# Probability Based Learning 

Lecture 7, DD2431 Machine Learning

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## Advantages of Probability Based Methods

- Work with sparse training data. More powerful than deterministic methods - decision trees - when training data is sparse.
- Results are interpretable. More transparent and mathematically rigorous than methods such as $A N N$, Evolutionary methods.
- Tool for interpreting other methods. Framework for formalizing other methods - concept learning, least squares.


## Outline

- Probability Theory Basics
$\checkmark$ Bayes' rule
$\checkmark$ MAP and ML estimation
$\checkmark$ Minimum Description Length principle
- Naïve Bayes Classifier
- EM Algorithm

Probability Theory Basics

## Random Variables

- A random variable $x$ denotes a quantity that is uncertain
$\checkmark$ the result of flipping a coin, $\checkmark$ the result of measuring the temperature
- The probability distribution $P(x)$ of a randam variable (r.v.) captures the fact that
$\checkmark$ the r.v. will have different values when observed and $\checkmark$ Some values occur more than others.


## Random Variables

- A discrete random variable takes values from a predefined set.
- For a Boolean discrete random variable this predefined set has two members - $\{0,1\}$, $\{$ yes, no $\}$ etc.
- A continuous random variable takes values that are real numbers.

discrete pdf

continuous pdf


## Joint Probabilities

- Consider two random variables $x$ and $y$.
- Observe multiple paired instances of $x$ and $y$. Some paired outcomes will occur more frequently.
- This information is encoded in the joint probability distribution $P(x, y)$.
- $P(\mathbf{x})$ denotes the joint probability of $\mathbf{x}=\left(x_{1}, \ldots, x_{K}\right)$.



## $\leftarrow$ discrete joint pdf

## Joint Probabilities (cont.)



Figure from Computer Vision: models, learning and inference by Simon Prince.

## Marginalization

The probability distribution of any single variable can be recovered from a joint distribution by summing for the discrete case

$$
P(x)=\sum_{y} P(x, y)
$$

and integrating for the continuous case

$$
P(x)=\int_{y} P(x, y) d y
$$

## Marginalization (cont.)



Figure from Computer Vision: models, learning and inference by Simon Prince.

## Conditional Probability

- The conditional probability of $x$ given that $y$ takes value $y^{*}$ indicates the different values of r.v. $x$ which we'll observe given that $y$ is fixed to value $y^{*}$.
- The conditional probability can be recovered from the joint distribution $P(x, y)$ :

$$
P\left(x \mid y=y^{*}\right)=\frac{P\left(x, y=y^{*}\right)}{P\left(y=y^{*}\right)}=\frac{P\left(x, y=y^{*}\right)}{\int_{x} P\left(x, y=y^{*}\right) d x}
$$

- Extract an appropriate slice, and then normalize it.


Figure from Computer Vision: models, learning and inference by Simon Prince.

## Bayes' Rule

## Bayes' Rule

$$
P(y \mid x)=\frac{P(x \mid y) P(y)}{P(x)}=\frac{P(x \mid y) P(y)}{\sum_{y} P(x \mid y) P(y)}
$$

Each term in Bayes' rule has a name:

- $P(y \mid x) \leftarrow$ Posterior (what we know about $y$ given $x$.)
- $P(y) \leftarrow$ Prior (what we know about $y$ before we consider $x$.)
- $P(x \mid y) \leftarrow$ Likelihood (propensity for observing a certain value of $x$ given a certain value of $y$ )
- $P(x) \leftarrow$ Evidence (a constant to ensure that the l.h.s. is a valid distribution)


## Bayes' Rule

In many of our applications $y$ is a discrete variable and $\mathbf{x}$ is a multi-dimensional data vector extracted from the world.

$$
P(y \mid \mathbf{x})=\frac{P(\mathbf{x} \mid y) P(y)}{P(\mathbf{x})}
$$

Then

- $P(\mathbf{x} \mid y) \leftarrow$ Likelihood represents the probability of observing data $\mathbf{x}$ given the hypothesis $y$.
- $P(y) \leftarrow$ Prior of $y$ represents the background knowledge of hypothesis $y$ being correct.
- $P(y \mid \mathbf{x}) \leftarrow$ Posterior represents the probability that hypothesis $y$ is true after data $\mathbf{x}$ has been observed.


## Learning and Inference

- Bayesian Inference: The process of calculating the posterior probability distribution $P(y \mid \mathbf{x})$ for certain data $\mathbf{x}$.
- Bayesian Learning: The process of learning the likelihood distribution $P(\mathbf{x} \mid y)$ and prior probability distribution $P(y)$ from a set of training points

$$
\left\{\left(\mathbf{x}_{1}, y_{1}\right),\left(\mathbf{x}_{2}, y_{2}\right), \ldots,\left(\mathbf{x}_{n}, y_{n}\right)\right\}
$$

## Example: Which Gender?

Task: Determine the gender of a person given their measured hair length.

## Notation:

- Let $g \in\{$ 'f', 'm'\} be a r.v. denoting the gender of a person.
- Let $x$ be the measured length of the hair.


## Information given:

- The hair length observation was made at a boy's school thus

$$
P\left(g=' m^{\prime}\right)=05, \quad P\left(g-\prime^{\prime} f^{\prime}\right)=.05
$$

- Knowledge of the likelihood distributions $P(x \mid g=$ ' f ' $)$ and $P(x \mid g=$ 'm' $)$


## Example: Which Gender?

Task: Determine the gender of a person given their measured hair length.
Notation:

- Let $g \in\left\{\right.$ ' $^{\prime}$ ', 'm'\} be a r.v. denoting the gender of a person.
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- Let $x$ be the measured length of the hair.


## Information given:

- The hair length observation was made at a boy's school thus

$$
P(g=' m ')=.95, \quad P\left(g='^{\prime} f^{\prime}\right)=.05
$$

- Knowledge of the likelihood distributions $P(x \mid g=$ ' f ') and $P(x \mid g=$ 'm')



## Example: Which Gender?

Task: Determine the gender of a person given their measured hair length $\Longrightarrow$ calculate $P(g \mid x)$.

## Solution:

Apply Bayes' Rule to get

$$
\begin{aligned}
P(g=' \mathrm{~m} ' \mid x) & =\frac{P\left(x \mid g=\mathrm{m}^{\prime}\right) P\left(g=\mathrm{m}^{\prime}\right)}{P(x)} \\
& =\frac{P(x \mid g=\text { 'm' }) P\left(g=\mathrm{m}^{\prime}\right)}{P\left(x \mid g=\mathrm{m}^{\prime}\right) P\left(g=\mathrm{f}^{\prime}\right)+P\left(x \mid g={ }^{\prime} \mathrm{m}^{\prime}\right) P\left(g=\mathrm{m}^{\prime}\right)}
\end{aligned}
$$

Can calculate $P\left(g={ }^{\prime} \mathrm{f}^{\prime} \mid x\right)=1-P\left(g={ }^{\prime} \mathrm{m}^{\prime} \mid x\right)$

## Selecting the most probably hypothesis

- Maximum A Posteriori (MAP) Estimate:

Hypothesis with highest probability given observed data

$$
\begin{aligned}
y_{\mathrm{MAP}} & =\arg \max _{y \in \mathcal{Y}} P(y \mid \mathbf{x}) \\
& =\arg \max _{y \in \mathcal{Y}} \frac{P(\mathbf{x} \mid y) P(y)}{P(\mathbf{x})} \\
& =\arg \max _{y \in \mathcal{Y}} P(\mathbf{x} \mid y) P(y)
\end{aligned}
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- Maximum Likelihood Estimate (MLE): Hypothesis with highest likelihood of generating observed data.


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- Maximum Likelihood Estimate (MLE):

Hypothesis with highest likelihood of generating observed data.

$$
y_{\mathrm{MLE}}=\arg \max _{y \in \mathcal{Y}} P(\mathbf{x} \mid y)
$$

Useful if we do not know prior distribution or if it is uniform.

## Example: Cancer or Not?

## Scenario:

A patient takes a lab test and the result comes back positive. The test returns a correct positive result in only $98 \%$ of the cases in which the disease is actually present, and a correct negative result in only $97 \%$ of the cases in which the disease is not present. Furthermore, $0.8 \%$ of the entire population have cancer.

## Scenario in probabilities:

- Priors:

$$
P(\text { disease })=.008 \quad P(\text { not disease })=.992
$$

- Likelihoods:

$$
\begin{array}{ll}
P(+\mid \text { disease })=.98 & P(+\mid \text { not disease })=.03 \\
P(-\mid \text { disease })=.02 & P(-\mid \text { not disease })=.97
\end{array}
$$

## Example: Cancer or Not?

## Find MAP estimate:

When test returned a positive result,

$$
\begin{aligned}
y_{\mathrm{MAP}} & =\arg \max _{y \in\{\text { disease, not disease }\}} P(y \mid+) \\
& =\arg \underset{y \in\{\text { disease, not disease }\}}{\max } P(+\mid y) P(y)
\end{aligned}
$$

Substituting in the correct values get

$$
P(+\mid \text { disease }) P(\text { disease })=.98 \times .008=.0078
$$

$$
P(+\mid \text { not disease }) P(\text { not disease })=.03 \times .992=.0298
$$

Therefore $y_{\mathrm{MAP}}=$ "not disease" .
The Posterior probabilities:


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\end{aligned}
$$

Therefore $y_{\mathrm{MAP}}=$ "not disease".
The Posterior probabilities:

$$
\begin{aligned}
P(\text { disease } \mid+) & =\frac{.0078}{(.0078+.0298)}=.21 \\
P(\text { not disease } \mid+) & =\frac{.0298}{(.0078+.0298)}=.79
\end{aligned}
$$

## Relation to Occams's Razor

## Occam's Razor:

Choose the simplest explanation for the observed data

- Information theoretic perspective Occam's razor corresponds to choosing the explanation requiring the fewest bits to represent.
- The optimal representation requires $-\log _{2} p(y \mid \mathbf{x})$ bits to store. (Remember: the Shannon information content)
- Minimum description length principle: Choose hypothesis

$$
\begin{aligned}
y_{\mathrm{MDL}} & =\arg \min _{y \in \mathcal{Y}}-\log _{2} P(y \mid \mathbf{x}) \\
& =\arg \min _{y \in \mathcal{Y}}-\log _{2} P(\mathbf{x} \mid y)-\log _{2} P(y)
\end{aligned}
$$

- The MDL estimate is equal to the MAP estimate

$$
y \text { Map }=\underset{y \in \mathcal{y}}{\arg \max } \log _{2} P(\mathrm{x} \mid y)+\log _{2} P(y)
$$

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y_{\mathrm{MAP}}=\arg \max _{y \in \mathcal{Y}} \log _{2} P(\mathbf{x} \mid y)+\log _{2} P(y)
$$

Naïve Bayes Classifier

## Feature Space

- Sensors give measurements which can be converted to features.
- Ideally a feature value is identical for all samples in one class.


Samples


Feature space

## Feature Space

- Sensors give measurements which can be converted to features.
- However in the real world


Samples
because of
$\checkmark$ Measurement noise
$\checkmark$ Intra-class variation
$\checkmark$ Poor choice of features

## Feature Space

End result: a $K$-dimensional space

- in which each dimension is a feature
- containing $n$ labelled samples (objects)



## Problem: Large Feature Space

- Size of feature space exponential in number of features.
- More features $\Longrightarrow$ potential for better description of the objects but...

More features $\Longrightarrow$ more difficult to model $P(\mathbf{x} \mid y)$.

- Extreme Solution: Naïve Bayes classifier $\checkmark$ All features (dimensions) regarded as indenendent. $\checkmark$ Model $k$ one-dimensional distributions instead of one $k$-dimensional distribution.


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- Extreme Solution: Naïve Bayes classifier
$\checkmark$ All features (dimensions) regarded as independent.
$\checkmark$ Model $k$ one-dimensional distributions instead of one $k$-dimensional distribution.


## Naïve Bayes Classifier

- One of the most common learning methods.
- When to use:
$\checkmark$ Moderate or large training set available.
$\checkmark$ Features $x_{i}$ of a data instance $\mathbf{x}$ are conditionally independent given classification (or at least reasonably independent, still works with a little dependence).
- Successful applications:
$\checkmark$ Medical diagnoses (symptoms independent)
$\checkmark$ Classification of text documents (words independent)


## Naïve Bayes Classifier

- $\mathbf{x}$ is a vector $\left(x_{1}, \ldots, x_{K}\right)$ of attribute or feature values.
- Let $\mathcal{Y}=\{1,2, \ldots, Y\}$ be the set of possible classes.
- The MAP estimate of $y$ is

$$
\begin{aligned}
y_{\mathrm{MAP}} & =\arg \max _{y \in \mathcal{Y}} P\left(y \mid x_{1}, \ldots, x_{K}\right) \\
& =\arg \max _{y \in \mathcal{Y}} \frac{P\left(x_{1}, \ldots, x_{K} \mid y\right) P(y)}{P\left(x_{1}, \ldots, x_{K}\right)} \\
& =\arg \max _{y \in \mathcal{Y}} P\left(x_{1}, \ldots, x_{K} \mid y\right) P(y)
\end{aligned}
$$

- Naïve Bayes assumption: $P\left(x_{1}, \ldots, x_{K} \mid y\right)=\prod_{k=1}^{K} P\left(x_{k} \mid y\right)$
- This give the Naïve Bayes classifier:



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$$
y_{\mathrm{MAP}}=\arg \max _{y \in \mathcal{Y}} P(y) \prod_{k=1}^{K} P\left(x_{k} \mid y\right)
$$

## Example: Play Tennis?

Question: Will I go and play tennis given the forecast?
My measurements:
(1) forecast $\in\{$ sunny, overcast, rainy $\}$,
(2) temperature $\in\{$ hot, mild, cool $\}$,
(3) humidity $\in\{$ high, normal $\}$,
(1) windy $\in\{$ false, true $\}$.

Possible decisions:
$y \in\{$ yes, no $\}$

## Example: Play Tennis?

What I did in the past:

| outlook | temp. | humidity | windy | play | outlook | temp. | humidity | windy | play |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| sunny | hot | high | false | no | sumny | mild | high | false | no |
| sunny | hot | high | true | no | sumny | cod | normal | false | yes |
| overcast | hot | high | false | yes | rainy | mild | normal | false | yes |
| rainy | mild | high | fake | yes | sumny | mild | normal | true | yes |
| rainy | cool | normal | false | yes | overcast | mild | high | true | yes |
| rainy | cool | normal | true | no | overcast | hot | normal | false | yes |
| overcast | cool | normal | true | yes | rainy | mild | high | true | no |

## Example: Play Tennis?

## Counts of when I played tennis (did not play)

| Outlook |  |  | Temperature |  |  | Humidity |  | Windy |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| 2 (3) | 4 (0) | 3 (2) | 2 (2) | 4 (2) | 3 (1) | 3 (4) | 6 (1) | 6 (2) | 3 (3) |

Prior of whether I played tennis or not

| Counts: | Play |  | Prior Probabilities: | Play |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | yes | no |  | yes | no |
|  | 9 | 5 |  | $\frac{9}{14}$ | $\frac{5}{14}$ |

Likelihood of attribute when tennis played $P\left(x_{i} \mid \mathrm{y}=\mathrm{yes}\right)\left(P\left(x_{i} \mid \mathrm{y}=\mathrm{no}\right)\right)$

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Counts of when I played tennis (did not play)

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Prior of whether I played tennis or not


Likelihood of attribute when tennis played $P\left(x_{i} \mid \mathrm{y}=\mathrm{yes}\right)\left(P\left(x_{i} \mid \mathrm{y}=\mathrm{no}\right)\right)$

| Outlook |  |  | Temperature |  |  | Humidity |  | Windy |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| $\frac{2}{9}\left(\frac{3}{5}\right)$ | $\frac{4}{9}\left(\frac{0}{5}\right)$ | $\frac{3}{9}\left(\frac{2}{5}\right)$ | $\frac{2}{9}\left(\frac{2}{5}\right)$ | $\frac{4}{9}\left(\frac{2}{5}\right)$ | $\frac{3}{9}\left(\frac{1}{5}\right)$ | $\frac{3}{9}\left(\frac{4}{5}\right)$ | $\frac{6}{9}\left(\frac{1}{5}\right)$ | $\frac{6}{9}\left(\frac{2}{5}\right)$ | $\frac{3}{9}\left(\frac{3}{5}\right)$ |

## Example: Play Tennis?

Inference: Use the learnt model to classify a new instance.
New instance:

$$
\mathbf{x}=(\text { sunny }, \text { cool, high, true })
$$

## Apply Naïve Bayes Classifier:

$$
y_{\mathrm{MAP}}=\arg \max _{y \in\{y \mathrm{yes}, \mathrm{no}\}} P(y) \prod_{i=1}^{4} P\left(x_{i} \mid y\right)
$$

$$
\begin{aligned}
& P(\text { yes }) P(\text { sunny } \mid \text { yes }) P(\text { cool } \mid \text { yes }) P(\text { high } \mid \text { yes }) P(\text { true } \mid \text { yes })=\frac{9}{14} \times \frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9}=.005 \\
& P(\text { no }) P(\text { sunny } \mid \text { no }) P(\text { cool } \mid \text { no }) P(\text { high } \mid \text { no }) P(\text { true } \mid \text { no })=\frac{5}{14} \times \frac{3}{5} \times \frac{1}{5} \times \frac{4}{5} \times \frac{3}{5}=.021 \\
& \Longrightarrow y_{\mathrm{MAP}}=\mathrm{nO}
\end{aligned}
$$

## Naïve Bayes: Independence Violation

- Conditional independence assumption:

$$
P\left(x_{1}, x_{2}, \ldots, x_{K} \mid y\right)=\prod_{k=1}^{K} P\left(x_{k} \mid y\right)
$$

often violated - but it works surprisingly well anyway!

- Note: Do not need the posterior probabilities $P(y \mid \mathrm{x})$ to be correct. Only need $y_{\text {MAP }}$ to be correct.
- Since dependencies ignored, naïve Bayes posteriors often unrealistically close to 0 or 1 .

Different attributes say the same thing to a higher degree than we expect as they are correlated in reality.

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- Note: Do not need the posterior probabilities $P(y \mid \mathbf{x})$ to be correct. Only need $y_{\text {map }}$ to be correct.
- Since dependencies ignored, naïve Bayes posteriors often unrealistically close to 0 or 1 .
Different attributes say the same thing to a higher degree than we expect as they are correlated in reality.


## Naïve Bayes: Estimating Probabilities

- Problem: What if none of the training instances with target value $y$ have attribute $x_{i}$ ? Then

$$
P\left(x_{i} \mid y\right)=0 \quad \Longrightarrow \quad P(y) \prod_{i=1}^{K} P\left(x_{i} \mid y\right)=0
$$

- Solution: Add as prior knowledge that $P\left(x_{i} \mid y\right)$ must be larger than 0 :

where
$n=$ number of training samples with label $y$
$n_{y}=$ number of training samples with label $y$ and value $x_{i}$
$p=$ prior estimate of $P\left(x_{i} \mid y\right)$
$m=$ weight given to prior estimate (in relation to data)


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$$

- Solution: Add as prior knowledge that $P\left(x_{i} \mid y\right)$ must be larger than 0 :

$$
P\left(x_{i} \mid y\right)=\frac{n_{y}+m p}{n+m}
$$

where
$n=$ number of training samples with label $y$
$n_{y}=$ number of training samples with label $y$ and value $x_{i}$
$p=$ prior estimate of $P\left(x_{i} \mid y\right)$
$m=$ weight given to prior estimate (in relation to data)

## Example: Spam detection

- Aim: Build a classifier to identify spam e-mails.
- How:

$$
\begin{aligned}
& \checkmark \text { Create dictionary of words and tokens } \mathcal{W}=\left\{w_{1}, \ldots, w_{L}\right. \\
& \text { These words should be those which are specific to spam or non-spam e-mails. } \\
& \checkmark \quad \text { E-mail is a concatenation, in order, of its words and } \\
& \text { tokens: } \mathrm{e}=\left(e_{1}, e_{2}, \ldots, e_{K}\right) \text { with } e_{i} \in \mathcal{W} . \\
& \checkmark \text { Must model and learn } \\
& P\left(e_{1}, e_{2}, \ldots, e_{K} \mid \text { spam }\right) \text { and } P\left(e_{1}, e_{2}, \ldots, e_{K} \mid \text { not spam }\right)
\end{aligned}
$$

## Example: Spam detection

- Aim: Build a classifier to identify spam e-mails.
- How:

Training
$\checkmark$ Create dictionary of words and tokens $\mathcal{W}=\left\{w_{1}, \ldots, w_{L}\right\}$. These words should be those which are specific to spam or non-spam e-mails.
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Email: E
Vector: e

Dear customer,
A fully licensed Online Pharmacy is offering pharmaceuticals:
brought to you directly from abroad
-produced by the same multinational corporations selling through the major US pharmacies
-priced up to 5 times cheaper as compared to major US pharmacies.
Enjoy the US dollar purchasing power on hittp://pharmacy-buyonline.com.ual

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Inference
$\checkmark$ Given an e-mail, $E$, compute $\mathbf{e}=\left(e_{1}, \ldots, e_{K}\right)$.
$\checkmark$ Use Bayes' rule to compute

$$
P\left(\text { spam } \mid e_{1}, \ldots, e_{K}\right) \propto P\left(e_{1}, \ldots,\left.e_{K}\right|_{\text {spam }}\right) P(\text { spam })
$$

## Example: Spam detection

- How is the joint probability distribution modelled?

$$
P\left(e_{1}, \ldots,\left.e_{K}\right|_{\text {spam }}\right)
$$

Remember $K$ will be very large and vary from e-mail to e-mail..

- Make conditional independence assumption:


Similarly

$$
P\left(e_{1}, \ldots, e_{K} \mid \text { not spam }\right)=\prod_{k=1}^{K} P\left(e_{k} \mid \text { not spam }\right)
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$$

- Have assumed the position of word is not important.


## Example: Spam detection

## Learning:

Assume one has $n$ training e-mails and their labels - spam /non-spam

$$
\mathcal{S}=\left\{\left(\mathbf{e}_{1}, y_{1}\right), \ldots,\left(\mathbf{e}_{n}, y_{n}\right)\right\}
$$

Note: $\mathbf{e}_{i}=\left(e_{i 1}, \ldots, e_{i K_{i}}\right)$.

## Example: Spam detection

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Create dictionary
(1) Make a union of all the distinctive words and tokens in $\mathbf{e}_{1}, \ldots, \mathbf{e}_{n}$ to create $\mathcal{W}=\left\{w_{1}, \ldots, w_{L}\right\}$. (Note: words such as and, the, ... omitted)

## Example: Spam detection

## Learning:

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$$

Note: $\mathbf{e}_{i}=\left(e_{i 1}, \ldots, e_{i K_{i}}\right)$.

## Learn probabilities

For $y \in\{$ spam, not spam $\}$
(1) Set $P(y)=\frac{\sum_{i=1}^{n} \operatorname{Ind}\left(y_{i}=y\right)}{n} \leftarrow$ proportion of e-mails from class $y$.
(2) $n_{y}=\sum_{i=1}^{n} K_{i} \times \operatorname{Ind}\left(y_{i}=y\right) \leftarrow$ total $\#$ of words in the class $y$ e-mails.
(3) For each word $w_{l}$ compute
$n_{y l}=\sum_{i=1}^{n} \operatorname{Ind}\left(y_{i}=y\right) \times\left(\sum_{k=1}^{K_{i}} \operatorname{Ind}\left(e_{i k}=w_{l}\right)\right) \leftarrow \#$ of occurrences of word $w_{l}$ in the class $y$ e-mails.
(4) $P\left(w_{l} \mid y\right)=\frac{n_{y l}+1}{n_{y}+|\mathcal{W}|} \leftarrow$ assume prior value of $P\left(w_{l} \mid y\right)$ is $1 /|\mathcal{W}|$.

## Example: Spam detection

Inference: Classify a new e-mail $\mathbf{e}^{*}=\left(e_{1}^{*}, \ldots, e_{K^{*}}^{*}\right)$

$$
y^{*}=\arg \max _{y \in\{-1,1\}} P(y) \prod_{k=1}^{K^{*}} P\left(e_{k}^{*} \mid y\right)
$$

## Summary so far

- Bayesian theory: Combines prior knowledge and observed data to find the most probable hypothesis.
- Naïve Bayes Classifier: All variables considered independent.


## Expectation-Maximization (EM) Algorithm

## Mixture of Gaussians

This distribution is a weight sum of $K$ Gaussian distributions

$$
\begin{aligned}
& P(x)=\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(x ; \mu_{k}, \sigma_{k}^{2}\right) \\
& \text { where } \pi_{1}+\cdots+\pi_{K}=1 \\
& \text { and } \pi_{k}>0(k=1, \ldots, K) .
\end{aligned}
$$

This model can describe complex multi-modal probability distributions by combining simpler distributions.

## Mixture of Gaussians

$$
P(x)=\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(x ; \mu_{k}, \sigma_{k}^{2}\right)
$$

- Learning the parameters of this model from training data $x_{1}, \ldots, x_{n}$ is not trivial - using the usual straightforward maximum likelihood approach.
- Instead learn parameters using the Expectation-Maximization (EM) algorithm.


## Mixture of Gaussians as a marginalization

We can interpret the Mixture of Gaussians model with the introduction of a discrete hidden/latent variable $h$ and $P(x, h)$ :

$$
\begin{aligned}
P(x)=\sum_{k=1}^{K} P(x, h=k) & =\sum_{k=1}^{K} P(x \mid h=k) P(h=k) \\
& =\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(x ; \mu_{k}, \sigma_{k}^{2}\right)
\end{aligned}
$$



## $\leftarrow$ mixture density

Figures taken from Computer Vision: models, learning and inference by Simon Prince.

## EM for two Gaussians

Assume: We know the pdf of $x$ has this form:

$$
P(x)=\pi_{1} \mathcal{N}\left(x ; \mu_{1}, \sigma_{1}^{2}\right)+\pi_{2} \mathcal{N}\left(x ; \mu_{2}, \sigma_{2}^{2}\right)
$$

where $\pi_{1}+\pi_{2}=1$ and $\pi_{k}>0$ for components $k=1,2$.
Unknown: Values of the parameters (Many!)

$$
\Theta=\left(\pi_{1}, \mu_{1}, \sigma_{1}, \mu_{2}, \sigma_{2}\right)
$$

Have: Observed $n$ samples $x_{1}, \ldots, x_{n}$ drawn from $p(x)$.
Want to: Estimate $\Theta$ from $x_{1}, \ldots, x_{n}$.
How would it be possible to get them all???

## EM for two Gaussians

For each sample $x_{i}$ introduce a hidden variable $h_{i}$

$$
h_{i}= \begin{cases}1 & \text { if sample } x_{i} \text { was drawn from } \mathcal{N}\left(x ; \mu_{1}, \sigma_{1}^{2}\right) \\ 2 & \text { if sample } x_{i} \text { was drawn from } \mathcal{N}\left(x ; \mu_{2}, \sigma_{2}^{2}\right)\end{cases}
$$

and come up with initial values

$$
\Theta^{(0)}=\left(\pi_{1}^{(0)}, \mu_{1}^{(0)}, \sigma_{1}^{(0)}, \mu_{2}^{(0)}, \sigma_{2}^{(0)}\right)
$$

for each of the parameters.
EM is an iterative algorithm which updates $\Theta^{(t)}$ using the following two steps...

## EM for two Gaussians: E-step

The responsibility of $k$-th Gaussian for each sample $x$ (indicated by the size of the projected data point)


Look at each sample $x$ along hidden variable $h$ in the E-step

Figure from Computer Vision: models, learning and inference by Simon Prince.

## EM for two Gaussians: E-step (cont.)

E-step: Compute the "posterior probability" that $x_{i}$ was generated by component $k$ given the current estimate of the parameters $\Theta^{(t)}$. (responsibilities)
for $i=1, \ldots n$

$$
\text { for } k=1,2
$$

$$
\gamma_{i k}^{(t)}=P\left(h_{i}=k \mid x_{i}, \Theta^{(t)}\right)
$$

$$
=\frac{\pi_{k}^{(t)} \mathcal{N}\left(x_{i} ; \mu_{k}^{(t)}, \sigma_{k}^{(t)}\right)}{\pi_{1}^{(t)} \mathcal{N}\left(x_{i} ; \mu_{1}^{(t)}, \sigma_{1}^{(t)}\right)+\pi_{2}^{(t)} \mathcal{N}\left(x_{i} ; \mu_{2}^{(t)}, \sigma_{2}^{(t)}\right)}
$$

Note: $\gamma_{i 1}^{(t)}+\gamma_{i 2}^{(t)}=1$ and $\pi_{1}+\pi_{2}=1$

## EM for two Gaussians: M-step

Fitting the Gaussian model for each of $k$-th constinuetnt. Sample $x_{i}$ contributes according to the responsibility $\gamma_{i k}$.

(dashed and solid lines for fit before and after update)
Look along samples $x$ for each $h$ in the M-step

## EM for two Gaussians: M-step (cont.)

M-step: Compute the Maximum Likelihood of the parameters of the mixture model given out data's membership distribution, the $\gamma_{i}^{(t)}$,s:
for $k=1,2$

$$
\begin{aligned}
\mu_{k}^{(t+1)} & =\frac{\sum_{i=1}^{n} \gamma_{i k}^{(t)} x_{i}}{\sum_{i=1}^{n} \gamma_{i k}^{(t)}} \\
\sigma_{k}^{(t+1)} & =\sqrt{\frac{\sum_{i=1}^{n} \gamma_{i k}^{(t)}\left(x_{i}-\mu_{k}^{(t+1)}\right)^{2}}{\sum_{i=1}^{n} \gamma_{i k}^{(t)}}} \\
\pi_{k}^{(t+1)} & =\frac{\sum_{i=1}^{n} \gamma_{i k}^{(t)}}{n}
\end{aligned}
$$

## EM in practice



## Summary

- Bayesian theory: Combines prior knowledge and observed data to find the most probable hypothesis.
- Naïve Bayes Classifier: All variables considered independent.
- EM algorithm: Learn probability destribiution (model parameters) in presence of hidden variables.
If you are interested in learning more take a look at:
C. M. Bishop, Pattern Recognition and Machine Learning, Springer Verlag 2006.

