# Data analysis and stochastic modeling 

## Lecture 5 - Mixture models and the EM algorithm

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## Multivariate Gaussian density

## Definition

$X$ is a Gaussian vector of dimension $p$ if any linear combination of its components $a^{\prime} X$ is a Gaussian in dimension 1.

$$
f(x)=\frac{1}{(2 \pi)^{n / 2}|\Sigma|^{1 / 2}} \exp \left\{-\frac{1}{2}(x-\mu)^{\prime} \Sigma^{-1}(x-\mu)\right\}
$$




Example of a multivariate Gaussian with $m=[21]$ and $\theta=\pi / 6$.

## Properties of the covariance matrix

The covariance matrix is symmetric, definite positive,

$$
\Sigma=V D V^{\prime}
$$

where
$V$ are the eigen vectors defining the principal axes (orientation of the density) and
$D$ are the eigen values defining the dispertion along the axes.

## Theorem

The components of a Gaussian vector are independent if and only if $\Sigma$ is a diagonal matrix, i.e. if the components are not correlated.

## Illustration of 2D Gaussians

From the correlation point of view
From the geometric point of view

$$
\Sigma=\left(\begin{array}{cc}
\sigma_{1}^{2} & \rho \sigma_{1} \sigma_{2} \\
\rho \sigma_{2} \sigma_{1} & \sigma_{2}^{2}
\end{array}\right)
$$

$$
V=\left(\begin{array}{cc}
\cos (\theta) & \sin (\theta) \\
\sin (\theta) & \cos (\theta)
\end{array}\right)
$$



$\theta=\pi / 6$
$D=\operatorname{diag}(41)$


$$
\begin{array}{r}
\theta=\pi / 6 \\
D=\operatorname{diag}(2
\end{array}
$$2)

## Isodensity ellipsoids

Isodensity curves are (hyper)ellipsoids whose equation is given by

$$
(x-\mu)^{\prime} \Sigma^{-1}(x-\mu)=c
$$



$90 \%$ of the samples lie whithin the pink ellipse 6)語IRISA

99\% of the samples lie whithin the red ellipse

## Why mixture models?


true distribution


Gaussian model


Mixture model

## Why mixture models?



## Mixture model - definition

A mixture model is a weighted sum of laws, the likelihood of a sample $x$ being given by

$$
f(x)=\sum_{i=1}^{K} \pi_{i} f_{i}(x)
$$

with the constraint that

$$
\sum_{i=1}^{K} \pi_{i}=1
$$

- $f_{i}()$ can be any density and the $f_{i}()$ 's need not be from the same family
- $f()$ is a density since $\int_{-\infty}^{\infty} f(x) d x=1$
- the model can extend to discrete variables


## Examples of mixture model densities






## Multivariate Gaussian mixture model

- Each component of the mixture is a multivariate Gaussian density

$$
f_{i}(x)=\frac{1}{(2 \pi)^{n / 2}\left|\Sigma_{i}\right|^{1 / 2}} \exp \left\{-\frac{1}{2}\left(x-\mu_{i}\right)^{\prime} \Sigma_{i}^{-1}\left(x-\mu_{i}\right)\right\}
$$

- Parameters of the model
- weights of each component (K)
$\triangleright$ mean vectors
(Kn)
$\triangleright$ covariance matrices

$$
(K n(n+1) / 2)
$$

- In practice, we often assume diagonal covariance matrices
$\triangleright$ much less parameters $\quad(K n \ll K n(n+1) / 2)$
$\triangleright$ much less computation (saves matrix inversion)
$\triangleright$ can be compensated with more components


## Gaussian mixture model


$\mathrm{x}_{1} \quad{ }^{2}$ [courtesy of ${ }^{-4}$ A. A. D'Souza and J-F. Bonastre]


## Gaussian mixture model



## Mixture models from the generative viewpoint

A sample is drawn according to the law of the component $f_{i}()$ of the mixture with probabiliy $\pi_{i}$.

Practically, sampling is a two step process

1. choose a component $i$ of the mixture according to the discrete law defined by the weights $w_{j}$
2. draw a sample according to the law $f_{i}()$

Example: $w=[0.3,0.7], f_{1}=\mathcal{N}(0,1), f_{2}=\mathcal{N}(2,1)$

## Mixture models from the generative viewpoint

Interpretation: [from a generative point of view,] the samples in a mixture model are drawn from either one of the component of the models with the proportion defined by the weights, i.e.

- for each component $i$, there is a set of samples distributed according to $f_{i}(x)$
- the proportion of such samples is given by $\pi_{i}$
$\Rightarrow$ hidden variable indicating the component to which a sample belong!


## Mixture models and hidden variables

The law of $x$ is the marginal over the hidden variable $Z$, i.e.

$$
f(x)=\sum_{i=1}^{K} \underbrace{\pi_{i}}_{P[Z=i]} \underbrace{f_{i}(x)}_{p(x \mid Z=i)}
$$



$$
\begin{gathered}
\text { Likelihood } \\
\Downarrow \\
(X)=\sum_{Z}(X, Z)
\end{gathered}
$$

## Mixture models and hidden variables

- Conditional density of $x$ given $z$

$$
p(x \mid z)=f_{z}(x)=\sum_{i=1}^{K} f_{i}(x) \mathbb{I}_{(z=i)}
$$

- Joint density of $(x, z)$

$$
p(x, z)=\pi_{z} f_{z}(x)=\left(\sum_{i=1}^{K} f_{i}(x) \mathbb{I}_{(z=i)}\right)\left(\sum_{i=1}^{K} \pi_{i} \mathbb{I}_{(z=i)}\right)
$$

- Marginal density of $x$

$$
p(x)=\sum_{z} p(x, z)=\sum_{z} \sum_{i} \pi_{i} f_{i}(x) \mathbb{I}_{(z=i)}=\sum_{i} \pi_{i} f_{i}(x)
$$

## Maximum likelihood parameter estimation

- Let $\mathbf{x}=\left\{x_{1}, \ldots, x_{N}\right\}$ be a set of training samples from which we want to estimate the parameters of a Gaussian mixture model with $K$ components, i.e.
$\triangleright$ weights $\left\{w_{1}, \ldots, w_{K}\right\}$,
$\triangleright$ mean vectors $\left\{\mu_{1}, \ldots, \mu_{2}\right\}$,
$\triangleright$ variance vectors $\left\{\sigma_{1}, \ldots, \sigma_{2}\right\}$.
- Maximum likelihood criterion

$$
\ln f(\mathbf{x})=\sum_{i=1}^{N} \ln \left(\sum_{j=1}^{K} w_{j} f_{j}\left(x_{i} ; \theta_{j}\right)\right)
$$

$\Rightarrow$ direct maximization (nearly) impossible!

## Direct maximum likelihood parameter estimation

- Directly solving the ML equations
$\triangleright$ they often do not exist!
$\triangleright$ complex equations when they do exist
- Gradient descent algorithms
$\triangleright$ non convex likelihood function $\Rightarrow$ non unicity of the solution
$\triangleright$ need for prior knowledge on the domain of $\theta$
- The Expectation-Maximization algorithm
$\triangleright$ nice and elegant solution!


## Maximum likelihood with complete data

- The set of training samples x is incomplete!
- Assume for each sample $x_{i}$, we know the component indicator function $z_{i}$
- The set $\left\{x_{1}, z_{1}, \ldots, x_{N}, z_{N}\right\}$ is known as complete data
- Maximum likelihood estimates can be obtained from the complete data, e.g.

$$
\widehat{w}_{i}=\frac{1}{N} \sum_{j=1}^{N} \mathbb{I}_{\left(z_{j}=i\right)} \quad \text { and } \quad \widehat{\mu}_{i}=\frac{\sum_{j=1} x_{j} \mathbb{I}_{\left(z_{j}=i\right)}}{\sum_{j=1}^{N} \mathbb{I}_{\left(z_{j}=i\right)}}
$$

$\Rightarrow$ but the variables $z_{j}$ are not known!

## The Expectation-Maximization principle

The Expectation-Maximization (EM) principle compensates for missing (aka latent) data, replacing them by their expectations.

## EM Iterative principle

1. estimate the missing variables given a current estimate of the parameters
2. estimate new parameters given the current estimate of the missing variables
3. repeat steps 1 and 2 until convergence

Note: this principle applies to many problems, not only for maximum likelihood parameter estimation!

## The auxiliary function

The EM algorithm aims at maximizing an auxiliary function defined as

$$
Q(\theta, \widehat{\theta})=E[\ln f(\mathbf{z}, \mathbf{x} ; \theta) \mid \mathbf{x} ; \widehat{\theta}]
$$

where $f(z, x ; \theta)$ is the likelihood function of the complete data.

## Estimation step

E compute the expected quantities in $Q(\theta, \widehat{\theta})$ (given $\widehat{\theta}=\theta_{n}$ )

## Maximization step

M maximize the auxiliary function w.r.t. the (true) parameters $\theta$ (given the expected quantities) to obtain a new estimate $\widehat{\theta}=\theta_{i+1}$, i.e.

$$
\theta_{i+1}=\arg \max _{\theta} Q\left(\theta, \theta_{i}\right)
$$

## Close-up on the auxiliary function

Assume we have a n -sample $\mathbf{x}=\left\{x_{1}, \ldots, x_{n}\right\}$ and already know a wide guess $\widehat{\theta}$ of the parameters $\theta$ that we seek to estimate.

The log-likelihood of the complete data is given by

$$
\begin{aligned}
\ln f_{\theta}(\mathbf{z}, \mathbf{x}) & =\ln \left(\prod_{i=1}^{n} P_{\theta}\left[Z_{i}=z_{i}\right] p_{\theta}\left(x_{i} \mid z_{i}\right)\right) \\
& =\sum_{i=1}^{n} \ln \underbrace{P_{\theta}\left[Z_{i}=z_{i}\right]}_{=\pi_{z_{i}}}+\ln \underbrace{p_{\theta}\left(x_{i} \mid z_{i}\right)}_{\text {e.g, } \mathcal{N}\left(\mu_{z_{i}}, \sigma_{z_{i}}\right)} \\
& =\sum_{j=1}^{K} \sum_{i=1}^{n} \ln \left(\pi_{j}\right) \mathbb{I}_{\left(j=z_{i}\right)}+\ln \left(p_{\theta_{j}}\left(x_{i}\right)\right) \mathbb{I}_{\left(j=z_{i}\right)}
\end{aligned}
$$

Hence the auxiliary function boils down to

$$
Q(\theta, \widehat{\theta})=\sum_{j=1}^{K} \sum_{i=1}^{n} \ln \left(\pi_{j}\right) E_{\widehat{\theta}}\left[\mathbb{I}_{\left(j=z_{i}\right)} \mid \mathbf{x}\right]+\ln \left(p_{\theta_{j}}\left(x_{i}\right)\right) E_{\widehat{\theta}}\left[\mathbb{I}_{\left(j=z_{i}\right.} \mid \mathbf{x}\right]
$$

## Maximizing the auxiliary function

Maximizing

$$
Q(\theta, \widehat{\theta})=\sum_{j=1}^{K} \sum_{i=1}^{n} \ln \left(\pi_{j}\right) E_{\widehat{\theta}}\left[\mathbb{I}_{\left(j=z_{i}\right)} \mid \mathbf{x}\right]+\ln \left(p_{\theta_{j}}\left(x_{i}\right)\right) E_{\widehat{\theta}}\left[\mathbb{I}_{\left(j=z_{i}\right)} \mid \mathbf{x}\right]
$$

w.r.t. $\pi_{j}$ under the constraints that weights sum to 1 yields

$$
\widehat{\pi_{j}} \leftarrow \frac{\sum_{i} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]}{\sum_{k} \sum_{i} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=k\right)} \mid \mathbf{x}\right]}
$$

Similarly, maximization w.r.t. the parameters $\theta_{j}$ of the log-likelihood of the $j$-th component, $\ln \left(p_{\theta_{j}}\left(x_{i}\right)\right)$, will yield a function of the expectations $E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]$, e.g., for a Gaussian density - details later

$$
\widehat{\mu}_{j} \leftarrow \frac{\sum_{i} x_{i} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]}{\sum_{i} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]}
$$

## A simple example

- $\mathbf{x}=\left\{x_{1}, \ldots, x_{N}\right\}$ from two classes with prior probabilities $\pi$ and $1-\pi$
- class indicator function $\mathbf{z}=\left\{z_{1}, \ldots, z_{N}\right\}, z_{i} \in\{0,1\}$
- joint distribution of ( $\mathbf{x}, \mathbf{z}$ )

$$
\begin{aligned}
\ln p_{\theta}(\mathbf{x}, \mathbf{z}) & =\sum_{i=1}^{N} \ln p_{\theta}\left(x_{i} \mid z_{i}\right)+\ln P_{\theta}\left[Z_{i}=z_{i}\right] \\
& =\sum_{i=1}^{N} \sum_{j \in\{0,1\}}\left(\ln p_{\theta_{j}}\left(x_{i}\right)+\ln P_{\theta}\left[Z_{i}=j\right]\right) \mathbb{I}_{\left(z_{i}=j\right)}
\end{aligned}
$$

- auxiliary function

$$
Q(\theta, \widehat{\theta})=\sum_{i=1}^{N} \sum_{j \in\{0,1\}}\left(\ln p_{\theta_{j}}\left(x_{i}\right)+\ln P_{\theta}\left[Z_{i}=j\right]\right) E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]
$$

## A simple example: maximization equations

- auxiliary function (cont'd)

$$
\begin{aligned}
& Q(\theta, \widehat{\theta})=\sum_{j \in\{0,1\}} \sum_{i=1}^{N} \ln p_{\theta_{j}}\left(x_{i}\right) E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right] \\
& \quad+\ln (\pi) \sum_{i=1}^{N} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=0\right)} \mid \mathbf{x}\right]+\ln (1-\pi) \sum_{i=1}^{N} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=1\right)} \mid \mathbf{x}\right]
\end{aligned}
$$

- Maximization w.r.t. $\pi$

$$
\pi \leftarrow \frac{\sum_{i} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=-1\right)} \mid \mathbf{x}\right]}{\sum_{j \in\{0,1\}} \sum_{i} E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]}
$$

- Maximization w.r.t. $\theta_{j}$
$\triangleright$ only depends on the expecation $E_{\theta^{n}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]$


## Simple example: expectation computation

The maximization (M-step) of $Q(\theta, \widehat{\theta})$ requires the computation of the expectations (E-step)

$$
E_{\widehat{\theta}}\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x}\right]=P_{\widehat{\theta}}\left[Z_{i}=j \mid x_{i}\right]=\gamma_{j}(i)
$$

for $i \in[1, N]$ and $j \in\{0,1\}$, which is given by (dropping $\widehat{\theta}$ to facilitate reading)

$$
P\left[Z_{i}=j \mid x_{i}\right]=\frac{p\left(x_{i} \mid Z_{i}=j\right) P\left[Z_{i}=j\right]}{\sum_{k \in\{0,1\}} p\left(x_{i} \mid Z_{i}=k\right) P\left[Z_{i}=k\right]}
$$

In our two class example, for $j=0$ we have

$$
p\left(x_{i} \mid Z_{i}=j\right) P\left[Z_{i}=j\right]=\widehat{p i} p_{\widehat{\theta}_{0}}\left(x_{i}\right)
$$

where $\widehat{\pi}$ and $\widehat{\theta}_{0}$ are the current estimates of the parameters.

## EM and hidden class

In all generality

$$
\gamma_{j}(i)=P_{\widehat{\theta}}\left[Z_{i}=j \mid x_{i}\right]=\frac{\widehat{\pi}_{j} p_{\widehat{\theta}_{j}}\left(x_{i}\right)}{\sum_{k} \widehat{\pi}_{k} p_{\widehat{\theta}_{k}}\left(x_{i}\right)}
$$

The latent variable $\gamma_{j}(i)$ indicates membership to a class as estimated from the current estimate $\widehat{\theta}$ of the parameters, we have the following interpretation:

- $P_{\widehat{\theta}}\left[Z_{i}=j \mid x_{i}\right]=$ degree $(\in[0,1])$ of membership to class $j$ of the $i$ 'th observation
- maximization relies on standard estimators based on the degree of membership (weighted standard estimators) [see Gaussian mixture example]


## EM from an algorithmic viewpoint

1. choose some initial (good) parameters $\theta_{0}$
2. $n \leftarrow 0$
3. while not happy (with convergence)
(a) for $i=1 \rightarrow N$ and $j=1 \rightarrow K$
compute the component posterior $\gamma_{j}^{(n)}(i)=P\left[Z_{i}=j \mid x_{i} ; \theta_{n}\right]$
(b) foreach paramter $\alpha$ in $\theta$
compute new parameter value $\alpha_{n+1}$ from the quantities $\gamma_{j}^{(n)}(i)$
(by maximizing $Q\left(\theta, \theta_{n}\right)$ )
(c) $n \leftarrow n+1$

## Properties of the EM algorithm

## Property 1

The serie of estimators $\left\{\theta_{n}\right\}$ is such that the likelihood of the data increases with each iteration of the algorithm.

It can be shown that

$$
\begin{aligned}
& Q\left(\theta, \theta_{i+1}\right)-Q\left(\theta, \theta_{i}\right)= \\
& \quad \ln p\left(\mathbf{x} ; \theta_{i+1}\right)-\ln p\left(\mathbf{x} ; \theta_{i}\right)+\underbrace{E\left[\left.\ln \frac{p\left(\mathbf{z} \mid \mathbf{x} ; \theta_{i+1}\right)}{p\left(\mathbf{z} \mid \mathbf{x} ; \theta_{i}\right)} \right\rvert\, \mathbf{x} ; \theta_{i}\right]}_{<0}
\end{aligned}
$$

which implies that

$$
Q\left(\theta, \theta_{i+1}\right) \geq Q\left(\theta, \theta_{i}\right) \Longrightarrow p\left(\mathbf{x} ; \theta_{i+1}\right) \geq p\left(\mathbf{x} ; \theta_{i}\right)
$$

## Properties of the EM algorithm

## Property 2

The EM algorithm enables the computation of the gradient of the log-likelihood function at the points $\theta_{i}$.

It can be verified that under some non very restrictive assumptions

$$
\left.\frac{\partial Q\left(\theta, \theta_{i}\right)}{\partial \theta}\right|_{\theta=\theta_{i}}=\left.\frac{\partial \ln f(\mathbf{x} ; \theta)}{\partial \theta}\right|_{\theta=\theta_{i}}+\underbrace{\left.\frac{\partial E\left[\ln p(\mathbf{z} \mid \mathbf{x} ; \theta) \mid \mathbf{x} ; \theta_{i}\right]}{\partial \theta}\right|_{\theta=\theta_{i}}}_{=0}
$$

## Convergence of the EM algorithm

## Property 1

The serie of estimators $\left\{\theta^{(n)}\right\}$ is such that the likelihood of the data increases with each iteration of the algorithm.

## Property 2

The EM algorithm enables the computation of the gradient of the log-likelihood function at the points $\theta_{i}$.

## The EM estimate converges toward stationary points of the

 log-likelihood function $\ln p(\mathbf{x} ; \theta)$.
## Convergence of the EM algorithm in practice

- The convergence is only guaranteed toward a local maximum of the likelihood function $\ln p(\mathbf{x} ; \theta)$.
$\triangleright$ need for a good initial guess $\theta_{0}$
$\triangleright$ need to avoid degenerate solutions!
- In practice, convergence is controled by two factors
$\triangleright$ increase of the log-likelihood of the data
$\triangleright$ fixed number of iterations
- Constraints on the parameter space are often used to avoid bad or degenerated solutions, e.g.
$\triangleright$ minimum variance floor
$\triangleright$ initialization based on (segmental) k-means algorithm


## EM for Gaussian mixtures

- Joint likelihood of ( $\mathbf{x}, \mathbf{z}$ )

$$
\ln f(\mathbf{x}, \mathbf{z})=\sum_{i=1}^{N} \sum_{j=1}^{K} \ln \left(w_{j} f\left(x_{i} ; \mu_{j}, \sigma_{j}\right)\right) \mathbb{I}_{\left(z_{i}=j\right)}
$$

- Auxiliary function

$$
\begin{aligned}
& Q\left(\theta, \theta_{n}\right) \propto \sum_{j=1}^{K} \sum_{i=1}^{N} \ln \left(w_{j}\right) E\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x} ; \theta_{n}\right] \\
& \quad-\frac{1}{2} \sum_{j=1}^{K} \sum_{i=1}^{N}\left(\sum_{k=1}^{d} \ln \left(\sigma_{j k}^{2}\right)+\frac{\left(x_{i k}-\mu_{j k}\right)^{2}}{\sigma_{j k}^{2}}\right) E\left[\mathbb{I}_{\left(z_{i}=j\right)} \mid \mathbf{x} ; \theta_{n}\right]
\end{aligned}
$$

## EM for Gaussian mixtures (cont'd)

- Compute the expectations at iteration $n$

$$
\gamma_{j}^{(n)}(i)=\frac{w_{j}^{(n)} f\left(x_{i} ; \mu_{j}^{(n)}, \sigma_{j}^{(n)}\right)}{\sum_{k} w_{k}^{(n)} f\left(x_{i} ; \mu_{k}^{(n)}, \sigma_{k}^{(n)}\right)}
$$

where the parameters correspond to the current estimate $\theta^{(n)}$.

- Maximization

$$
w_{j}^{(n+1)}=\frac{\sum_{i=1}^{N} \gamma_{j}^{(n)}(i)}{\sum_{k=1}^{K} \sum_{i=1}^{N} \gamma_{k}^{(n)}(i)} \quad \mu_{j k}^{(n+1)}=\frac{\sum_{i=1}^{N} \gamma_{j}^{(n)}(i) x_{i k}}{\sum_{i=1}^{N} \gamma_{j}^{(n)}(i)}
$$

## The EM at work: initialization


[courtesy of A. W. Moore and J-F. Bonastre]

## The EM at work: iteration 1


[courtesy of A. W. Moore and J-F. Bonastre]

## The EM at work: iteration 2


[courtesy of A. W. Moore and J-F. Bonastre]

## The EM at work: iteration 3


[courtesy of A. W. Moore and J-F. Bonastre]

## The EM at work: iteration 4


$\square$
[courtesy of A. W. Moore and J-F. Bonastre]

## The EM at work: iteration 20


[courtesy of A. W. Moore and J-F. Bonastre]

## The EM at work: another example



## EM and k-means clustering

- Maximum likelihood estimates with known class membership

$$
\widehat{w}_{i}=\frac{1}{N} \sum_{j=1}^{N} \mathbb{I}_{\left(z_{j}=i\right)} \quad \widehat{\mu}_{i}=\frac{\sum_{j=1}^{N} x_{j} \mathbb{I}_{\left(z_{j}=i\right)}}{\sum_{j=1}^{N} \mathbb{I}_{\left(z_{j}=i\right)}}
$$

- EM estimates with unknown class membership

$$
\widehat{w}_{i}=\frac{1}{N} \sum_{j=1}^{N} E\left[\mathbb{I}_{\left(z_{j}=i\right)} \mid \mathbf{x}, \theta_{n}\right]
$$

$$
\widehat{\mu}_{i}=\frac{\sum_{j=1}^{N} x_{j} E\left[\mathbb{I}_{\left(z_{j}=i\right)} \mid \mathbf{x}, \theta_{n}\right]}{\sum_{j=1}^{N} E\left[\mathbb{I}_{\left(z_{j}=i\right)} \mid \mathbf{x}, \theta_{n}\right]}
$$

## EM and k-means clustering



## A practical use of the Gaussian law


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## EM, sufficient statistics and the exponential family

- Joint density is from the exponential family

$$
f(\mathbf{x}, \mathbf{z} ; \theta)=\exp \left(\alpha(\theta)^{\prime} a(\mathbf{x}, \mathbf{z})+b(\mathbf{x}, \mathbf{z})-\beta(\theta)\right)
$$

- E-step $\Rightarrow$ estimate the sufficient statistic $a(\mathbf{x}, \mathbf{z})$ by computing its expectation under the posterior law given a current estimation of the parameters
- Examples:

$$
\begin{array}{ll}
\sum_{j} \mathbb{I}_{\left(z_{j}=i\right)} & \longrightarrow \sum_{j} E\left[\mathbb{I}_{\left(z_{j}=i\right)} \mid \mathbf{x} ; \theta_{n}\right] \\
\sum_{j} x_{j} \mathbb{I}_{\left(z_{j}=i\right)} & \longrightarrow \sum_{j} x_{j} E\left[\mathbb{I}_{\left(z_{j}=i\right)} \mid \mathbf{x} ; \theta_{n}\right] \\
\sum_{j}\left(x_{j}-\widehat{\mu}_{j}\right)^{2} \mathbb{I}_{\left(z_{j}=i\right)} & \longrightarrow
\end{array}
$$

## The LDA topic mixture model

## I eat fish and vegetables.

Fishes are pets.
My kitten eats fish.


Topic 247

| word | prob. |
| ---: | :---: |
| DRUGS | .069 |
| DRUG | .060 |
| MEDICINE | .027 |
| EFFECTS | .026 |
| BODY | .023 |
| MEDICINES | .019 |
| PAIN | .016 |
| PERSON | .016 |
| MARIJUANA | .014 |
| LABEL | .012 |
| ALCOHOL | .012 |
| DANGEROUS | .011 |
| ABUSE | .009 |
| EFFECT | .009 |
| KNOWN | .008 |
| PILLS | .008 |

Topic 5

| word | prob. |
| ---: | :---: |
| RED | .202 |
| BLUE | .099 |
| GREEN | .096 |
| YELLOW | .073 |
| WHITE | .048 |
| COLOR | .048 |
| BRIGHT | .030 |
| COLORS | .029 |
| ORANGE | .027 |
| BROWN | .027 |
| PINK | .017 |
| LOOK | .017 |
| BLACK | .016 |
| PURPLE | .015 |
| CROSS | .011 |
| COLORED | .009 |

Topic 43

| word | prob. |
| ---: | ---: |
| MIND | .081 |
| THOUGHT | .066 |
| REMEMBER | .064 |
| MEMORY | .037 |
| THINKING | .030 |
| PROFESSOR | .028 |
| FELT | .025 |
| REMEMBERED | .022 |
| netrouGHTS | .020 |
| FORGOTTEN | .020 |
| MOMENT | .020 |
| THINK | .019 |
| THING | .016 |
| WONDER | .014 |
| FORGET | .012 |
| RECALL | .012 |

Topic 56

| word | prob. |
| ---: | ---: |
| DOCTOR | .074 |
| DR. | .063 |
| PATIENT | .061 |
| HOSPITAL | .049 |
| CARE | .046 |
| MEDICAL | .042 |
| NURSE | .031 |
| PATIENTS | .029 |
| DOCTORS | .028 |
| HEALTH | .025 |
| MEDICINE | .017 |
| NURSING | .017 |
| DENTAL | .015 |
| NURSES | .013 |
| PHYSICIAN | .012 |
| HOSPITALS | .011 |

Figure 1. An illustration of four (out of 300) topics extracted from the TASA corpus.

## Variants

The EM principle enables many variants when the E-step and/or the M-step are intractable

- Monte-Carlo EM: replace the exact computation of the expected quantities by some Monte-Carlo approximations obtained using the current parameters
- Generalized EM: simply increase the auxiliary function rather than maximizing it, e.g. using a gradient algorithm
- Variational EM: replace the auxiliary function $Q$ by a more simple variational approximation based on factorial distribution $Q \simeq \prod_{i} Q_{i}$.
- ...


## Choosing the number of components

- Experimentations...
- Information criterion

$$
\mathcal{I}(\mathbf{x}, \theta)=\ln p(\mathbf{x} ; \theta)-g(\# \text { parameters, } \# \text { data })
$$

$\triangleright$ Akaike
$\triangleright$ Bayesian Information criterion (BIC)
$\triangleright \ldots$

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