#### 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:

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

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

$$P(a < X \le b) = P(X \le b) - P(X \le a)$$
$$= F(b) - F(a)$$

## Background: pdf

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

$$p(x) = \frac{d}{dx}F(x) = F'(x)$$
$$F(x) = \int_{-\infty}^{x} p(x)dx$$

- 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)

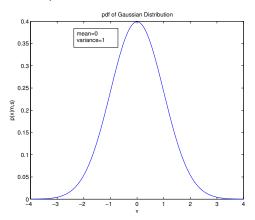
- The Gaussian (or Normal) distribution is the most common (and easily analysed) continuous distribution
- It is also a reasonable model in many situations (the famous "bell curve")
- If a (scalar) variable has a Gaussian distribution, then it has a probability density function with this form:

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

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

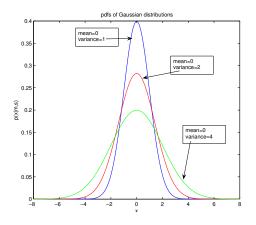
#### Plot of Gaussian distribution

- 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  $(\mu=0, \, \sigma^2=1)$ :



## Properties of the Gaussian distribution

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



#### Parameter estimation

- Estimate mean and variance parameters of a Gaussian from data x<sub>1</sub>, x<sub>2</sub>,...,x<sub>N</sub>
- Use the following as the estimates:

$$\hat{\mu}=rac{1}{N}\sum_{n=1}^{N}x_n$$
 (mean)  $\hat{\sigma}^2=rac{1}{N}\sum_{n=1}^{N}(x_n-\hat{\mu})^2$  (variance)

## Example: ML estimation of the mean

Consider the log likelihood of a set of N training data points  $\{x_1, \ldots, x_N\}$  being generated by a Gaussian with mean  $\mu$  and variance  $\sigma^2$ :

$$L = \ln p(\{x_1, \dots, x_N\} | \mu, \sigma^2) = -\frac{1}{2} \sum_{n=1}^{N} \left( \frac{(x_n - \mu)^2}{\sigma^2} - \ln \sigma^2 - \ln(2\pi) \right)$$
$$= -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi)$$

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  $\mathbf{x} = (x_1, \dots, x_D)^T$  follows a multivariate Gaussian (or normal) distribution if it has a probability density function of the following form:

$$p(\mathbf{x} \,|\, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = rac{1}{(2\pi)^{D/2} |\boldsymbol{\Sigma}|^{1/2}} \exp\left(-rac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})
ight)$$

The pdf is parameterised by the mean vector  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_D)^T$  and the covariance matrix  $\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_{11} & \dots & \sigma_{1D} \\ \vdots & \ddots & \vdots \\ \sigma_{D1} & \dots & \sigma_{DD} \end{pmatrix}$ .

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

#### Covariance matrix

• The mean vector  $\mu$  is the expectation of x:

$$\mu = E[x]$$

 The covariance matrix Σ is the expectation of the deviation of x from the mean:

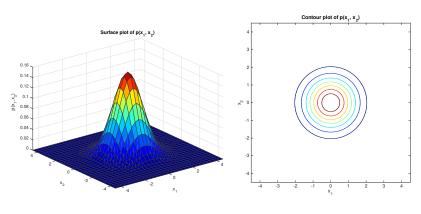
$$\Sigma = E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T]$$

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

$$\sigma_{ij} = E[(x_i - \mu_i)(x_j - \mu_j)] = E[(x_j - \mu_j)(x_i - \mu_i)] = \sigma_{ji}$$

- The sign of the covariance helps to determine the relationship between two components:
  - If  $x_j$  is large when  $x_i$  is large, then  $(x_i \mu_i)(x_j \mu_j)$  will tend to be positive;
  - If  $x_j$  is small when  $x_i$  is large, then  $(x_i \mu_i)(x_j \mu_j)$  will tend to be negative.

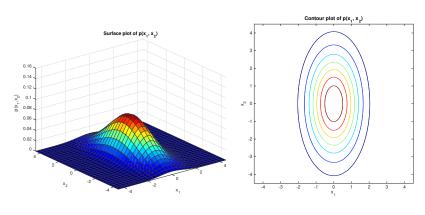
## Spherical Gaussian



$$oldsymbol{\mu} = \left( egin{array}{c} 0 \ 0 \end{array} 
ight) \qquad oldsymbol{\Sigma} = \left( egin{array}{c} 1 & 0 \ 0 & 1 \end{array} 
ight) \qquad 
ho_{12} = 0$$

NB: Correlation coefficient  $\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$   $(-1 \le \rho_{ij} \le 1)$ 

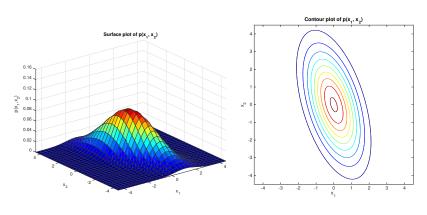
## Diagonal Covariance Gaussian



$$oldsymbol{\mu} = \left( egin{array}{c} 0 \ 0 \end{array} 
ight) \qquad oldsymbol{\Sigma} = \left( egin{array}{c} 1 & 0 \ 0 & 4 \end{array} 
ight) \qquad 
ho_{12} = 0$$

NB: Correlation coefficient  $\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$   $(-1 \le \rho_{ij} \le 1)$ 

#### Full covariance Gaussian



$$\mu = \left( egin{array}{c} 0 \ 0 \end{array} 
ight) \qquad oldsymbol{\Sigma} = \left( egin{array}{cc} 1 & -1 \ -1 & 4 \end{array} 
ight) \qquad 
ho_{12} = -0.5$$

NB: Correlation coefficient  $\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$   $(-1 \le \rho_{ij} \le 1)$ 

## Parameter estimation of a multivariate Gaussian distribution

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

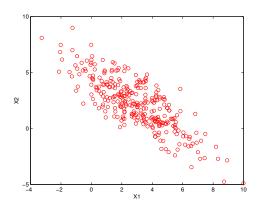
$$\hat{\mu} = \frac{1}{N} \sum_{t=1}^{N} \mathbf{x}_n$$

$$\hat{\Sigma} = \frac{1}{N} \sum_{t=1}^{N} (\mathbf{x}_n - \hat{\mu}) (\mathbf{x}_n - \hat{\mu})^T$$

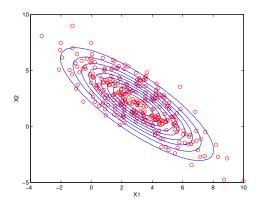
where 
$$\mathbf{x}_{n} = (x_{n,1}, \dots, x_{n,D})^{T}$$
.

NB: T denotes either the number of samples or vector transpose depending on context.

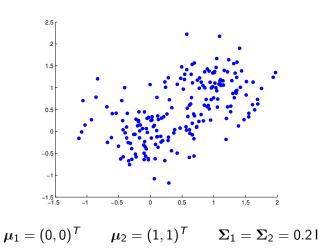
## Example data



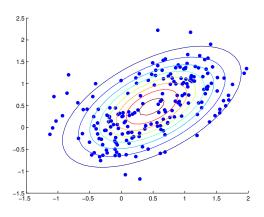
## Maximum likelihood fit to a Gaussian



## Data in clusters (example 1)



## Example 1 fit by a Gaussian



$$\mu_1 = (0,0)^T$$
  $\mu_2 = (1,1)^T$   $\Sigma_1 = \Sigma_2 = 0.2 \, \mathrm{I}$ 

#### Mixture model

- A more powerful form of density estimation is to introduce multiple components to the model, each with its own probability density. This is called a mixture model or a mixture density
- Can view this as a generative model
  - Choose a random mixture component C based on a prior probability P(C = m)
  - ② Generate a data point x from the chosen component using a density function p(x|C=m)
    - \*\*The component C is not observed\*\*
- We can calculate the probability density of x as

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

• We use shorthand notation P(m), p(x|m)

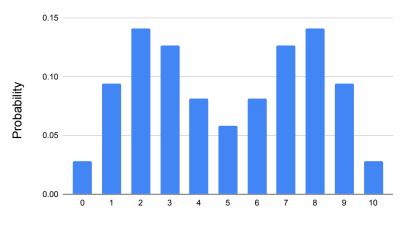
## Simple example

- Suppose we have two identical bags, each containing a
  different proportion of blue balls. In each trial, we randomly
  chose a bag with probability 0.5 and pull out k balls (with
  replacement).
- What is the distribution of X, the number of blue balls sampled?

$$P(X=i) = \frac{1}{2}Bin(k,\alpha_1) + \frac{1}{2}Bin(k,\alpha_2)$$

where  $\alpha_1,\alpha_2$  are the proportions of blue balls in the respective bags

## Simple example



Number of blue balls, X

Example for 
$$\alpha_1 = \frac{1}{4}$$
,  $\alpha_2 = \frac{3}{4}$ ,  $k = 10$ 

#### Gaussian mixture model

 The most important mixture model is the Gaussian Mixture Model (GMM), where the component densities are Gaussians

$$p(\mathbf{x}) = \sum_{m=1}^{M} P(m) p(\mathbf{x} \mid m) = \sum_{m=1}^{M} P(m) \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_{m}, \boldsymbol{\Sigma}_{m})$$

## Estimating the parameters of a mixture model

- Define the indicator variable  $z_{mn} = 1$  if component m generated data point  $x_n$  (and 0 otherwise)
- If z<sub>mn</sub> wasn't hidden then we could count the number of observed data points generated by m:

$$N_m = \sum_{n=1}^N z_{mn}$$

 And use the observations assigned to each component to estimate the parameters using maximum likelihood estimation

### In our simple example

- Suppose we repeat the experiment (trial) n times
- $z_{mn}$  indicates if bag m was chosen on the nth trial
- If  $x_n$  is the number of blue balls drawn on the *n*th trial

$$\hat{\alpha}_m = \frac{\sum_{n=1}^N z_{mn} x_n}{k \times N_m}$$

 If the bags were not chosen with identical probability, we could estimate this probability with

$$\hat{P}(m) = \frac{1}{N} \sum_{n} z_{mn} = \frac{N_m}{N}$$

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

Estimate the mean, covariance and mixing parameters as:

$$\hat{\boldsymbol{\mu}}_{m} = \frac{\sum_{n} z_{mn} \boldsymbol{x}_{n}}{N_{m}}$$

$$\hat{\boldsymbol{\Sigma}}_{m} = \frac{\sum_{n} z_{mn} (\boldsymbol{x}_{n} - \hat{\boldsymbol{\mu}}_{m}) (\boldsymbol{x}_{n} - \hat{\boldsymbol{\mu}}_{m})^{T}}{N_{m}}$$

$$\hat{P}(m) = \frac{1}{N} \sum_{n} z_{mn} = \frac{N_{m}}{N}$$

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

- *Problem:* we don't know  $z_{mn}$  which mixture component a data point comes from...
- Instead we use the EM algorithm: estimate the posterior probability P(m|x), which gives the probability that component m was responsible for generating data point x, using an initial set of parameters,  $\lambda_0$
- At each iteration, we maximise

$$\sum_{m} P(m|x;\lambda_0) \log P(x,m;\lambda)$$

$$P(m|x; \lambda_0) = \frac{p(x|m) P(m)}{p(x)} = \frac{p(x|m) P(m)}{\sum_{m'=1}^{M} p(x|m') P(m')}$$

(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  $P(m|x_n)$ :

$$N_m^* = \sum_{n=1}^N P(m | x_n)$$

- We can imagine this as assigning data points to component m weighted by the component occupation probability  $P(m|x_n)$
- In the bag example: imagine estimating which bag has been chosen at the *n*th trial, based on the number of blue balls drawn (and our earlier estimates of the parameters)
- It is possible to prove that the EM algorithm is guaranteed to increase the likelihood at each iteration

#### For the GMM

Estimate the mean, variance and prior probabilities as:

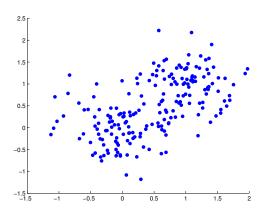
$$\hat{\mu}_{m} = \frac{\sum_{n} P(m|\mathbf{x}_{n}) \mathbf{x}_{n}}{\sum_{n} P(m|\mathbf{x}_{n})} = \frac{\sum_{n} P(m|\mathbf{x}_{n}) \mathbf{x}_{n}}{N_{m}^{*}}$$

$$\hat{\Sigma}_{m} = \frac{\sum_{n} P(m|\mathbf{x}_{n}) (\mathbf{x}_{n} - \hat{\mu}_{m}) (\mathbf{x}_{n} - \hat{\mu}_{m})^{T}}{\sum_{n} P(m|\mathbf{x}_{n})}$$

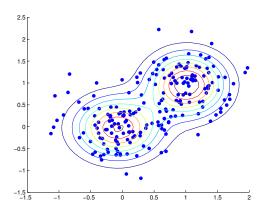
$$= \frac{\sum_{n} P(m|\mathbf{x}_{n}) (\mathbf{x}_{n} - \hat{\mu}_{m}) (\mathbf{x}_{n} - \hat{\mu}_{m})^{T}}{N_{m}^{*}}$$

$$\hat{P}(m) = \frac{1}{N} \sum_{n} P(m|\mathbf{x}_{n}) = \frac{N_{m}^{*}}{N}$$

## Example 1 fit using a GMM

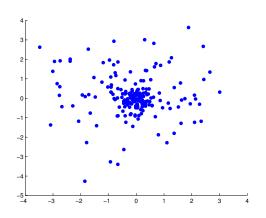


## Example 1 fit using a GMM



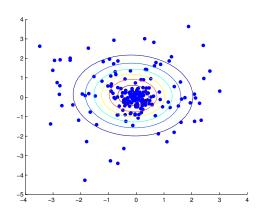
Fitted with a two component GMM using EM

## Peakily distributed data (Example 2)



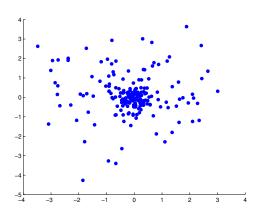
$$\mu_1 = \mu_2 = [0 \quad 0]^T \qquad \Sigma_1 = 0.1$$
I  $\Sigma_2 = 2$ I

## Example 2 fit by a Gaussian

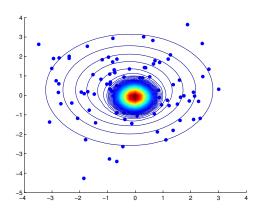


$$\mu_1 = \mu_2 = [0 \quad 0]^T \qquad \Sigma_1 = 0.1$$
l  $\Sigma_2 = 2$ l

## Example 2 fit by a GMM

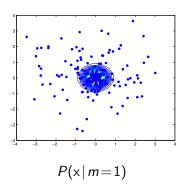


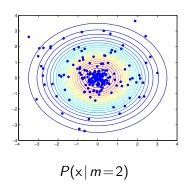
## Example 2 fit by a GMM



Fitted with a two component GMM using EM

## Example 2: component Gaussians





#### 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 GMM-based speech recognition systems might have as many as 30,000 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:

$$b_j(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$$

We need to estimate parameters  $\hat{\mu}_j$ ,  $\hat{\Sigma}_j$  for each state j. Use the EM algorithm to weight each sample  $\mathbf{x}_t$  by the occupation probability  $\gamma_i(t)$ :

$$\hat{\boldsymbol{\mu}}_j = \frac{\sum_{t=1}^T \gamma_j(t) \boldsymbol{x}_t}{\sum_{t=1}^T \gamma_j(t)}$$

And likewise for the covariance matrices:

$$\hat{\boldsymbol{\Sigma}}_j = \frac{\sum_{t=1}^T \gamma_j(t) (\boldsymbol{x}_t - \hat{\boldsymbol{\mu}}_j) (\boldsymbol{x}_t - \hat{\boldsymbol{\mu}}_j)^T}{\sum_{t=1}^T \gamma_j(t)}$$

## 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:

$$b_j(\mathbf{x}) = p(\mathbf{x} | q = j) = \sum_{m=1}^{M} c_{jm} \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_{jm}, \boldsymbol{\Sigma}_{jm})$$

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  $\gamma_{im}(t)$ : the probability of occupying mixture component m of state j at time t.

 $(\mathcal{E}_{tm}(i))$  in Jurafsky and Martin's SLP)

 Re-estimate the parameters of component m of state i as follows

$$egin{aligned} \hat{m{\mu}}_{jm} &= rac{\sum_{t=1}^{T} \gamma_{jm}(t) m{x}_t}{\sum_{t=1}^{T} \gamma_{jm}(t)} \ \hat{m{\Sigma}}_{jm} &= rac{\sum_{t=1}^{T} \gamma_{jm}(t) (m{x}_t - \hat{m{\mu}}_{jm}) (m{x}_t - \hat{m{\mu}}_{jm})^T}{\sum_{t=1}^{T} \gamma_{jm}(t)} \end{aligned}$$

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

$$\hat{c}_{jm} = rac{\sum_{t=1}^{T} \gamma_{jm}(t)}{\sum_{m'=1}^{M} \sum_{t=1}^{T} \gamma_{jm'}(t)}$$

## 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: GMMs

\* Renals and Hain (2010). "Speech Recognition", Computational Linguistics and Natural Language Processing Handbook, Clark, Fox and Lappin (eds.), Blackwells: section 2.2.