial distribution. Let $\theta$ be the probability that a sample $x_{j}$ is equal to 1 , and ( $1-\theta$ ) the probability of being 0 . (Note: $Y$ is here univariate, therefore is not in bold)
- Note: The binomial distribution here could model both the distribution of class labels $y_{j}$ AND the distribution of feature values $x_{i}$ in case of discrete features. The purpose is just to see how MLE applies to these types of distributions.
- Consider the PMF (probability mass function) of a Binomial distribution where $r$ is the number of times we observe $x=1$ in $n$ trials (e.g., the PMF modeling the probability of observing $r$ " $1 s$ " in the $n$ samples in $D$ ):

$$
P(D ; \theta)=\frac{n!}{r!(n-r)!} \theta^{r}(1-\theta)^{n-r}
$$

So, if the MODEL is a Binomial distribution, the only parameter is $\theta$ the probability $P(x=1)$

## MLE for Binomial Distribution

- The likelihood for $\theta$ based on the observation of $n$ samples is defined as the joint probability distribution of observing a sequence of n binary values $\left(y_{1}, y_{2}, \ldots, y_{n}\right)$ such that every $y_{i}$ is either 1 or 0 . Since $\left(y_{1}, y_{2}, \ldots, y_{n}\right)$ are i.i.d. observations of the random variable $X$, the joint distribution is:

$$
\begin{gathered}
L_{D}(\boldsymbol{\theta})=P(D ; \theta)=\prod_{i=1}^{n} P\left(y_{i} ; \boldsymbol{\theta}\right)=\theta^{r}(1-\theta)^{n-r} \\
\text { such that: } \theta+(1-\theta)=1 \text { and } \theta \geq 0
\end{gathered}
$$

- Note that the constant $\frac{n!}{r!(n-r)!}$ of the binomial distribution is not necessary in the likelihood formula. Since the $L_{D}(\boldsymbol{\theta})$ is a function on $\boldsymbol{\theta}$, and $\frac{n!}{r!(n-r)!}$ is a fixed constant, it does not affect the MLE (maximization).
- The constant values in the expression of $P\left(x_{i} ; \boldsymbol{\theta}\right)$ are statistically irrelevant.


## MLE for Binomial Distribution

- Note that the values of $r$ and $n$ - $r$ in previous formula are, respectively, $N_{1}$ (the number of observed samples where $Y=1$ ) and $N_{o}$ (the number of samples with $Y=0$ ) in $D\left(|D|=n=N_{1}+N_{0}\right)$. They represent a sufficient statistics to estimate the parameter $\theta$ of the binomial distribution
- We can employ MLE to estimate $\theta$ using the log-likelihood:

$$
l_{D}(\theta)=\log \left(L_{D}(\boldsymbol{\theta})\right)=N_{1} \log \theta+N_{0} \log (1-\theta)
$$

- With $\theta+(1-\theta)=1$
- Taking derivative $\frac{\partial\left(l_{D}(\theta)\right)}{\partial(\theta)}$ and equating it to 0 we obtain (log is the natural log):

Note: $\hat{\theta}$ is our ESTIMATE of the parameter, given the evidence

$$
\frac{N_{1}}{\theta}=\frac{N_{0}}{1-\theta} \rightarrow \hat{\theta}=\frac{N_{1}}{N_{0}+N_{1}}=\frac{N_{1}}{|D|}=\frac{N_{1}}{n}
$$

## MLE for Multinomial Distribution

- Suppose that $D=\left(x_{1}, x_{2}, \ldots, x_{n}\right)$ represents n i.i.d. samples ( $n=|D|$ ) of a random variable X . The random variable is now multinomial, i.e., it can assume one out of k different values each with probability $\theta_{j}$ (e.g., assigning a category label to a document in a predictive task )
- Consider the PMF of a Multinomial distribution:

$$
P(D ; \theta)=\frac{n!}{r_{1}!r_{2}!\ldots r_{k}!} \theta_{1}^{r_{1}} \theta_{2}^{r_{2}} \ldots \theta_{k}^{r_{k}}=\frac{n!}{r_{1}!r_{2}!\ldots r_{k}!} \prod_{j=1}^{k} \theta_{j}^{r_{j}}
$$

Where $r_{j}$ is the number of occurrences of the outcome $j$. Each $r_{j}$ can be estimated by the dataset D.

- Notice that in the multinomial distribution, the Maximum likelihood parameter vector $\boldsymbol{\theta}$ is composed by a set of k probabilities $\theta_{1} \theta_{2} \ldots \theta_{k}$ of observing each possible outcome $X=x_{j}$.


## MLE for Multinomial Distribution

- Since $\left(x_{1}, x_{2}, \ldots, x_{n}\right)$ are i.i.d., the joint distribution is:
(1) $L_{D}(\boldsymbol{\theta})=P(D ; \boldsymbol{\theta})=\prod_{i=1}^{n} P\left(x_{i} ; \boldsymbol{\theta}\right)=\prod_{j=1}^{k} \theta_{j}^{r_{j}}$ such that: $\sum_{i} \theta_{i}=1$ and $\theta_{i} \geq 0 \forall i$
- Since the $L_{D}(\boldsymbol{\theta})$ is a function on $\boldsymbol{\theta}, \frac{n!}{r_{1}!r_{2}!\ldots r_{k}!}$ is a fixed constant, it does not affect the MLE (maximization)! As before, the constants are statistically irrelevant.
- In this case the «sufficient statistics» are $r_{1}, r_{2} \ldots r_{k}$, e.g. the observations of the of |D| values xi of the multinomial random variable X (we observe $r_{1}$ times value $\mathrm{x}_{1}$, ecc.)
- To calculate the log-likelihood and incorporating constraints (the «such that» above) we can use the Lagrangian method


## Lagrangian optimization

Given a function $f(x)$ and a set of constraints $c_{1}, . . c_{n}$, a Lagrangian is a function $L\left(f, c_{1}, . . c_{n}, \alpha_{1}, . . \alpha_{n}\right)$ that "incorporates" the constraints in the optimization problem

$$
L(x, \alpha)=f(x)-\sum \alpha_{i} c_{i}(x)
$$

Karush-Kuhn-Tucker (KKT) conditions: The optimum is at a point where

2) $\alpha_{i} \geq 0$
3) $\alpha_{i} c_{i}(x)=0 \forall i \quad$ This condition is known as complementarity condition (it means that at least one of $\alpha_{i}, \mathrm{c}_{\mathrm{i}}(\mathrm{x})$ must be zero).

## MLE optimization with Lagrangian

- MLE optimization then implies first, incorporating the constraints with lagrangians
- From previous equation (1) by applying the log and incorporating constraints ( $\alpha$ is the lagrangian coefficient), we obtain:

$$
l_{D}(\theta)=\sum_{j} r_{j} \log \theta_{j}+\alpha\left(1-\sum_{j} \theta_{j}\right)
$$

- Next, we apply the partial derivatives vrs. each $\theta_{j}$ and set them to zero, and solve equations considering that $\sum_{j} \theta_{j}=1$

$$
\theta_{j}=\frac{r_{j}}{\sum_{i} r_{i}}=\frac{r_{j}}{|D|}=\frac{r_{j}}{n}
$$

## MLE for supervised learning

- Previous formulas estimate the probability of observing a given value $x_{j}$ in an «unconditional» setting, that is: we estimate the likelihood of observing a given «outcome» in the data, regardless of the function $y=f(x)$ that generates these outcomes.
- The MLE principle is:

$$
\theta_{M L E}=\operatorname{argmax}_{\theta}(P(D ; \theta))
$$

- Where $\theta$ are the parameters of $M$, a model that may represent the distribution of data, e.g. a binomial.
- We now need to apply MLE to a supervised context where we consider both input and output data ( $x$ and $y$ )

$$
\theta_{M L E}=\operatorname{argmax}_{\theta}(P(D ;(\boldsymbol{x}, \theta)))
$$

## Example of prediction with MLE

- Suppose we have univariate multinomial instances $x$ describing a unique feature: the age of citizens (values are, e.g.: A: [16-20) B:[20-23) C[23-28) D [28, 100]), the class label is binary and represents their average cellular phone bill, where $Y=0 \rightarrow$ less than $€ 100$, $Y=1 \quad \gg=€ 100$
- Step 1: we partition our data (patients) in two subsets $\mathrm{D}_{\mathrm{Y}=0}$ and $\mathrm{D}_{\mathrm{Y}=1}$;
- Step 2: we assume that x follows a multinomial distribution, and we estimate, for each subset $\mathrm{D}_{\mathrm{Y}=\mathrm{i}}$ separately, the model parameters $\Theta_{D_{Y=i}}$ using the log-likelyhood maximization seen above
- Step 3: given a new unseen instance $x^{\prime}$, we predict the class $Y$ as

$$
Y=\operatorname{argmax}_{j}\left(P\left(x^{\prime} ; Y=j\right)\right)
$$

- in practice this will be the most likely bill range for citizens aged in the range $A, B, C$ or $D$, to which $x$ belongs. We select the class value $j$ that maximizes the probabilty that $x$ has been generated by the model $\mathrm{M}\left(\mathrm{D}_{Y=j}\right)$ with parameters $\boldsymbol{\Theta}_{D_{Y=i}}$


## MLE for continuous variables



Suppose we have data points representing the average of past grades of students in a class (so we have only one feature for each instance, a univariate problem, but now the variable is continuous), and we want to predict if they will pass a new test. (in our train set $D$, red passed test $T_{i}$, green did not). So here $x$ is continuous, $y$ is binary. In the histogram, $x$ is the average, y is the \% of the population with that average value, the color distinguishes the distribution (in our sample) of those who passed and those who not passed.

## MLE for Gaussian distribution

- Given our data, let's suppose that the model for input variable X (average grade) follows approximately a Gaussian distribution
- So the model $M$ is (probability density of $X$ in C ):

$$
p(x \mid C)=\frac{1}{\sqrt{2 \pi} \sigma_{c}} \exp \left(-\frac{\left(x-\mu_{C}\right)^{2}}{2 \sigma_{C}^{2}}\right)
$$

- Note, as for the discrete case before, that $\boldsymbol{\theta}$ parameters ( $\sigma_{C=1} \mu_{C=1} ; \sigma_{C=0} \mu_{C=0}$ ) are DIFFERENT for each class C (those who passed and those who didn't).
- In the example we have just two classes (the output C is binomial) and one feature (univariate, continuous) but this applies in general to multiple classes and multiple features - each would follow a Gaussian)


## Example (3): fitting the model with data



We need to find, for each subset of samples (in our example, students who passed test Ti and those who did'nt), the values of $\theta$ parameters $\sigma, \mu$ of the Gaussian, such that $P\left(D_{C} ; \theta\right)$ best «fits» the observed data.

## Example: MLE for Gaussian distributions

- Let $D_{C i}$ be the subset of D of instances with class $\mathrm{C}=\mathrm{C}_{\mathrm{i}}(0$ or 1 ) and lets' use a superscript to denote different instances $\boldsymbol{x}^{(i)}$ in $D_{C i}$ (so that for multi-variate observations we can denote with subscripts their features).
- We then have for the log-likelyhood (we omit the Ci subscript to avoid overloading the notation and furthermore $\left|D_{C i}\right|=N$ ):
$x^{(n)}$ is the $n$-th
observation inD

$$
\begin{array}{r}
l_{D}(\boldsymbol{\theta})=-\ln \left(\prod_{n=1}^{N} \frac{1}{\sqrt{2 \pi} \sigma} \exp \left(-\frac{\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{2}}\right)\right) \\
=\sum_{n=1}^{N} \ln (\sqrt{2 \pi} \sigma)+\sum_{n=1}^{N} \frac{\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{2}}=\frac{N}{2} \ln \left(2 \pi \sigma^{2}\right)+\sum_{n=1}^{N} \frac{\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{2}}
\end{array}
$$

We have two parameters, $\mu$ and $\sigma$

## Computing partial derivatives

- We then apply the derivative $\frac{\partial(l)}{\partial \mu}$ to the log likelihood and set to zero

$$
\begin{aligned}
& =\frac{\partial\left(\frac{N}{2} \ln \left(2 \pi \sigma^{2}\right)+\sum_{n=1}^{N} \frac{\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{2}}\right)}{\partial \mu}=\frac{d\left(\sum_{n=1}^{N} \frac{\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{2}}\right)}{d \mu} \\
& =\frac{-\sum_{n=1}^{N} 2\left(x^{(n)}-\mu\right)}{2 \sigma^{2}}=-\sum_{n=1}^{N} \frac{\left(x^{(n)}-\mu\right)}{\sigma^{2}}=\frac{N \mu-\sum_{n=1}^{N} x^{(n)}}{\sigma^{2}}
\end{aligned}
$$

- Setting to zero the derivative ( $\rightarrow$ numerator must be $=0$ ), we obtain:

$$
\mu=\frac{1}{N} \sum_{n=1}^{N} x^{(n)}
$$

## Computing partial derivatives

- Next, we compute derivative $\frac{\partial l}{\partial \sigma}$ and set it to 0
,

$$
\begin{aligned}
&=\frac{\partial\left(\frac{N}{2} \ln \left(2 \pi \sigma^{2}\right)+\sum_{n=1}^{N} \frac{\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{2}}\right)}{\partial \sigma^{2}} \\
&=\frac{N}{2} \frac{1}{2 \pi \sigma^{2}} 2 \pi+\frac{\sum_{n=1}^{N}\left(x^{(n)}-\mu\right)^{2}}{2}\left(\frac{-1}{\sigma^{4}}\right) \\
&=\frac{N}{2 \sigma^{2}}-\frac{\sum_{n=1}^{N}\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{4}} \\
& 0=\frac{N}{2 \sigma^{2}}-\frac{\sum_{n=1}^{N}\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{4}}=\frac{N \sigma^{2}-\sum_{n=1}^{N}\left(x^{(n)}-\mu\right)^{2}}{2 \sigma^{4}} \\
& \sigma^{2}=\frac{1}{N} \sum_{n=1}^{N}\left(x^{(n)}-\mu\right)^{2}
\end{aligned}
$$

(which is a rather obvious result.. )
This generalizes in a straightforward way to the multivariate case (multiple features): now $\boldsymbol{x}^{\boldsymbol{n}} \boldsymbol{\sigma}, \boldsymbol{\mu}$ are vectors, and we compute partial derivatives

$$
\frac{\partial l}{\partial \mu_{i}}, \frac{\partial l}{\partial \sigma_{i}}
$$

## When the model parameters have been estimated, how is a new prediction made with MLE?

Given a new instance $\mathbf{x}$ (we now suppose $\mathbf{x}$ is a vector), and having estimated the parameters of the generative models for each possible class, we compute $P\left(\mathbf{x} \mid C_{i}\right)$ for each model, and compute the argmax


## Maximum A Posteriori (MAP) another generative model

- MAP is an alternative probabilistic formulation of ML problems, still belonging to the generative class of models
- In short, the essential difference wrt MLE is in what is modeled using probability theory. MLE first, learns a joint probability $\boldsymbol{L}_{\boldsymbol{D}}(\boldsymbol{\theta})=\boldsymbol{f}(\boldsymbol{D} ; \boldsymbol{\theta})$ and then, to predict a class, estimates the argmax of $P(X=x ; Y=y i)$ for every output value or class
- MAP uses a Bayesan approach: The formulation is a conditional probability $A / B$ rather than a joint probability A;B.
- MAP estimates conditional probabilities rather than the parameters of a distribution


## Maximum A Posteriori estimate

- In MAP, the probabilistic model M is: $P(Y=y \mid \boldsymbol{X}=\boldsymbol{x})(\mathrm{P}(\mathrm{y} \mid \mathbf{x})$ for short), the conditional probability of class label $y$, given the observation of an instance $\mathbf{x}$
- The prediction is computed as $\mathrm{y} *=\operatorname{argmax}_{y j}\left(\mathrm{P}\left(Y=y_{j} \mid \mathrm{X}=\mathbf{x}\right)\right)$ (remember, in MLE we computed the joint probability $\mathrm{P}(\mathbf{x} ; \mathrm{Y}(\mathbf{x}))$ !!)
- As for MLE, we need to estimate the parameters $\boldsymbol{\theta}$ of M

```
Learn the values of model parameters that
maximize the the conditional probability of a class
label y given the observation of x. Model
parameters are probabilities.
```

- The solution of the problem is based on the Bayes theorem


## Maximum a posteriori estimate learning

- Similarly to MLE, we estimate $y_{i}$ by maximizing a probability function distribution, which is for MAP:

$$
y^{*}=\operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i} \mid X=\boldsymbol{x}\right)\right)
$$

- In probability calculus, often estimating $P(a \mid b)$ is easier that estimating $P(b \mid a)$ so MAP applies the Bayes theorem to invert conditional probabilities

$$
\begin{gathered}
y^{*}=\operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i} \mid X=\boldsymbol{x}\right)\right)=\operatorname{argmax}_{y_{i}}\left(\frac{P\left(Y=y_{i}\right) P\left(X=\boldsymbol{x} \mid Y=y_{i}\right)}{P(X=\boldsymbol{x})}\right) \\
\approx \operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) P\left(X=\boldsymbol{x} \mid Y=y_{i}\right)\right)
\end{gathered}
$$

- Note that since the denominator $P(X=\boldsymbol{x})$ is common to all the probabilities, it does not affect the ranking in the argmax computation. No need to compute it!!!
- Also note that the problem is now formuled both in terms of prior probabilities (the $P\left(Y=y_{i}\right)$ ) of the random variable to be predicted, and conditional probabilities $\mathrm{P}(\mathrm{X} \mid \mathrm{Y})$

Given previous formula, how does MAP works?

Conditionals Priors

$$
\theta_{M A P}=\underset{\theta}{\arg \max } P(X \mid \theta) P(\theta)
$$

$$
\begin{array}{ll}
=\underset{\theta}{\arg \max } \log P(X \mid \theta)+\log P(\theta) & \text { Apply log } \\
=\underset{\theta}{\arg \max } \log \prod_{i} P\left(x_{i} \mid \theta\right)+\log P(\theta) & \begin{array}{l}
\text { Use property of independence } \\
\text { of observations }
\end{array}
\end{array}
$$

$$
=\underset{\theta}{\arg \max } \sum_{i} \log P\left(x_{i} \mid \theta\right)+\log P(\theta)
$$

Change product with sum (property of logs)

# Probabilistic Classification with MAP (multinomial, multivariate $X$ and $Y$ ) 

- Let $\boldsymbol{Y}$ be a univariate multinomial random variable for the output class $Y$ which takes values

$$
\left\{y_{1}, y_{2}, \ldots, y_{n}\right\} \text { ( } n \text { possible classifications for our instances). }
$$

- Let $X$ be a multivariate multinomial random variable describing input instances consisting of $\boldsymbol{d}$ features
- $\left.\boldsymbol{x}:<X_{1}, X_{2}, \ldots, X_{d}\right\rangle$, let $x_{j}$ be a possible value for the feature $X_{j}(j=1, \ldots, d)$
- Remember: we now use uppercase Xi for features, to suggest that features are random variables, lowercase for instances xi (random vectors) of $X$ in $D$.
- Since features Xi are multinomial (multiple values), for our classification task, we need to compute the conditional probabilities:

$$
\begin{gathered}
P\left(Y=y_{i} \mid X=\boldsymbol{x}:<X_{1}=x_{1}, \ldots, X_{d}=x_{d}>\right) \text { for } i=1, \ldots, n \\
\text { (e.g. } P(Y=\text { positive } \mid X=\boldsymbol{x}:<\text { color }=\text { blue, shape }=\text { circle }>) \text { ) }
\end{gathered}
$$

Remember:

- Multinomial is a random variable that can take a finite number of values
- Multivariate is a random vector made of multiple random variables


## Probabilistic Classification

$$
\begin{aligned}
& P\left(Y=y_{i} \mid X=x<X_{1}=x_{1}, \ldots, X_{d}=x_{d}>\right) \text { for } i=1, \ldots, n \\
& \text { (e.g. } P(Y=\text { positive } \mid X=\boldsymbol{x}<\text { color }=\text { blue, shape }=\text { circle }>) \text { ) }
\end{aligned}
$$

- the objective is to classify a new unseen instance $\boldsymbol{x}$ by first estimating the probability of each possible classification $y_{i}$, given the observation of feature values of the instance to be classified
- To estimate $P\left(Y=y_{i} \mid \boldsymbol{X}=\boldsymbol{x}\right)$ we use a learning set $\mathbf{D}$ of pairs $(\boldsymbol{x}, Y(x))$
- Summary notation:
- $i$ is index of class values ( $Y$ is univariate and multinomial)
- $j$ is index of features ( $X$ is multivariate, $X j$ are multinomial)
- uppercase $X_{j}$ is a feature, lowercase $x_{j}$ is a value
- Bold lowercase $\mathbf{x}$ is a specific instance in $\mathrm{D}(\mathbf{x} \in X)$ - here the idea is that uppercase represents a random variable, lowercase an observation.
- We omit the superscript h of instances $\mathbf{x}^{\mathrm{h}}$ in D (unless strictly necessary) to avoid overloading the notation


## How can we compute

$$
P\left(Y=y_{i} \mid X=\boldsymbol{x}\right) ? ?
$$

- Example: we observe the instance $\mathbf{x}<$ color $=$ red, shape $=$ circle> (two symbolic features) and there are two possible classes $\mathbf{Y}<\mathrm{y}_{1}=$ positive, $\mathrm{y}_{2}=$ negative $>$
- Possible values for features are: color:\{red,blue\} ; shape:\{circle, square\}
- We need to compute:

$$
\begin{aligned}
& P(\text { positive } \mid \text { red circle })=\frac{P(\text { positive red circle })}{P(\text { red circle })} \\
& P(\text { negative } \mid \text { red circle })=\frac{P(\text { positive red circle })}{P(\text { red circle })}
\end{aligned}
$$

- So we need to estimate the joint probabilities (e.g. P(positive^red^circle))
- The joint probability distribution for a set of random independent variables gives the probability of every combination of values


## Joint probability tables

$P($ shape $=$ circle, color $=$ blue,$C=$ positive $)$

Class $=$ positive

|  | circle | square |
| :--- | :--- | :--- |
| red | 0.20 | 0.02 |
| blue | 0.02 | 0.01 |

Class $=$ negative

|  | circle | square |
| :--- | :--- | :--- |
| red | 0.05 | 0.30 |
| blue | 0.20 | 0.20 |

- The probability of all possible conjunctions (= assignments of values to some subset of features) can be estimated from the training set, by summing the appropriate subset of values from the joint distribution.
$P($ red circle $)=P($ red circle positive $)+P($ red circle negative $)=0.20+0.05=0.25$
- If all joint probabilities can be estimated, all conditional probabilities can be

$$
\begin{aligned}
& \text { calculated. } \\
& \quad P(\text { positive } \mid \text { red } \wedge \text { circle })=\frac{P(\text { positive } \wedge r e d ~}{P(\text { circle })} \\
& P(\text { red } \wedge \text { circle })
\end{aligned}=\frac{0.20}{0.25}=0.80
$$

## Example

Consider this learning set D of 5 annotated instances:

- $\mathbf{x}^{1}$ (red, circle), positive
- $\mathbf{x}^{2}$ (red,square), negative
- $\mathbf{x}^{3}$ (blue,circle), positive
- $\mathbf{x}^{4}($ red, circle), negative
- $\mathbf{x}^{5}$ (red, circle), positive

$$
P(\text { positive } \mid r e d \wedge \text { circle })=\frac{P(\text { positive } \wedge r e d \wedge \text { circle })}{P(r e d \wedge \text { circle })}=\frac{\frac{2}{5}}{\frac{3}{5}}=\frac{2}{3}
$$

## Probabilistic Classification

- However, given no other assumptions, this requires tables assigning a probability to each category label for each possible combination of feature values in the instance space $\mathbf{X}$, which is impossible to accurately estimate from a reasonably-sized training set $\mathbf{D}$.
- E.g $P\left(Y=y_{i} \mid X_{1}=x_{1}, X_{2}=x_{2}, \ldots, X_{d}=x_{d}\right)$ for all $y_{i}$ and $x_{j}$ Assuming that $Y$ and all $X_{i}$ are binomial, and we have $\boldsymbol{d}$ features, we need $\mathbf{2}^{\boldsymbol{d}}$ entries to estimate $P\left(Y=p o s \mid X=\boldsymbol{x}^{\boldsymbol{k}}\right)$ for each of the $\mathbf{2}^{\boldsymbol{d}}$ possible combinations of feature values since:
- $P(Y=n e g \mid X=\boldsymbol{x})=1=1-P(Y=\operatorname{pos} \mid X=\boldsymbol{x})$
- Given:
- An unclassified random vector $\boldsymbol{x}$, which is represented by $d$ discrete features (e.g. binomial or multinomial)
- A multinomial classification function $Y(\mathbf{x})$ with possible values $\left\{y_{1}, \ldots, y_{m}\right\}$


## Summary MAP so far

- The target of the probabilistic classifier is to classify $\boldsymbol{x}$ based on:
$y^{*}=\operatorname{argmax}_{y_{i}}\left(P\left(y_{i} \mid \boldsymbol{x}\right)\right)$
(the most likely classification given the specific combination of feature values in $\boldsymbol{x}$ )
- The parameters of the model are the $P\left(y_{i} \mid \boldsymbol{x}\right)$
- We need to estimate $P\left(y_{i} \mid \boldsymbol{x}\right)$ for all $y_{i}$, using the evidence provided by the previously seen instances $\left\langle x_{i}, y_{i}\right\rangle$ in $D$
- Quite likely, the specific combination of feature values of $\boldsymbol{x}$ is not in the learning set: even if values are boolean, there are $\mathbf{2}^{\text {d }}$ possible combinations! So how do we go about it?


## Naïve Bayes classifier: <br> an ML algorithm based on MAP

## Naïve Bayes Model

Let's define the model:

- We are given an evidence represented by an annotated learning set $D$ of classified instances ( $x, y$ ).
- Consider an instance $\boldsymbol{x}$ as a random vector of $d$ random variables

$$
<X_{1}, X_{2}, \ldots, X_{d}>
$$

- Each $X_{j}$ feature can assume a discrete value $x_{k} \in\left\{1, \ldots, d_{j}\right\}$ (i.e. binary or multinomial)
- The class variable is a multinomial random variable $Y$ that can take a set of values $y_{i}$ with $\mathrm{i}=1, . ., n$, usually categorical (e.g., red, blue,..)

Naïve Bayes assumption: all the $X_{i}$ are statistically independent

## Naïve Bayes Model

- Our goal is to make a prediction, based on a conditional probability model $P(Y \mid X)$, whose parameters can be estimated considering the dataset D (Training)
- For MAP and Bayes Theorem, this requires to compute (see previous slides):

$$
y^{*}=\operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) P\left(X=\boldsymbol{x} \mid Y=y_{i}\right)\right)
$$

Where x is a vector of feature values $<X_{1}=x_{1}, X_{2}=x_{2}, \ldots, X_{d}=x_{d}>$

## Naïve Bayes Model

How can we calculate $P\left(X=\boldsymbol{x}<x_{1}, \ldots, x_{d}>\mid Y=y_{i}\right)$ ?

$$
P\left(\boldsymbol{x}=<X_{1}=x_{1}, X_{2}=x_{2}, \ldots, X_{d}=x_{d}>\mid Y=y_{i}\right)=
$$

## By Independence assumption (e.g. Naïve Bayes Assumption):

$$
=\prod_{j=1}^{d} P\left(X_{j}=x_{j} \mid Y=y_{i}\right)
$$

We assume that features' random variables are also statistically independent!

To classify a new instance we apply the MAP formulation + NB assumption:

$$
\begin{gathered}
y^{*} \approx \operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) P\left(X=\boldsymbol{x} \mid Y=y_{i}\right)\right)= \\
\operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) \prod_{j=1}^{d} P\left(X_{j}=x_{j} \mid Y=y_{i}\right)\right)
\end{gathered}
$$

## Naïve Bayes Model

Now, we have to estimate the priors $P\left(Y=y_{i}\right)$ and the conditionals $P\left(X_{j}=\right.$ $x_{j} \mid Y=y_{i}$ ) (our parameters)

- $P\left(Y=y_{i}\right)$ can be estimated directly from the learning set D , since categories are complete and disjoint
- Next we use again likelyhood to estimate two sets of parameters $\theta^{1}$ and $\theta^{2}$ :
- $\theta^{1}: P\left(Y=y_{i}\right)$ (the priors)
- $\theta^{2}: P\left(X_{j}=x_{j} \mid Y=y_{i}\right)=\frac{P\left(X_{j}=x_{j} Y ; Y=y_{i}\right)}{P\left(Y=y_{i}\right)}$ (the conditionals)


## Naïve Bayes Model

- The estimate of parameters depend on the random variable distribution:
$>$ Categorical Distributions (e.g. Binomial, Multinomial, Geometric)
> Gaussian, exponential..
$>$ Etc.
- Let first suppose that both $Y$ and the $X_{j}$ follow a multinomial distribution, then (for what we have seen in previous slides ), using the likelyhood maximization:

$$
\boldsymbol{\theta}_{i}^{1}=\frac{N\left(y_{i}\right)}{|D|} \quad \boldsymbol{\theta}_{i j}^{2}=\frac{N\left(x_{j}, y_{i}\right)}{N\left(y_{i}\right)}
$$

- Where $N\left(y_{i}\right)$ is the number of instances classified $y_{i}$ in the training set (so $\boldsymbol{\theta}_{i}^{1}$ are the priors);
- Where $N\left(x_{j}, y_{i}\right)$ is the number of times the label $y_{i}$ is seen in conjunction with feature value $x_{j}$ in D : number of instances in D in which $X_{j}=x_{j}$ and $Y=y_{i}$

Note that these formulas are obtained exactly as for the MLE case (see previous slides): we consider the log of the multinomial for each random variable, then take the derivative and equate to 0 (ignoring the constant values).

## Naïve Bayes Model

## Make Predictions

Finally to make a prediction for a new instace $\boldsymbol{x}=<X_{1}=x_{1}, X_{2}=x_{2}, \ldots, X_{d}=x_{d}>$ we must calculate:

$$
\begin{gathered}
y^{*} \approx \operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) P\left(X=x \mid Y=y_{i}\right)\right)= \\
\operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) \prod_{j=1}^{d} P\left(X_{j}=x_{j} \mid Y=y_{i}\right)\right)=
\end{gathered}
$$

$$
\operatorname{argmax}_{y_{i}}\left(\frac{N\left(y_{i}\right)}{|D|} \prod_{j=1}^{d} \frac{N\left(x_{j}, y_{i}\right)}{N\left(y_{i}\right)}\right)
$$

- Where $N\left(y_{i}\right)$ is the number of instances classified with label $y_{i}$ in the training set;
- Where $N\left(x_{j}, y_{i}\right)$ is the number of times the label $y_{i}$ is seen in conjunction with the feature $\mathrm{Xj}=x_{j}$


## Naïve Bayes Model Example

| $\mathbf{X}$ | X1 |  | X2 | X3 |
| :--- | :--- | :--- | :--- | :--- |
| 1 | med | red | circ | pos |
| 2 | sm | blue | tri | pos |
| 3 | med | red | tri | pos |
| 4 | lg | grn | circ | pos |
| 5 | lg | red | circ | pos |
| 6 | sm | blue | circ | pos |
| 7 | sm | red | sqr | pos |
| 8 | med | red | circ | pos |
| 9 | $\lg$ | red | sqr | neg |
| 10 | sm | blue | tri | neg |
| 11 | med | grn | circ | neg |
| 12 | med | grn | tri | neg |
| 13 | lg | red | circ | neg |
| 14 | sm | blue | sqr | neg |
| 15 | sm | blue | tri | neg |
| 16 | lg | grn | sqr | neg |

$$
|D|=16, d=3
$$

$$
\begin{aligned}
& \mathrm{X} 1=\text { size } \mathrm{X} 2=\text { color } \mathrm{X} 3=\text { shape } \\
& \mathrm{X} 1=\{\text { small, medium, large }\} \\
& \mathrm{X} 2=\{\text { red, green, blue }\} \\
& \mathrm{X} 3=\{\text { triangle, } \text { square, circle }\} \\
& \mathrm{Y}=\{\text { pos, } \mathrm{ne} \text { \} }\}
\end{aligned}
$$

## Naïve Bayes Model Example

- Urns represent occurrences of feature values in training set D. Red urns are positive, blue negative. Separate urns indicate statistical independence of features (sampling of values from each urn does not affect the others).


Category


## Naïve Bayes Inference Problem

Let's say we have a new unclassified instance $x$ : $\langle$ large, red, circle $\rangle$.
We need to estimate, using the learning set D , the class label $y i$ that maximizes the probability of observing $x$ : < large, red, circle $>$. Is it more likely to extract this combination from red or from blue urns?


Category


Positive


## How?

## We fill urns using the available dataset D



Now we can compute parameters $\theta_{i}^{1}$ and $\theta_{i j}^{2}$


## Using parameters we can classify unseen instances

For example, $\mathbf{x}$ :<medium ,red, circle> $\mathbf{y}=$ ?

| For example, $\mathbf{x}:<$ medium, red, circle> $\mathbf{y}=$ ? |
| :--- |
| Probability $\mathrm{Y}=$ positive $\mathrm{Y}=$ negative <br> $\mathrm{P}(Y)$ 0.5 0.5 <br> $\boldsymbol{y}^{*} \approx \operatorname{argmax}_{y_{i}}\left(\boldsymbol{\theta}_{i}^{1} \prod_{j=1}^{d} \boldsymbol{\theta}_{i j}^{2}\right)$   <br>  $3 / 8$ $2 / 8$ <br>  $5 / 8$ $2 / 8$ <br> $\mathrm{P}($ circle $\mid Y)$ $5 / 8$ $2 / 8$ |

$\mathrm{P}($ positive $\mid X)=\mathrm{P}($ positive $) * \mathrm{P}($ medium $\mid$ positive $) * \mathrm{P}($ red $\mid$ positive $) * \mathrm{P}($ circle $\mid$ positive $) / \mathrm{P}(\mathrm{X})$ $0.5 \quad * \quad 3 / 8 \quad * \quad 5 / 8 \quad * \quad 5 / 8$

$$
=0,073
$$

$$
\begin{gathered}
y^{*}=\operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i} \mid X=x\right)\right)=\operatorname{argmax}_{y_{i}}\left(\frac{P\left(Y=y_{i}\right) P\left(X=x \mid Y=y_{i}\right)}{P(X=x)}\right) \\
\approx \operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) P\left(X=x \mid Y=y_{i}\right)\right)
\end{gathered}
$$

Note: sum is not 1 since we ignore the denominator of original formulation $P(X=x)$

## Naive Bayes Summary

Classify any new unseen instance $\boldsymbol{x}=\left(X_{1}, \ldots, X d\right)$ as:

$$
y^{*} \approx \operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) P\left(X=x \mid Y=y_{i}\right)\right)=\operatorname{argmax}_{y_{i}}\left(P\left(Y=y_{i}\right) \prod_{j=1}^{d} P\left(X_{j}=x_{j} \mid Y=y_{i}\right)\right)
$$

- To do this based on training examples, estimate the parameters from the training examples in D :
- For each label value of the classification variable (hypothesis) $y_{i}$

$$
\hat{P}\left(Y=y_{j}\right):=\text { estimate } P\left(y_{i}\right)
$$

- For each attribute value of $x_{j}$ of each datum instance

$$
P\left(X_{j}=x_{j} \mid Y=y_{i}\right):=\boldsymbol{e s t i m a t e} P\left(x_{j} \mid y_{i}\right)
$$

## Estimating Probabilities

- Usually, as in previous example, probabilities are estimated based on observed frequencies in the training data.
- If $D$ contains $N\left(y_{i}\right)$ examples in category $y_{i}$, and $N\left(x_{j}, y_{i}\right)$ of these $N\left(y_{i}\right)$ examples have value $x_{j}$ for feature $X_{j}$, then:

$$
P\left(X_{j}=x_{j} \mid Y=y_{i}\right)=\frac{N\left(x_{j}, y_{i}\right)}{N\left(y_{i}\right)}
$$

- However, estimating such probabilities from small training sets is error-prone (bias in the estimate, as we have seen)
- If - due only to low chance - a rare feature value, $X_{j}=x_{j}$ is never observed in the training data, then our estimate

$$
P\left(X_{j}=x_{j} \mid Y=y_{i}\right)=0
$$

- If $X_{j}=x_{j}$ actually occurs in a test instance, $\boldsymbol{x}$, the result is that $\forall y_{i}: P\left(Y=y_{i} \mid \boldsymbol{x}\right)=0$ (since individual probability estimates are multiplied)


## Probability Estimation Example

Test Instance $x$ :
<medium, red, circle>
No instances in D with Size=medium!

| $\begin{aligned} & P(\text { positive } \mid x)=0.5 * 0.0 * 1.0 * 1.0 / P(x)=0 \\ & P(\text { negative } \mid x)=0.5 * 0.0 * 0.5 * 0.5 / P(x)=0 \end{aligned}$ |  |  |  |  | Probability | positive | negative |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  | $\mathrm{P}(Y)$ | 0.5 | 0.5 |
|  |  |  |  |  | $\mathrm{P}($ small $\mid Y)$ | 0.5 | 0.5 |
| Ex | Size | Color | Shape | Category | $\mathrm{P}($ medium \| $Y$ ) | 0.0 | 0.0 |
|  |  |  |  |  | $\mathrm{P}($ large $\mid Y)$ | 0.5 | 0.5 |
| 1 | small | red | circle | positive | $\mathrm{P}(\mathrm{red} \mid Y)$ | 1.0 | 0.5 |
| 2 | large | red | circle | positive | P (blue \| $Y$ ) | 0.0 | 0.5 |
|  |  |  |  |  | $\mathrm{P}($ green $\mid Y$ ) | 0.0 | 0.0 |
| 3 | small | red | triangle | negative | P (square $\mid Y$ ) | 0.0 | 0.0 |
| 4 | large | blue | circle | negative | $\mathrm{P}($ triangle $\mid Y$ ) | 0.0 | 0.5 |
|  |  |  |  |  | P (circle $\mid Y$ ) | 1.0 | 0.5 |

## Smoothing

- To account for estimation from small samples, probability estimates are adjusted or smoothed.
- Laplace smoothing using an $m$-estimate assumes that each feature is given a prior probability, $p$, that is assumed to have been previously observed in a "virtual" sample of size $m$.

$$
P\left(X_{j}=x_{j} \mid Y=y_{i}\right)=\frac{N\left(x_{j}, y_{i}\right)+m p}{N\left(y_{i}\right)+m}
$$

- For binary features, $p$ is simply assumed to be 0.5 , while it can be set to $\frac{1}{k}$ where k is the number of values that $x_{j}$ can assume.


## Laplace Smoothing Example

- Assume training set contains 10 positive examples, and the feature "Size" has 3 values, but 1 value (size=medium) is not observed in $D$ :
>4: small
$>0$ : medium
>6: large
- Estimate parameters as follows (if we set $m=1, p=1 / 3$ )
$>P($ small $\mid$ positive $)=(4+1 / 3) /(10+1)=0.394$
$>P($ medium $\mid$ positive $)=(0+1 / 3) /(10+1)=0.03$
$>P($ large $\mid$ positive $)=(6+1 / 3) /(10+1)=0.576$
$>P($ small or medium or large $\mid$ positive $)=1.0$


## Naïve Bayses (MAP) with Continuous Distributions

- If $X$ is a continuous (univariate) random variable rather than a discrete one, need another way to calculate $P\left(X=x_{j} \mid Y=y_{i}\right)$.
- Assume that $X$ has a Gaussian distribution whose mean and variance depend on $Y$.
- During training, for each combination of the continuous values of $X$ and a class value $y_{i}$ for $Y$, estimate a mean $\mu_{i}$, and standard deviation $\sigma_{i}$ based on the observed values of feature $X$ in class $y_{i}$ in the training data. E.g., $\mu_{i}$ is the mean value of $\underline{X}$ observed in instances for which $Y=y_{i}$ in $D$
- During testing, estimate $P\left(X=x_{j} \mid Y=y_{i}\right)$ for a given observation $X=x_{j}$, using the Gaussian distribution defined by $\mu_{i}$ and $\sigma_{i}$.

$$
P\left(X=x_{j} \epsilon R \mid Y=y_{i}\right)=\frac{1}{\sigma_{i} \sqrt{2 \pi}} \exp \left(\frac{-\left(X_{j}-\mu_{i}\right)^{2}}{2 \sigma_{i}^{2}}\right)
$$

Probability of observing the value $x_{j}$ (our current observation) given that the class is $y_{i}$

## Comments on Naïve Bayes

- May work well despite strong assumption of conditional independence.
- Although it does not produce accurate probability estimates when its independence assumptions are violated, it may still pick the correct maximumprobability class in many cases.
- Does not perform any search of the hypothesis space. Directly constructs a hypothesis from parameter estimates that are easily calculated from the training data.
- Not guaranteed consistency with training data.
- Typically handles noise well since it does not even focus on completely fitting the training data.


## More

- Likelihood Function and MLE: LINK, LINK, LINK, LINK, LINK, LINK, LINK, LINK
- MLE VS MAP: LINK, LINK, LINK,LINK, LINK, LINK
- Naïve Bayes LINK, LINK, LINK, LINK
- Note that what we said also applies to DEEP models. For example, $\mathbf{x}$ can be the "deep" representation of an instance (e.g., an image), and we want to infer the model $M$ that underlies the generation of our images (inferring M can be easier if we capture the "invariants" of the input).
- See here an introduction to deep generatve models

