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)

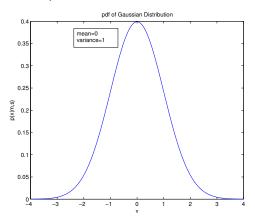
- The Gaussian (or Normal) distribution is the most common (and easily analysed) continuous distribution
- It is also a reasonable model in many situations (the famous "bell curve")
- If a (scalar) variable has a Gaussian distribution, then it has a probability density function with this form:

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

- The Gaussian is described by two parameters:
 - the mean μ (location)
 - the variance σ^2 (dispersion)

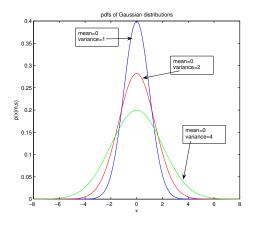
Plot of Gaussian distribution

- 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 x₁, x₂,...,x_N
- 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 μ and variance σ^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 μ 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:

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

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

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• The 1-dimensional Gaussian is a special case of this pdf

The multivariate Gaussian distribution

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$$ho(\mathbf{x} | oldsymbol{\mu}, oldsymbol{\Sigma}) = rac{1}{(2\pi)^{D/2} |oldsymbol{\Sigma}|^{1/2}} \exp\left(-rac{1}{2}(\mathbf{x} - oldsymbol{\mu})^T oldsymbol{\Sigma}^{-1}(\mathbf{x} - oldsymbol{\mu})
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- The 1-dimensional Gaussian is a special case of this pdf
- The argument to the exponential $0.5(\mathbf{x} \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} \boldsymbol{\mu})$ is referred to as a *quadratic form*.

Covariance matrix

• The mean vector μ is the expectation of x:

$$\mu = E[x]$$

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

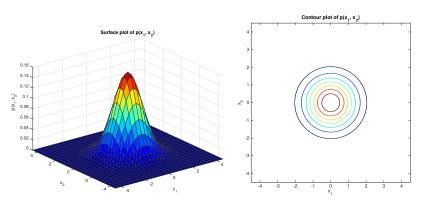
$$\Sigma = E[(x - \mu)(x - \mu)^T]$$

• Σ 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.

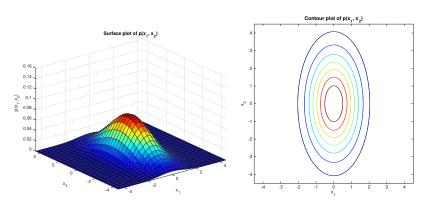
Spherical Gaussian



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

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

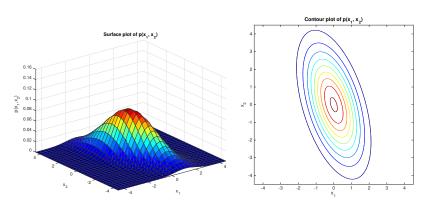
Diagonal Covariance Gaussian



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

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:

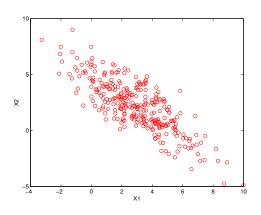
$$\hat{\mu} = \frac{1}{N} \sum_{t=1}^{N} \mathbf{x}_n$$

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

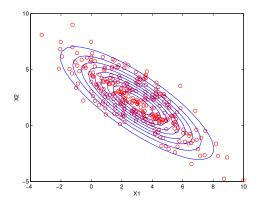
where
$$\mathbf{x}_{n} = (x_{n,1}, \dots, x_{n,D})^{T}$$
.

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

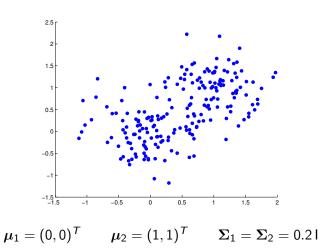
Example data



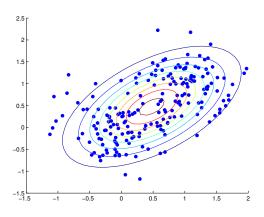
Maximum likelihood fit to a Gaussian



Data in clusters (example 1)



Example 1 fit by a Gaussian

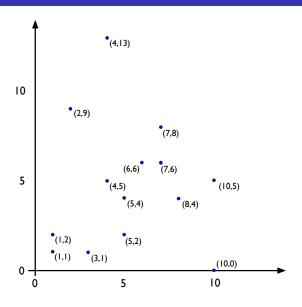


$$m{\mu}_1 = (0,0)^T \qquad m{\mu}_2 = (1,1)^T \qquad m{\Sigma}_1 = m{\Sigma}_2 = 0.2 \, \mathsf{I}$$

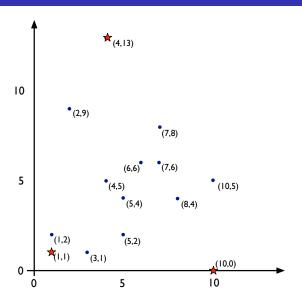
k-means clustering

- 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

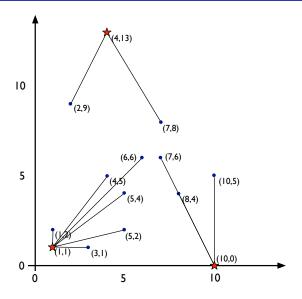
k-means example: data set



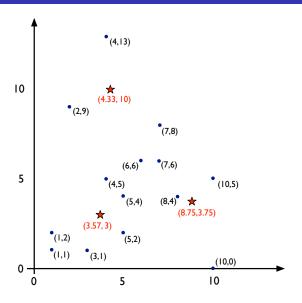
k-means example: initialisation



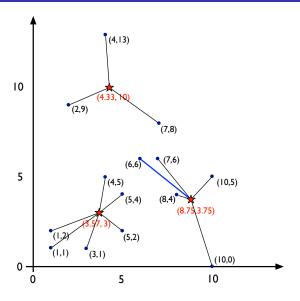
k-means example: iteration 1 (assign points to clusters)



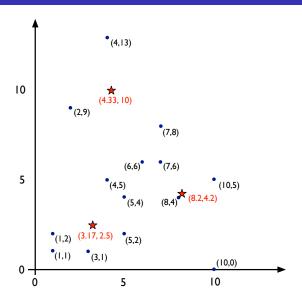
k-means example: iteration 1 (recompute centres)



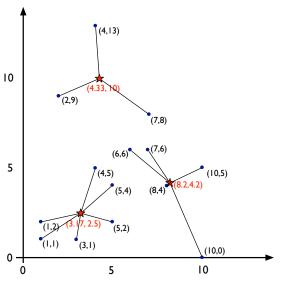
k-means example: iteration 2 (assign points to clusters)



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:

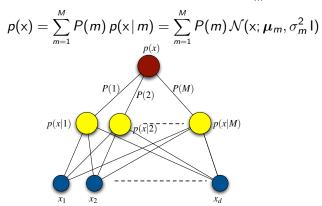
$$p(x) = \sum_{m=1}^{M} P(m)p(x|m)$$

- This is called a *mixture model* or a *mixture density*
- p(x|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(x|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 $\mathcal{N}(\mathsf{x}; \boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m)$ has mean $\boldsymbol{\mu}_m$ and a spherical covariance $\boldsymbol{\Sigma}_m = \sigma_m^2 \mathbf{I}$



GMM Parameter estimation when we know which component generated the data

- Define the indicator variable $z_{mn} = 1$ if component m generated data point x_n (and 0 otherwise)
- If z_{mn} 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 estimate the mean, variance and mixing parameters as:

$$\hat{\mu}_m = \frac{\sum_n z_{mn} \mathbf{x}_n}{N_m}$$

$$\hat{\sigma}_m^2 = \frac{\sum_n z_{mn} || \mathbf{x}_n - \hat{\mu}_m ||^2}{N_m}$$

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

GMM 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, λ_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 λ_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 $P(m|\mathbf{x}_n)$:

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

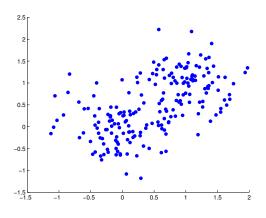
- We can imagine this as assigning data points to component m weighted by the component occupation probability $P(m|x_t)$
- Estimate the mean, variance and prior probabilities as:

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

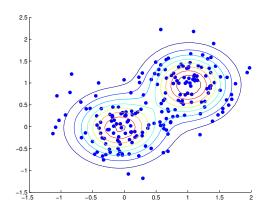
$$\hat{\sigma}_{m}^{2} = \frac{\sum_{n} P(m|\boldsymbol{x}_{n}) \|\boldsymbol{x}_{n} - \hat{\boldsymbol{\mu}}_{m}\|^{2}}{\sum_{n} P(m|\boldsymbol{x}_{n})} = \frac{\sum_{n} P(m|\boldsymbol{x}_{n}) \|\boldsymbol{x}_{n} - \hat{\boldsymbol{\mu}}_{m}\|^{2}}{N_{m}^{*}}$$

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

Example 1 fit using a GMM

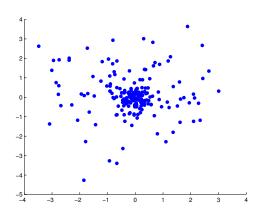


Example 1 fit using a GMM



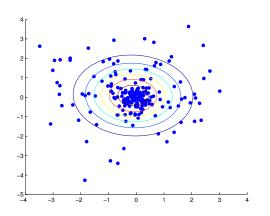
Fitted with a two component GMM using EM

Peakily distributed data (Example 2)



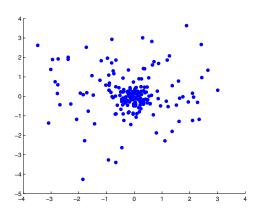
$$oldsymbol{\mu}_1 = oldsymbol{\mu}_2 = [0 \quad 0]^T \qquad oldsymbol{\Sigma}_1 = 0.1 \mathbf{I} \qquad oldsymbol{\Sigma}_2 = 2 \mathbf{I}$$

Example 2 fit by a Gaussian

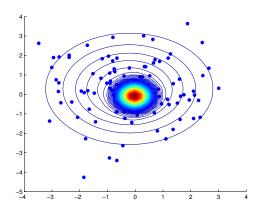


$$\mu_1 = \mu_2 = [0 \quad 0]^T \qquad \Sigma_1 = 0.1 \mathbf{I} \qquad \Sigma_2 = 2 \mathbf{I}$$

Example 2 fit by a GMM

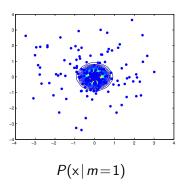


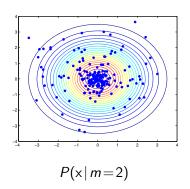
Example 2 fit by a GMM



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 speech recognition systems can have 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:

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

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

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

And likewise for the covariance matrices:

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

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:

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

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

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

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

• 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: HMMs

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