## Bayesian Learning

Olive slides: Alpaydin
Black slides: Mitchell.

## Bayesian Learning

- Probabilistic approach to inference.
- Quantities of interest are governed by prob. dist. and optimal decisions can be made by reasoning about these prob.
- Learning algorithms that directly deal with probabilities.
- Analysis framework for non-probabilistic methods.


## Two Roles for Bayesian Methods

Provides practical learning algorithms:

- Naive Bayes learning
- Bayesian belief network learning
- Combine prior knowledge (prior probabilities) with observed data
- Requires prior probabilities

Provides useful conceptual framework

- Provides "gold standard" for evaluating other learning algorithms
- Additional insight into Occam's razor


## Basic Probability Formulas

- Product Rule: probability $P(A \wedge B)$ of a conjunction of two events A and B :

$$
P(A, B)=P(B, A)=P(A \wedge B)=P(A \mid B) P(B)=P(B \mid A) P(A)
$$

- Sum Rule: probability of a disjunction of two events $A$ and $B$ :

$$
P(A \vee B)=P(A)+P(B)-P(A \wedge B)
$$

- Theorem of total probability: if events $A_{1}, \ldots, A_{n}$ are mutually exclusive with $\sum_{i=1}^{n} P\left(A_{i}\right)=1$, then

$$
P(B)=\sum_{i=1}^{n} P\left(B \mid A_{i}\right) P\left(A_{i}\right)
$$

## Bayes Theorem

$$
P(h \mid D)=\frac{P(D \mid h) P(h)}{P(D)}
$$

- $P(h)=$ prior probability that $h$ holds, before seeing the training data
- $P(D)=$ prior probability of observing training data $D$
- $P(D \mid h)=$ probability of observing $D$ in a world where $h$ holds
- $P(h \mid D)=$ probability of $h$ holding given observed data $D$
- Some useful tricks:
- $P(h, D)=P(D, h)$
- $P(h \mid D)=\frac{P(h, D)}{P(D)}$
- $P(D, h)=P(D \mid h) P(h)$, from $P(D \mid h)=\frac{P(D, h)}{P(h)}$


## Bayes Theorem: Example

Does patient have cancer or not?
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, . 001 of the entire population have this cancer.

$$
\begin{array}{cl}
P(\text { cancer })= & P(\neg \text { cancer })= \\
P(\oplus \mid \text { cancer })= & P(\ominus \mid \text { cancer })= \\
P(\oplus \mid \neg \text { cancer })= & P(\ominus \mid \neg \text { cancer })=
\end{array}
$$

How does $P($ cancer $\mid \oplus)$ compare to $P(\neg$ cancer $\mid \oplus)$ ?

## Bayes Theorem: Example

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, .001 of the entire population have this cancer.

$$
\begin{array}{cl}
P(\text { cancer })=0.001, \text { given } & P(\neg \text { cancer })=1-P(\text { cancer })=1-0.001=0.999 \\
P(\oplus \mid \text { cancer })=0.98, \text { given } & P(\ominus \mid \text { cancer })=1-P(\oplus \mid \text { cancer })=1-0.98=0.02 \\
P(\oplus \mid \neg \text { cancer })=1-P(\ominus \mid \neg \text { cancer }) & P(\ominus \mid \neg \text { cancer })=0.97, \text { given } \\
=1-0.97=0.03 &
\end{array}
$$

How does $P($ cancer $\mid \oplus)$ compare to $P(\neg$ cancer $\mid \oplus)$ ?

$$
\begin{aligned}
P(\text { cancer } \mid \oplus) & =\frac{P(\oplus \mid \text { cancer }) P(\text { cancer })}{P(\oplus)} \\
& =\frac{0.98 \times 0.001}{P(\oplus)} \\
& =\frac{0.00098}{P(\oplus, \text { cancer })+P(\oplus, \neg \text { cancer })} \\
& =\frac{0.00098}{P(\oplus \mid \text { cancer }) P(\text { cancer })+P(\oplus \mid \neg \text { cancer }) P(\neg \text { cancer })} \\
& =\frac{0.00098}{0.98 \times 0.001+0.03 \times 0.999}=0.031664
\end{aligned}
$$

## Conditional Independence

Definition: $X$ is conditionally independent of $Y$ given $Z$ if the probability distribution governing $X$ is independent of the value of $Y$ given the value of $Z$; that is, if

$$
\left(\forall x_{i}, y_{j}, z_{k}\right) P\left(X=x_{i} \mid Y=y_{j}, Z=z_{k}\right)=P\left(X=x_{i} \mid Z=z_{k}\right)
$$

more compactly, we write

$$
P(X \mid Y, Z)=P(X \mid Z)
$$

Example: Thunder is conditionally independent of Rain, given Lightning

$$
P(\text { Thunder } \mid \text { Rain }, \text { Lightning })=P(\text { Thunder } \mid \text { Lightning })
$$

## Choosing Hypotheses

$$
P(h \mid D)=\frac{P(D \mid h) P(h)}{P(D)}
$$

## Generally want the most probable hypothesis given the training data

Maximum a posteriori hypothesis $h_{M A P}$ :

$$
\begin{aligned}
h_{M A P} & =\arg \max _{h \in H} P(h \mid D) \\
& =\arg \max _{h \in H} \frac{P(D \mid h) P(h)}{P(D)} \\
& =\arg \max _{h \in H} P(D \mid h) P(h)
\end{aligned}
$$

## Choosing Hypotheses

- If all hypotheses are equally probable a priori:

$$
P\left(h_{i}\right)=P\left(h_{j}\right), \forall h_{i}, h_{j},
$$

then, $h_{M A P}$ reduces to:

$$
h_{M L} \equiv \underset{h \in H}{\operatorname{argmax}} P(D \mid h) .
$$

$\rightarrow$ Maximum Likelihood hypothesis.

## Brute Force MAP Hypothesis Learner

1. For each hypothesis $h$ in $H$, calculate the posterior probability

$$
P(h \mid D)=\frac{P(D \mid h) P(h)}{P(D)}
$$

2. Output the hypothesis $h_{M A P}$ with the highest posterior probability

$$
h_{M A P}=\underset{h \in H}{\operatorname{argmax}} P(h \mid D)
$$

## Learning A Real Valued Function



Consider any real-valued target function $f$
Training examples $\left\langle x_{i}, d_{i}\right\rangle$, where $d_{i}$ is noisy training value

- $d_{i}=f\left(x_{i}\right)+e_{i}$
- $e_{i}$ is random variable (noise) drawn independently for each $x_{i}$ according to some Gaussian distribution with mean=0

Then the maximum likelihood hypothesis $h_{M L}$ is the one that minimizes the sum of squared errors:

$$
h_{M L}=\arg \min _{h \in H} \sum_{i=1}^{m}\left(d_{i}-h\left(x_{i}\right)\right)^{2}
$$

## Setting up the Stage

- Probability density function:

$$
p\left(x_{0}\right) \equiv \lim _{\epsilon \rightarrow 0} \frac{1}{\epsilon} P\left(x_{0} \leq x<x_{0}+\epsilon\right)
$$

- ML hypothesis

$$
h_{M L}=\underset{h \in H}{\operatorname{argmax}} p(D \mid h)
$$

- Training instances $\left\langle x_{1}, \ldots, x_{m}\right\rangle$ and target values $\left\langle d_{1}, \ldots, d_{m}\right\rangle$, where $d_{i}=f\left(x_{i}\right)+e_{i}$.
- Assume training examples are mutually independent given $h$,

$$
h_{M L}=\underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} p\left(d_{i} \mid h\right)
$$

Note: $p(a, b \mid c)=p(a \mid b, c) \cdot p(b \mid c)=p(a \mid c) \cdot p(b \mid c)$

## Derivation of ML for Func. Approx.

From $h_{M L}=\operatorname{argmax}_{h \in H} \prod_{i=1}^{m} p\left(d_{i} \mid h\right)$ :

- Since $d_{i}=f\left(x_{i}\right)+e_{i}$ and $e_{i} \sim \mathcal{N}\left(0, \sigma^{2}\right)$, it must be:

$$
d_{i} \sim \mathcal{N}\left(f\left(x_{i}\right), \sigma^{2}\right)
$$

- $x \sim \mathcal{N}\left(\mu, \sigma^{2}\right)$ means random variable $x$ is normally distributed with mean $\mu$ and variance $\sigma^{2}$.
- Using pdf of $\mathcal{N}$ :

$$
\begin{gathered}
h_{M L}=\underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} \frac{1}{\sqrt{2 \pi \sigma^{2}}} e^{-\frac{\left(d_{i}-\mu\right)^{2}}{2 \sigma^{2}}} . \\
h_{M L}=\underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} \frac{1}{\sqrt{2 \pi \sigma^{2}}} e^{-\frac{\left(d_{i}-h\left(x_{i}\right)\right)^{2}}{2 \sigma^{2}}} .
\end{gathered}
$$

## Derivation of ML

$$
h_{M L}=\underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} \frac{1}{\sqrt{2 \pi \sigma^{2}}} e^{-\frac{\left(d_{i}-h\left(x_{i}\right)\right)^{2}}{2 \sigma^{2}}}
$$

- Get rid of constant factor $\frac{1}{\sqrt{2 \pi \sigma^{2}}}$, and put on log:

$$
\begin{align*}
h_{M L} & =\underset{h \in H}{\operatorname{argmax}} \ln \prod_{i=1}^{m} e^{-\frac{\left(d_{i}-h\left(x_{i}\right)\right)^{2}}{2 \sigma^{2}}} \\
& =\underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} \ln e^{-\frac{\left(d_{i}-h\left(x_{i}\right)\right)^{2}}{2 \sigma^{2}}} \\
& =\underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m}-\frac{\left(d_{i}-h\left(x_{i}\right)\right)^{2}}{2 \sigma^{2}} \\
& =\underset{h \in H}{\operatorname{argmin}} \sum_{i=1}^{m}\left(d_{i}-h\left(x_{i}\right)\right)^{2} \tag{2}
\end{align*}
$$

## Least Square as ML

Assumptions

- Observed training values $d_{i}$ generated by adding random noise to true target value, where noise has a normal distribution with zero mean.
- All hypotheses are equally probable (uniform prior).
- Note: it is possible that $M A P \neq M L$ !

Limitations

- Possible noise in $x_{i}$ not accounted for.


## Minimum Description Length

Occam's razor: prefer the shortest hypothesis.

$$
\begin{aligned}
& h_{M A P}=\underset{h \in H}{\operatorname{argmax}} P(D \mid h) P(h) \\
& h_{M A P}=\underset{h \in H}{\operatorname{argmax}} \log _{2} P(D \mid h)+\log _{2} P(h) \\
& h_{M A P}=\underset{h \in H}{\operatorname{argmin}}-\log _{2} P(D \mid h)-\log _{2} P(h)
\end{aligned}
$$

Surprisingly, the above can be interpreted as $h_{M A P}$ preferring shorter hypotheses, assuming a particular encoding scheme is used for the hypothesis and the data.

According to information theory, the shortest code length for a message occurring with probability $p_{i}$ is $-\log _{2} p_{i}$ bits.

## MDL

$$
h_{M A P}=\underset{h \in H}{\operatorname{argmin}}-\log _{2} P(D \mid h)-\log _{2} P(h)
$$

- $L_{C}(i)$ : description length of message $i$ with respect to code $C$.
- $-\log _{2} P(h)$ : description length of $h$ under optimal coding $C_{H}$ for the hypothesis space $H$.

$$
L_{C_{H}}(h)=-\log _{2} P(h)
$$

- $-\log _{2} P(D \mid h)$ : description length of training data $D$ given hypothesis $h$, under optimal encoding $C_{D \mid H}$.

$$
L_{C_{D \mid H}}(D \mid h)=-\log _{2} P(D \mid h)
$$

- Finally, we get:

$$
h_{M A P}=\underset{h \in H}{\operatorname{argmin}} L_{C_{D \mid H}}(D \mid h)+L_{C_{H}}(h)
$$

## MDL

- MAP:

$$
h_{M A P}=\underset{h \in H}{\operatorname{argmin}} L_{C_{D \mid H}}(D \mid h)+L_{C_{H}}(h)
$$

- MDL: Choose $h_{M D L}$ such that:

$$
h_{M D L}=\underset{h \in H}{\operatorname{argmin}} L_{C_{1}}(h)+L_{C_{2}}(D \mid h)
$$

which is the hypothesis that minimizes the combined length of the hypotheis itself, and the data described by the hypothesis.

- $h_{M D L}=h_{M A P}$ if $C_{1}=C_{H}$ and $C_{2}=C_{D \mid H}$.


## Bayes Optimal Classifier

- What is the most probable hypothesis given the training data, vs. What is the most probable classification?
- Example:
- $P\left(h_{1} \mid D\right)=0.4, P\left(h_{2} \mid D\right)=0.3, P\left(h_{3} \mid D\right)=0.3$.
- Given a new instance $x, h_{1}(x)=1, h_{2}(x)=0, h_{3}(x)=0$.
- In this case, probability of $x$ being positive is only 0.4 .


## Bayes Optimal Classification

If a new instance can take classification $v_{j} \in V$, then the probability $P\left(v_{j} \mid D\right)$ of correct classification of new instance being $v_{j}$ is:

$$
P\left(v_{j} \mid D\right)=\sum_{h_{i} \in H} P\left(v_{j} \mid h_{i}\right) P\left(h_{i} \mid D\right)
$$

Thus, the optimal classification is

$$
\underset{v_{j} \in V}{\operatorname{argmax}} \sum_{h_{i} \in H} P\left(v_{j} \mid h_{i}\right) P\left(h_{i} \mid D\right) .
$$

## Bayes Optimal Classifier

What is the assumption for the following to work?

$$
P\left(v_{j} \mid D\right)=\sum_{h_{i} \in H} P\left(v_{j} \mid h_{i}\right) P\left(h_{i} \mid D\right)
$$

Let's consider $H=\{h, \neg h\}$ :

$$
\begin{aligned}
P(v \mid D)= & P(v, h \mid D)+P(v, \neg h \mid D) \\
= & \frac{P(v, h, D)}{P(D)}+\frac{P(v, \neg h, D)}{P(D)} \\
= & \frac{P(v \mid h, D) P(h \mid D) P(D)}{P(D)} \\
& +\frac{P(v \mid \neg h, D) P(\neg h \mid D) P(D)}{P(D)} \\
& \{\text { if } P(v \mid h, D)=P(v \mid h), \text { etc. }\} \\
= & P(v \mid h) P(h \mid D)+P(v \mid \neg h) P(\neg h \mid D)
\end{aligned}
$$

## Bayes Optimal Classifier: Example

- $P\left(h_{1} \mid D\right)=0.4, P\left(h_{2} \mid D\right)=0.3, P\left(h_{3} \mid D\right)=0.3$.
- Given a new instance $x, h_{1}(x)=1, h_{2}(x)=0, h_{1}(x)=0$.
- $P\left(\ominus \mid h_{1}\right)=0, P\left(\oplus \mid h_{1}\right)=1$, etc.
$-P(\oplus \mid D)=0.4+0+0, P(\ominus \mid D)=0+0.3+0.3=0.6$
- Thus, $\operatorname{argmax}_{v \in O\{\oplus, \ominus\}} P(v \mid D)=\ominus$.
- Bayes optimal classifiers maximize the probability that a new instance is correctly classified, given the available data, hypothesis space $H$, and prior probabilities over $H$.
- Some oddities: The resulting hypotheis can be outside of the hypothesis space.


## Gibbs Sampling

Finding $\operatorname{argmax}_{v \in V} P(v \mid D)$ by considering every hypothesis $h \in H$ can be infeasible. A less optimal, but error-bounded version is Gibbs sampling:

1. Randomly pick $h \in H$ with probability $P(h \mid D)$.
2. Use $h$ to classify the new instance $x$.

The result is that missclassification rate is at most $2 \times$ that of BOC.

## Naive Bayes Classifier

Given attribute values $\left\langle a_{1}, a_{2}, \ldots, a_{n}\right\rangle$, give the classification $v \in V$ :

$$
\begin{gathered}
v_{M A P}=\underset{v_{j} \in V}{\operatorname{argmax}} P\left(v_{j} \mid a_{1}, a_{2}, \ldots, a_{n}\right) \\
v_{M A P}=\underset{v_{j} \in V}{\operatorname{argmax}} \frac{P\left(a_{1}, a_{2}, \ldots, a_{n} \mid v_{j}\right) P\left(v_{j}\right)}{P\left(a_{1}, a_{2}, \ldots, a_{n}\right)} \\
=\underset{v_{j} \in V}{\operatorname{argmax}} P\left(a_{1}, a_{2}, \ldots, a_{n} \mid v_{j}\right) P\left(v_{j}\right)
\end{gathered}
$$

- Want to estimate $P\left(a_{1}, a_{2}, \ldots, a_{n} \mid v_{j}\right)$ and $P\left(v_{j}\right)$ from training data.


## Naive Bayes

- $P\left(v_{j}\right)$ is easy to calculate: Just count the frequency.
- $P\left(a_{1}, a_{2}, \ldots, a_{n} \mid v_{j}\right)$ takes the number of posible instances $\times$ number of possible target values.
- $P\left(a_{1}, a_{2}, \ldots, a_{n} \mid v_{j}\right)$ can be approximated as

$$
P\left(a_{1}, a_{2}, \ldots, a_{n} \mid v_{j}\right)=\prod_{i} P\left(a_{i} \mid v_{j}\right)
$$

- From this naive Bayes classifier is defined as:

$$
v_{N B}=\underset{v_{j} \in V}{\operatorname{argmax}} P\left(v_{j}\right) \prod_{i} P\left(a_{i} \mid v_{j}\right)
$$

- Naive Bayes only takes number of distinct attribute values $\times$ number of distinct target values.

Naive Bayes uses cond. indep. to justify

$$
\begin{aligned}
P(X, Y \mid Z) & =P(X \mid Y, Z) P(Y \mid Z) \\
& =P(X \mid Z) P(Y \mid Z)
\end{aligned}
$$

## Naive Bayes Algorithm

Naive_Bayes_Learn(examples)
For each target value $v_{j}$

$$
\hat{P}\left(v_{j}\right) \leftarrow \text { estimate } P\left(v_{j}\right)
$$

For each attribute value $a_{i}$ of each attribute $a$

$$
\hat{P}\left(a_{i} \mid v_{j}\right) \leftarrow \text { estimate } P\left(a_{i} \mid v_{j}\right)
$$

$$
v_{N B}=\underset{v_{j} \in V}{\operatorname{argmax}} \hat{P}\left(v_{j}\right) \prod_{i} \hat{P}\left(x_{i} \mid v_{j}\right)
$$

## Naive Bayes: Example

Consider PlayTennis again, and new instance:

$$
\begin{gathered}
x=\langle\text { Outlk }=\text { sun }, \text { Temp }=\text { cool }, \text { Humid }=\text { high }, \text { Wind }=\text { strong }\rangle \\
V=\{\text { Yes,No }\}
\end{gathered}
$$

Want to compute:

$$
\begin{gathered}
v_{N B}=\underset{v_{j} \in V}{\operatorname{argmax}} P\left(v_{j}\right) \prod_{i} P\left(x_{i} \mid v_{j}\right) \\
P(Y) P(\operatorname{sun} \mid Y) P(\operatorname{cool} \mid Y) P(\text { high } \mid Y) P(\text { strong } \mid Y)=.005 \\
P(N) P(\operatorname{sun} \mid N) P(\operatorname{cool} \mid N) P(\text { high } \mid N) P(\text { strong } \mid N)=.021
\end{gathered}
$$

Thus, $v_{N B}=N o$

## Naive Bayes: Subtleties

1. Conditional independence assumption is often violated

$$
P\left(a_{1}, a_{2} \ldots a_{n} \mid v_{j}\right)=\prod_{i} P\left(a_{i} \mid v_{j}\right)
$$

- ...but it works surprisingly well anyway. Note don't need estimated posteriors $\hat{P}\left(v_{j} \mid x\right)$ to be correct; need only that

$$
\underset{v_{j} \in V}{\operatorname{argmax}} \hat{P}\left(v_{j}\right) \prod_{i} \hat{P}\left(a_{i} \mid v_{j}\right)=\underset{v_{j} \in V}{\operatorname{argmax}} P\left(v_{j}\right) P\left(a_{1} \ldots, a_{n} \mid v_{j}\right)
$$

- Naive Bayes posteriors often unrealistically close to 1 or 0 .


## Naive Bayes: Subtleties

What if none of the training instances with target value $v_{j}$ have attribute value $a_{i}$ ? Then

$$
\begin{gathered}
\hat{P}\left(a_{i} \mid v_{j}\right)=0, \text { and... } \\
\hat{P}\left(v_{j}\right) \prod_{i} \hat{P}\left(a_{i} \mid v_{j}\right)=0
\end{gathered}
$$

Typical solution is Bayesian estimate for $\hat{P}\left(a_{i} \mid v_{j}\right)$

$$
\hat{P}\left(a_{i} \mid v_{j}\right) \leftarrow \frac{n_{c}+m p}{n+m}
$$

where

- $n$ is number of training examples for which $v=v_{j}$,
- $n_{c}$ number of examples for which $v=v_{j}$ and $a=a_{i}$
- $p$ is prior estimate for $\hat{P}\left(a_{i} \mid v_{j}\right)$
- $m$ is weight given to prior (i.e. number of "virtual" examples)


## Extra Slides: Will be covered, time permitting

## Expectation Maximization (EM)

When to use:

- Data is only partially observable
- Unsupervised clustering (target value unobservable)
- Supervised learning (some instance attributes unobservable)

Some uses:

- Train Bayesian Belief Networks
- Unsupervised clustering (AUTOCLASS)
- Learning Hidden Markov Models


## EM for Estimating $k$ Means

## Given:

- Instances from $X$ generated by mixture of $k$ Gaussian distributions
- Unknown means $\left\langle\mu_{1}, \ldots, \mu_{k}\right\rangle$ of the $k$ Gaussians
- Don't know which instance $x_{i}$ was generated by which Gaussian

Determine:

- Maximum likelihood estimates of $\left\langle\mu_{1}, \ldots, \mu_{k}\right\rangle$

Think of full description of each instance as $y_{i}=\left\langle x_{i}, z_{i 1}, z_{i 2}\right\rangle$, where

- $z_{i j}$ is 1 if $x_{i}$ generated by $j$ th Gaussian
- $x_{i}$ observable
- $z_{i j}$ unobservable


## EM for Estimating $k$ Means

EM Algorithm: Pick random initial $h=\left\langle\mu_{1}, \mu_{2}\right\rangle$, then iterate
step: Calculate the expected value $E\left[z_{i j}\right]$ of each hidden variable $z_{i j}$, assuming the current hypothesis $h=\left\langle\mu_{1}, \mu_{2}\right\rangle$ holds.

$$
\begin{aligned}
E\left[z_{i j}\right] & =\frac{p\left(x=x_{i} \mid \mu=\mu_{j}\right)}{\sum_{n=1}^{2} p\left(x=x_{i} \mid \mu=\mu_{n}\right)} \\
& =\frac{e^{-\frac{1}{2 \sigma^{2}}\left(x_{i}-\mu_{j}\right)^{2}}}{\sum_{n=1}^{2} e^{-\frac{1}{2 \sigma^{2}}\left(x_{i}-\mu_{n}\right)^{2}}}
\end{aligned}
$$

step: Calculate a new maximum likelihood hypothesis $h^{\prime}=\left\langle\mu_{1}^{\prime}, \mu_{2}^{\prime}\right\rangle$, assuming the value taken on by each hidden variable $z_{i j}$ is its expected value $E\left[z_{i j}\right]$ calculated above. Replace $h=\left\langle\mu_{1}, \mu_{2}\right\rangle$ by $h^{\prime}=\left\langle\mu_{1}^{\prime}, \mu_{2}^{\prime}\right\rangle$.

$$
\mu_{j} \leftarrow \frac{\sum_{i=1}^{m} E\left[z_{i j}\right] x_{i}}{\sum_{i=1}^{m} E\left[z_{i j}\right]}
$$

## EM Algorithm

```
Converges to local maximum likelihood }
and provides estimates of hidden variables }\mp@subsup{z}{ij}{
```

In fact, local maximum in $E[\ln P(Y \mid h)]$

- $Y$ is complete (observable plus unobservable variables) data
- Expected value is taken over possible values of unobserved variables in $Y$


## General EM Problem

Given:

- Observed data $X=\left\{x_{1}, \ldots, x_{m}\right\}$
- Unobserved data $Z=\left\{z_{1}, \ldots, z_{m}\right\}$
- Parameterized probability distribution $P(Y \mid h)$, where
$-Y=\left\{y_{1}, \ldots, y_{m}\right\}$ is the full data $y_{i}=x_{i} \cup z_{i}$
- $h$ are the parameters

Determine:

- $h$ that (locally) maximizes $E[\ln P(Y \mid h)]$


## General EM Method

Define likelihood function $Q\left(h^{\prime} \mid h\right)$ which calculates $Y=X \cup Z$ using observed $X$ and current parameters $h$ to estimate $Z$

$$
Q\left(h^{\prime} \mid h\right) \leftarrow E\left[\ln P\left(Y \mid h^{\prime}\right) \mid h, X\right]
$$

EM Algorithm:
Estimation (E) step: Calculate $Q\left(h^{\prime} \mid h\right)$ using the current hypothesis $h$ and the observed data $X$ to estimate the probability distribution over $Y$.

$$
Q\left(h^{\prime} \mid h\right) \leftarrow E\left[\ln P\left(Y \mid h^{\prime}\right) \mid h, X\right]
$$

Maximization (M) step: Replace hypothesis $h$ by the hypothesis $h^{\prime}$ that maximizes this $Q$ function.

$$
h \leftarrow \underset{h^{\prime}}{\operatorname{argmax}} Q\left(h^{\prime} \mid h\right)
$$

## Derivation of $k$-Means

- Hypothesis $h$ is parameterized by $\theta=\left\langle\mu_{1} \ldots \mu_{k}\right\rangle$.
- Observed data $X=\left\{\left\langle x_{i}\right\rangle\right\}$
- Hidden variables $Z=\left\{\left\langle z_{i 1}, \ldots, z_{i k}\right\rangle\right\}$ :
- $z_{i k}=1$ if input $x_{i}$ is generated by th $k$-th normal dist.
- For each input, $k$ entries.
- First, start with defining $\ln p(Y \mid h)$.


## Deriving $\ln P(Y \mid h)$

$$
p\left(y_{i} \mid h^{\prime}\right)=p\left(x_{i}, z_{i 1}, z_{i 2}, \ldots, z_{i k} \mid h^{\prime}\right)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} e^{-\frac{1}{2 \sigma^{2}} \sum_{j=1}^{k} z_{i j}\left(x_{i}-\mu_{j}^{\prime}\right)^{2}}
$$

Note that the vector $\left\langle z_{i 1}, \ldots, z_{i k}\right\rangle$ contains only a single 1 and all the rest are 0 .

$$
\begin{aligned}
\ln P\left(Y \mid h^{\prime}\right) & =\ln \prod_{i=1}^{m} p\left(y_{i} \mid h^{\prime}\right) \\
& =\sum_{i=1}^{m} \ln p\left(y_{i} \mid h^{\prime}\right) \\
& =\sum_{i=1}^{m}\left(\ln \frac{1}{\sqrt{2 \pi \sigma^{2}}}-\frac{1}{2 \sigma^{2}} \sum_{j=1}^{k} z_{i j}\left(x_{i}-\mu_{j}^{\prime}\right)^{2}\right)
\end{aligned}
$$

## Deriving $E[\ln P(Y \mid h)]$

Since $P\left(Y \mid h^{\prime}\right)$ is a linear function of $z_{i j}$, and since $E[f(z)]=f(E[z])$,

$$
\begin{aligned}
E\left[\ln P\left(Y \mid h^{\prime}\right)\right] & =E\left[\sum_{i=1}^{m}\left(\ln \frac{1}{\sqrt{2 \pi \sigma^{2}}}-\frac{1}{2 \sigma^{2}} \sum_{j=1}^{k} z_{i j}\left(x_{i}-\mu_{j}^{\prime}\right)^{2}\right)\right] \\
& =\sum_{i=1}^{m}\left(\ln \frac{1}{\sqrt{2 \pi \sigma^{2}}}-\frac{1}{2 \sigma^{2}} \sum_{j=1}^{k} E\left[z_{i j}\right]\left(x_{i}-\mu_{j}^{\prime}\right)^{2}\right)
\end{aligned}
$$

Thus,

$$
\begin{aligned}
Q\left(h^{\prime} \mid h\right) & =Q\left(\left\langle\mu_{1}^{\prime}, \ldots, \mu_{k}^{\prime}\right\rangle \mid h\right) \\
& =\sum_{i=1}^{m}\left(\ln \frac{1}{\sqrt{2 \pi \sigma^{2}}}-\frac{1}{2 \sigma^{2}} \sum_{j=1}^{k} E\left[z_{i j}\right]\left(x_{i}-\mu_{j}^{\prime}\right)^{2}\right)
\end{aligned}
$$

Finding $\operatorname{argmax}_{h^{\prime}} Q\left(h^{\prime} \mid h\right)$
With

$$
E\left[z_{i j}\right]=\frac{e^{-\frac{1}{2 \sigma^{2}}\left(x_{i}-\mu_{j}\right)^{2}}}{\sum_{n=1}^{2} e^{-\frac{1}{2 \sigma^{2}}\left(x_{i}-\mu_{n}\right)^{2}}}
$$

we want to find $h^{\prime}$ such that

$$
\begin{aligned}
\underset{h^{\prime}}{\operatorname{argmax}} Q\left(h^{\prime} \mid h\right) & =\underset{h^{\prime}}{\operatorname{argmax}} \sum_{i=1}^{m}\left(\ln \frac{1}{\sqrt{2 \pi \sigma^{2}}}-\frac{1}{2 \sigma^{2}} \sum_{j=1}^{k} E\left[z_{i j}\right]\left(x_{i}-\mu_{j}^{\prime}\right)^{2}\right) \\
& =\underset{h^{\prime}}{\operatorname{argmin}} \sum_{i=1}^{m} \sum_{j=1}^{k} E\left[z_{i j}\right]\left(x_{i}-\mu_{j}^{\prime}\right)^{2},
\end{aligned}
$$

which is minimized by

$$
\mu_{j} \leftarrow \frac{\sum_{i=1}^{m} E\left[z_{i j}\right] x_{i}}{\sum_{i=1}^{m} E\left[z_{i j}\right]} .
$$

## Deriving the Update Rule

Set the derivative of the quantity to be minimized to be zero:

$$
\begin{aligned}
& \frac{\partial}{\partial \mu_{j}^{\prime}} \sum_{i=1}^{m} \sum_{j=1}^{k} E\left[z_{i j}\right]\left(x_{i}-\mu_{j}^{\prime}\right)^{2} \\
&= \frac{\partial}{\partial \mu_{j}^{\prime}} \sum_{i=1}^{m} E\left[z_{i j}\right]\left(x_{i}-\mu_{j}^{\prime}\right)^{2} \\
&=2 \sum_{i=1}^{m} E\left[z_{i j}\right]\left(x_{i}-\mu_{j}^{\prime}\right)=0 \\
& \sum_{i=1}^{m} E\left[z_{i j}\right] x_{i}-\sum_{i=1}^{m} E\left[z_{i j}\right] \mu_{j}^{\prime}=0 \\
& \sum_{i=1}^{m} E\left[z_{i j}\right] x_{i}=\mu_{j}^{\prime} \sum_{i=1}^{m} E\left[z_{i j}\right] \\
& \mu_{j}^{\prime}=\frac{\sum_{i=1}^{m} E\left[z_{i j}\right] x_{i}}{\sum_{i=1}^{m} E\left[z_{i j}\right]}
\end{aligned}
$$

## Losses and Risks

$\square$ Actions: $\alpha_{i}$
$\square$ Loss of $\alpha_{i}$ when the state is $C_{k}: \lambda_{i k}$
$\square$ Expected risk (Duda and Hart, 1973)

$$
\begin{aligned}
& R\left(\alpha_{i} \mid \mathbf{x}\right)=\sum_{k=1}^{K} \lambda_{i k} P\left(c_{k} \mid \mathbf{x}\right) \\
& \text { choose } \alpha_{i} \text { if } R\left(\alpha_{i} \mid \mathbf{x}\right)=\min _{k} R\left(\alpha_{k} \mid \mathbf{x}\right)
\end{aligned}
$$

## Losses and Risks: 0/1 Loss

$$
\begin{aligned}
& \lambda_{i k}=\left\{\begin{array}{l}
0 \text { if } i=k \\
1 \text { if } i \neq k
\end{array}\right. \\
& \begin{aligned}
R\left(\alpha_{i} \mid \mathbf{x}\right) & =\sum_{k=1}^{k} \lambda_{i k} P\left(C_{k} \mid \mathbf{x}\right) \\
& =\sum_{k \neq i} P\left(C_{k} \mid \mathbf{x}\right) \\
& =1-P\left(C_{i} \mid \mathbf{x}\right)
\end{aligned}
\end{aligned}
$$

For minimum risk, choose the most probable class

## Losses and Risks: Reject

$$
\begin{aligned}
& \lambda_{i k}= \begin{cases}0 & \text { if } i=k \\
\lambda & \text { if } i=K+1, \quad 0<\lambda<1 \\
1 & \text { otherwise }\end{cases} \\
& \qquad R\left(\alpha_{K+1} \mid \mathbf{x}\right)=\sum_{k=1}^{K} \lambda P\left(C_{k} \mid \mathbf{x}\right)=\lambda \\
& \quad R\left(\alpha_{i} \mid \mathbf{x}\right)=\sum_{k \neq i} P\left(C_{k} \mid \mathbf{x}\right)=1-P\left(C_{i} \mid \mathbf{x}\right) \\
& \text { choose } C_{i} \\
& \text { if } P\left(C_{i} \mid \mathbf{x}\right)>P\left(C_{k} \mid \mathbf{x}\right) \forall k \neq i \text { and } P\left(C_{i} \mid \mathbf{x}\right)>1-\lambda \\
& \text { reject } \quad \text { otherwise }
\end{aligned}
$$

## Discriminant Functions

$$
\begin{gathered}
\text { choose } C_{i} \text { if } g_{i}(\mathbf{x})=\max _{k} g_{k}(\mathbf{x}) \\
g_{i}(\mathbf{x})=\left\{\begin{array}{l}
-R\left(\alpha_{i} \mid \mathbf{x}\right) \\
P\left(C_{i} \mid \mathbf{x}\right) \\
p\left(\mathbf{x} \mid C_{i}\right) P\left(C_{i}\right)
\end{array}\right. \\
K \text { decision regions } \mathcal{R}_{1}, \ldots, \mathcal{R}_{K}(\mathbf{x}), i=1, \ldots, K \\
\mathcal{R}=\left\{\mathbf{x} \mid g_{i}(\mathbf{x})=\max _{k} g_{k}(\mathbf{x})\right\}
\end{gathered}
$$

## $K=2$ Classes

$\square$ Dichotomizer ( $K=2$ ) vs Polychotomizer ( $K>2$ )
$\square g(x)=g_{1}(x)-g_{2}(x)$

$$
\text { choose }\left\{\begin{array}{l}
C_{1} \text { if } g(\mathbf{x})>0 \\
C_{2} \text { otherwise }
\end{array}\right.
$$

$\square$ Log odds: $\log \frac{P\left(C_{1} \mid \mathbf{x}\right)}{P\left(C_{2} \mid \mathbf{x}\right)}$

## Utility Theory

$\square$ Prob of state $k$ given exidence $\mathbf{x}: ~ P\left(S_{k} \mid x\right)$
$\square$ Utility of $\alpha_{i}$ when state is $k$ : $U_{i k}$
$\square$ Expected utility:

$$
\begin{aligned}
& E U\left(\alpha_{i} \mid \mathbf{x}\right)=\sum_{k} U_{i k} P\left(S_{k} \mid \mathbf{x}\right) \\
& \text { Choose } \alpha_{i} \text { if } E U\left(\alpha_{i} \mid \mathbf{x}\right)=\max _{j} E U\left(\alpha_{j} \mid \mathbf{x}\right)
\end{aligned}
$$

## Association Rules

$\square$ Association rule: $X \rightarrow Y$
$\square$ People who buy/click/visit/enjoy $X$ are also likely to buy/click/visit/enjoy Y.
$\square$ A rule implies association, not necessarily causation.

## Association measures

$\square$ Support $(X \rightarrow Y)$ :

$$
P(X, Y)=\frac{\#\{\text { customerswho bought } X \text { and } Y\}}{\#\{\text { customers }\}}
$$

$\square$ Confidence $(X \rightarrow Y)$ :

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

$\square$ Lift $(X \rightarrow Y): \quad=\frac{\#\{\text { customerswho bought } X \text { and } Y\}}{\#\{\text { customerswho bought } X\}}$

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

## References

