## Gaussian Mixture Models

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## Overview

## GMMs

- Univariate and multivariate Gaussians
- Gaussian mixture models
- GMM estimation with the EM algorithm
- Using GMMs with HMMs


## Background: cdf

Consider a real valued random variable $X$

- Cumulative distribution function (cdf) $F(x)$ for $X$ :

$$
F(x)=P(X \leq x)
$$

- To obtain the probability of falling in an interval we can do the following:

$$
\begin{aligned}
P(a<X \leq b) & =P(X \leq b)-P(X \leq a) \\
& =F(b)-F(a)
\end{aligned}
$$

## Background: pdf

- The rate of change of the cdf gives us the probability density function (pdf), $p(x)$ :

$$
\begin{aligned}
& p(x)=\frac{d}{d x} F(x)=F^{\prime}(x) \\
& F(x)=\int_{-\infty}^{x} p(x) \mathrm{d} x
\end{aligned}
$$

- $p(x)$ is not the probability that $X$ has value $x$. But the pdf is proportional to the probability that $X$ lies in a small interval centred on $x$.
- Notation: $p$ for pdf, $P$ for probability


## The Gaussian distribution (univariate)

- The Gaussian (or Normal) distribution is the most common (and easily analysed) continuous distribution
- It is also a reasonable model in many situations (the famous "bell curve")
- If a (scalar) variable has a Gaussian distribution, then it has a probability density function with this form:

$$
p\left(x \mid \mu, \sigma^{2}\right)=\mathcal{N}\left(x ; \mu, \sigma^{2}\right)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(\frac{-(x-\mu)^{2}}{2 \sigma^{2}}\right)
$$

- The Gaussian is described by two parameters:
- the mean $\mu$ (location)
- the variance $\sigma^{2}$ (dispersion)


## Plot of Gaussian distribution

- Gaussians have the same shape, with the location controlled by the mean, and the spread controlled by the variance
- One-dimensional Gaussian with zero mean and unit variance $\left(\mu=0, \sigma^{2}=1\right)$ :



## Properties of the Gaussian distribution

$\mathcal{N}\left(x ; \mu, \sigma^{2}\right)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(\frac{-(x-\mu)^{2}}{2 \sigma^{2}}\right)$


## Parameter estimation

- Estimate mean and variance parameters of a Gaussian from data $x_{1}, x_{2}, \ldots, x_{N}$
- Use the following as the estimates:

$$
\begin{aligned}
\hat{\mu} & \left.=\frac{1}{N} \sum_{n=1}^{N} x_{n} \quad \text { (mean }\right) \\
\hat{\sigma}^{2} & =\frac{1}{N} \sum_{n=1}^{N}\left(x_{n}-\hat{\mu}\right)^{2} \quad \text { (variance) }
\end{aligned}
$$

## Example: ML estimation of the mean

Consider the log likelihood of a set of $N$ training data points $\left\{x_{1}, \ldots, x_{N}\right\}$ being generated by a Gaussian with mean $\mu$ and variance $\sigma^{2}$ :

$$
\begin{aligned}
L=\ln p\left(\left\{x_{1}, \ldots, x_{N}\right\} \mid \mu, \sigma^{2}\right) & =-\frac{1}{2} \sum_{n=1}^{N}\left(\frac{\left(x_{n}-\mu\right)^{2}}{\sigma^{2}}-\ln \sigma^{2}-\ln (2 \pi)\right) \\
& =-\frac{1}{2 \sigma^{2}} \sum_{n=1}^{N}\left(x_{n}-\mu\right)^{2}-\frac{N}{2} \ln \sigma^{2}-\frac{N}{2} \ln (2 \pi)
\end{aligned}
$$

By maximising the the log likelihood function with respect to $\mu$ we can show that the maximum likelihood estimate for the mean is indeed the sample mean:

$$
\hat{\mu}=\frac{1}{N} \sum_{n=1}^{N} x_{n}
$$

## The multivariate Gaussian distribution

- The $D$-dimensional vector $x=\left(x_{1}, \ldots, x_{D}\right)^{T}$ follows a multivariate Gaussian (or normal) distribution if it has a probability density function of the following form:

$$
p(\times \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})=\frac{1}{(2 \pi)^{D / 2}|\boldsymbol{\Sigma}|^{1 / 2}} \exp \left(-\frac{1}{2}(\mathrm{x}-\boldsymbol{\mu})^{T} \boldsymbol{\Sigma}^{-1}(\mathrm{x}-\boldsymbol{\mu})\right)
$$

The pdf is parameterised by the mean vector $\boldsymbol{\mu}=\left(\mu_{1}, \ldots, \mu_{D}\right)^{T}$ and the covariance matrix $\boldsymbol{\Sigma}=\left(\begin{array}{ccc}\sigma_{11} & \ldots & \sigma_{1 D} \\ \vdots & \ddots & \vdots \\ \sigma_{D 1} & \cdots & \sigma_{D D}\end{array}\right)$.

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- The 1-dimensional Gaussian is a special case of this pdf
- The argument to the exponential $0.5(\times-\mu)^{T} \boldsymbol{\Sigma}^{-1}(\mathrm{x}-\boldsymbol{\mu})$ is referred to as a quadratic form.


## Covariance matrix

- The mean vector $\boldsymbol{\mu}$ is the expectation of x :

$$
\boldsymbol{\mu}=E[\mathrm{x}]
$$

- The covariance matrix $\boldsymbol{\Sigma}$ is the expectation of the deviation of $x$ from the mean:

$$
\boldsymbol{\Sigma}=E\left[(\mathrm{x}-\boldsymbol{\mu})(\mathrm{x}-\boldsymbol{\mu})^{T}\right]
$$

- $\Sigma$ is a $D \times D$ symmetric matrix:

$$
\sigma_{i j}=E\left[\left(x_{i}-\mu_{i}\right)\left(x_{j}-\mu_{j}\right)\right]=E\left[\left(x_{j}-\mu_{j}\right)\left(x_{i}-\mu_{i}\right)\right]=\sigma_{j i}
$$

- The sign of the covariance helps to determine the relationship between two components:
- If $x_{j}$ is large when $x_{i}$ is large, then $\left(x_{i}-\mu_{i}\right)\left(x_{j}-\mu_{j}\right)$ will tend to be positive;
- If $x_{j}$ is small when $x_{i}$ is large, then $\left(x_{i}-\mu_{i}\right)\left(x_{j}-\mu_{j}\right)$ will tend to be negative.


## Spherical Gaussian



NB: Correlation coefficient $\rho_{i j}=\frac{\sigma_{i j}}{\sqrt{\sigma_{i i} \sigma_{i j}}} \quad\left(-1 \leq \rho_{i j} \leq 1\right)$

## Diagonal Covariance Gaussian



NB: Correlation coefficient $\rho_{i j}=\frac{\sigma_{i j}}{\sqrt{\sigma_{i i} \sigma_{i j}}} \quad\left(-1 \leq \rho_{i j} \leq 1\right)$

## Full covariance Gaussian



NB: Correlation coefficient $\rho_{i j}=\frac{\sigma_{i j}}{\sqrt{\sigma_{i i} \sigma_{j j}}} \quad\left(-1 \leq \rho_{i j} \leq 1\right)$

## Parameter estimation of a multivariate Gaussian distribution

- It is possible to show that the mean vector $\hat{\boldsymbol{\mu}}$ and covariance matrix $\hat{\boldsymbol{\Sigma}}$ that maximise the likelihood of the training data are given by:

$$
\begin{aligned}
\hat{\boldsymbol{\mu}} & =\frac{1}{N} \sum_{t=1}^{N} x_{n} \\
\hat{\boldsymbol{\Sigma}} & =\frac{1}{N} \sum_{t=1}^{N}\left(x_{n}-\hat{\boldsymbol{\mu}}\right)\left(x_{n}-\hat{\boldsymbol{\mu}}\right)^{T}
\end{aligned}
$$

where $\boldsymbol{x}_{n}=\left(x_{n, 1}, \ldots, x_{n, D}\right)^{T}$.
NB: $T$ denotes either the number of samples or vector transpose depending on context.

## Example data



## Maximum likelihood fit to a Gaussian



## Data in clusters (example 1)



## Example 1 fit by a Gaussian



$$
\boldsymbol{\mu}_{1}=(0,0)^{T} \quad \boldsymbol{\mu}_{2}=(1,1)^{T} \quad \boldsymbol{\Sigma}_{1}=\boldsymbol{\Sigma}_{2}=0.2 \mathrm{l}
$$

## k-means clustering

- k-means is an automatic procedure for clustering unlabelled data
- Requires a prespecified number of clusters
- Clustering algorithm chooses a set of clusters with the minimum within-cluster variance
- Guaranteed to converge (eventually)
- Clustering solution is dependent on the initialisation


## k-means example: data set



## k-means example: initialisation



## k-means example: iteration 1 (assign points to clusters)



## k-means example: iteration 1 (recompute centres)



## k-means example: iteration 2 (assign points to clusters)



## k-means example: iteration 2 (recompute centres)



## k-means example: iteration 3 (assign points to clusters)



No changes, so converged

## Mixture model

- A more flexible form of density estimation is made up of a linear combination of component densities:

$$
p(x)=\sum_{m=1}^{M} P(m) p(x \mid m)
$$

- This is called a mixture model or a mixture density
- $p(\mathrm{x} \mid m)$ : component densities
- $P(m)$ : mixing parameters
- Generative model:
(1) Choose a mixture component based on $P(m)$
(2) Generate a data point $x$ from the chosen component using $p(\times \mid m)$


## Gaussian mixture model

- The most important mixture model is the Gaussian Mixture Model (GMM), where the component densities are Gaussians
- Consider a GMM, where each component Gaussian $\mathcal{N}\left(x ; \boldsymbol{\mu}_{m}, \boldsymbol{\Sigma}_{m}\right)$ has mean $\boldsymbol{\mu}_{m}$ and a spherical covariance $\boldsymbol{\Sigma}_{m}=\sigma_{m}^{2}$ I

$$
p(\mathrm{x})=\sum_{m=1}^{M} P(m) p(\mathrm{x} \mid m)=\sum_{m=1}^{M} P(m) \mathcal{N}\left(\mathrm{x} ; \boldsymbol{\mu}_{m}, \sigma_{m}^{2} \mathrm{l}\right)
$$

## GMM Parameter estimation when we know which component generated the data

- Define the indicator variable $z_{m n}=1$ if component $m$ generated data point $\boldsymbol{x}_{n}$ (and 0 otherwise)
- If $z_{m n}$ wasn't hidden then we could count the number of observed data points generated by $m$ :

$$
N_{m}=\sum_{n=1}^{N} z_{m n}
$$

- And estimate the mean, variance and mixing parameters as:

$$
\begin{aligned}
\hat{\boldsymbol{\mu}}_{m} & =\frac{\sum_{n} z_{m n} \boldsymbol{x}_{n}}{N_{m}} \\
\hat{\sigma}_{m}^{2} & =\frac{\sum_{n} z_{m n}\left\|\boldsymbol{x}_{n}-\hat{\boldsymbol{\mu}}_{m}\right\|^{2}}{N_{m}} \\
\hat{P}(m) & =\frac{1}{N} \sum_{n} z_{m n}=\frac{N_{m}}{N}
\end{aligned}
$$

## GMM Parameter estimation when we don't know which component generated the data

- Problem: we don't know $z_{m n}$ - which mixture component a data point comes from...
- Instead we use the EM algorithm: estimate the posterior probability $P(m \mid x)$, which gives the probability that component $m$ was responsible for generating data point $\times$, using an initial set of parameters, $\lambda_{0}$
- At each iteration, we maximise

$$
\begin{gathered}
\sum_{m} P\left(m \mid x, \lambda_{0}\right) \log P(x \mid m, \lambda) \\
P\left(m \mid x, \lambda_{0}\right)=\frac{p(x \mid m) P(m)}{p(x)}=\frac{p(x \mid m) P(m)}{\sum_{m^{\prime}=1}^{M} p\left(x \mid m^{\prime}\right) P\left(m^{\prime}\right)}
\end{gathered}
$$

(dropping the dependence on $\lambda_{0}$ for clarity)

## Soft assignment

- We can view the EM algorithm as estimating "soft counts" for the data points, based on the component occupation probabilities $P\left(m \mid \boldsymbol{x}_{n}\right)$ :

$$
N_{m}^{*}=\sum_{n=1}^{N} P\left(m \mid \boldsymbol{x}_{n}\right)
$$

- We can imagine this as assigning data points to component $m$ weighted by the component occupation probability $P\left(m \mid \boldsymbol{x}_{t}\right)$
- Estimate the mean, variance and prior probabilities as:

$$
\begin{aligned}
\hat{\boldsymbol{\mu}}_{m} & =\frac{\sum_{n} P\left(m \mid \boldsymbol{x}_{n}\right) \boldsymbol{x}_{n}}{\sum_{n} P\left(m \mid \boldsymbol{x}_{n}\right)}=\frac{\sum_{n} P\left(m \mid \boldsymbol{x}_{n}\right) \boldsymbol{x}_{n}}{N_{m}^{*}} \\
\hat{\sigma}_{m}^{2} & =\frac{\sum_{n} P\left(m \mid \boldsymbol{x}_{n}\right)\left\|\boldsymbol{x}_{n}-\hat{\boldsymbol{\mu}}_{m}\right\|^{2}}{\sum_{n} P\left(m \mid \boldsymbol{x}_{n}\right)}=\frac{\sum_{n} P\left(m \mid \boldsymbol{x}_{n}\right)\left\|\boldsymbol{x}_{n}-\hat{\boldsymbol{\mu}}_{m}\right\|^{2}}{N_{m}^{*}} \\
\hat{P}(m) & =\frac{1}{n} \sum_{n} P\left(m \mid \boldsymbol{x}_{n}\right)=\frac{N_{m}^{*}}{n}
\end{aligned}
$$

## Example 1 fit using a GMM



## Example 1 fit using a GMM



Fitted with a two component GMM using EM

## Peakily distributed data (Example 2)



$$
\boldsymbol{\mu}_{1}=\boldsymbol{\mu}_{2}=\left[\begin{array}{llll}
0 & 0
\end{array}\right]^{T} \quad \boldsymbol{\Sigma}_{1}=0.11 \quad \boldsymbol{\Sigma}_{2}=21
$$

## Example 2 fit by a Gaussian



$$
\boldsymbol{\mu}_{1}=\boldsymbol{\mu}_{2}=\left[\begin{array}{llll}
0 & 0
\end{array}\right]^{T} \quad \boldsymbol{\Sigma}_{1}=0.11 \quad \boldsymbol{\Sigma}_{2}=21
$$

## Example 2 fit by a GMM



## Example 2 fit by a GMM



Fitted with a two component GMM using EM

## Example 2: component Gaussians



$$
P(x \mid m=1)
$$



$$
P(x \mid m=2)
$$

## Comments on GMMs

- GMMs trained using the EM algorithm are able to self organise to fit a data set
- Individual components take responsibility for parts of the data set (probabilistically)
- Soft assignment to components not hard assignment - "soft clustering"
- GMMs scale very well, e.g.: large speech recognition systems can have $30,000 \mathrm{GMMs}$, each with 32 components: sometimes 1 million Gaussian components!! And the parameters all estimated from (a lot of) data by EM


## HMMs with Gaussian observation probabilities

We can use a Gaussian distribution to model the observation probability:

$$
b_{j}(\mathrm{x})=\mathcal{N}\left(\mathrm{x} ; \boldsymbol{\mu}_{j}, \boldsymbol{\Sigma}_{j}\right)
$$

We need to find estimate parameters $\hat{\boldsymbol{\mu}}_{j}, \hat{\boldsymbol{\Sigma}}_{j}$ for each state $j$. Use the EM algorithm to weight each sample $x_{t}$ by the occupation probability $\gamma_{j}(t)$ :

$$
\hat{\boldsymbol{\mu}}_{j}=\frac{\sum_{t=1}^{T} \gamma_{j}(t) x_{t}}{\sum_{t=1}^{T} \gamma_{j}(t)}
$$

And likewise for the covariance matrices:

$$
\hat{\boldsymbol{\Sigma}}_{j}=\frac{\sum_{t=1}^{T} \gamma_{j}(t)\left(x_{t}-\hat{\boldsymbol{\mu}}_{j}\right)\left(x-\hat{\boldsymbol{\mu}}_{j}\right)^{T}}{\sum_{t=1}^{T} \gamma_{j}(t)}
$$

## Extension to Gaussian mixture model (GMM)

- The assumption of a Gaussian distribution at each state is very strong; in practice the acoustic feature vectors associated with a state may be strongly non-Gaussian
- In this case an M-component Gaussian mixture model is an appropriate density function:

$$
b_{j}(\mathrm{x})=p(\mathrm{x} \mid q=j)=\sum_{m=1}^{M} c_{j m} \mathcal{N}\left(\mathrm{x} ; \boldsymbol{\mu}_{j m}, \boldsymbol{\Sigma}_{j m}\right)
$$

Given enough components, this family of functions can model any distribution.

- Train using the EM algorithm again, in which the component occupation probabilities are estimated along with the state occupation probabilities in the E-step


## EM training of HMM/GMM

- Rather than estimating the state-time alignment, we estimate the component/state-time alignment, and component-state occupation probabilities $\gamma_{j m}(t)$ : the probability of occupying mixture component $m$ of state $j$ at time $t$.
( $\xi_{t m}(j)$ in Jurafsky and Martin's SLP)
- Re-estimate the parameters of component $m$ of state $j$ as follows

$$
\begin{aligned}
\hat{\boldsymbol{\mu}}_{j m} & =\frac{\sum_{t=1}^{T} \gamma_{j m}(t) \boldsymbol{x}_{t}}{\sum_{t=1}^{T} \gamma_{j m}(t)} \\
\hat{\boldsymbol{\Sigma}}_{j m} & =\frac{\sum_{t=1}^{T} \gamma_{j m}(t)\left(\boldsymbol{x}_{t}-\hat{\boldsymbol{\mu}}_{j m}\right)\left(\boldsymbol{x}-\hat{\boldsymbol{\mu}}_{j m}\right)^{T}}{\sum_{t=1}^{T} \gamma_{j m}(t)}
\end{aligned}
$$

- The mixture coefficients are re-estimated in a similar way to transition probabilities:

$$
\hat{c}_{j m}=\frac{\sum_{t=1}^{T} \gamma_{j m}(t)}{\sum_{m^{\prime}=1}^{M} \sum_{t=1}^{T} \gamma_{j m^{\prime}}(t)}
$$

## Doing the computation

- The forward, backward and Viterbi recursions result in a long sequence of probabilities being multiplied
- This can cause floating point underflow problems
- In practice computations are performed in the log domain (in which multiplies become adds)
- Working in the log domain also avoids needing to perform the exponentiation when computing Gaussians


## References: HMMs

- Gales and Young (2007). "The Application of Hidden Markov Models in Speech Recognition", Foundations and Trends in Signal Processing, 1 (3), 195-304: section 2.2.
- Jurafsky and Martin (2008). Speech and Language Processing (2nd ed.): sections 6.1-6.5; 9.2; 9.4. (Errata at http://www.cs.colorado.edu/~martin/SLP/Errata/ SLP2-PIEV-Errata.html)
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- Renals and Hain (2010). "Speech Recognition", Computational Linguistics and Natural Language Processing Handbook, Clark, Fox and Lappin (eds.), Blackwells.

