Gaussian Mixture Models

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Automatic Speech Recognition— ASR Lecture 6
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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), $p(x)$:

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

- $p(x)$ 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)

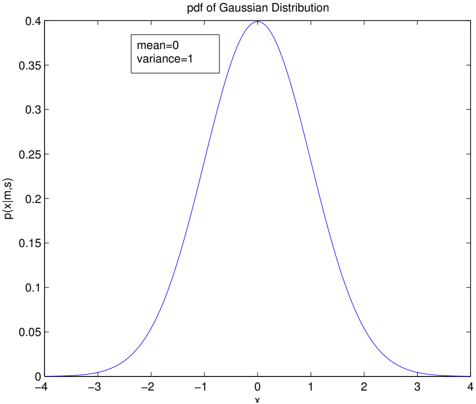
- The Gaussian (or Normal) distribution is the most common (and easily analysed) continuous distribution
- It is also a reasonable model in many situations (the famous "bell curve")
- If a (scalar) variable has a Gaussian distribution, then it has a probability density function with this form:

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

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

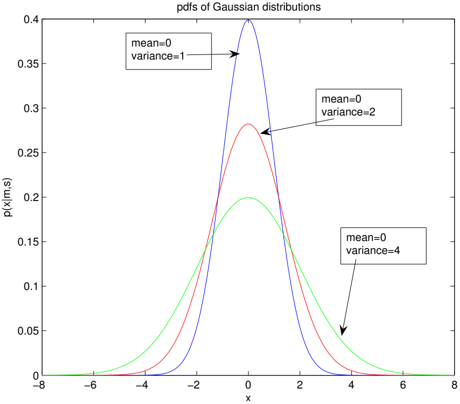
Plot of Gaussian distribution

- 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 $x_1, x_2, \ldots, x_N$
- Use the following as the estimates:

$$\hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x_n \qquad \text{(mean)}$$

$$\hat{\sigma}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \hat{\mu})^2 \qquad \text{(variance)}$$

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:

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

$$= -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi)$$

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

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

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

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

Covariance matrix

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

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

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

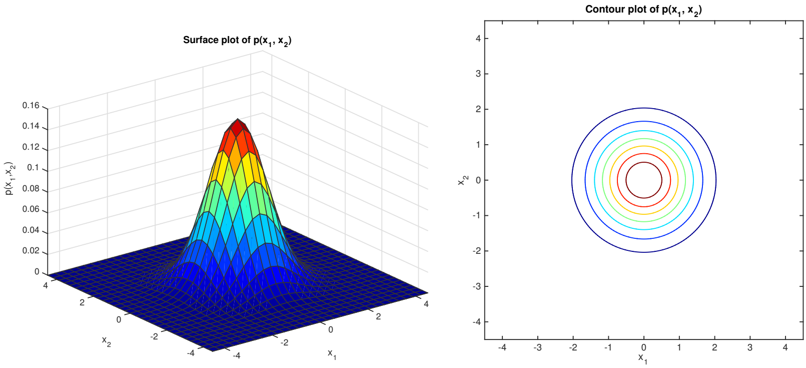
$$\boldsymbol{\Sigma} = E[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T]$$

- $\boldsymbol{\Sigma}$ 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.

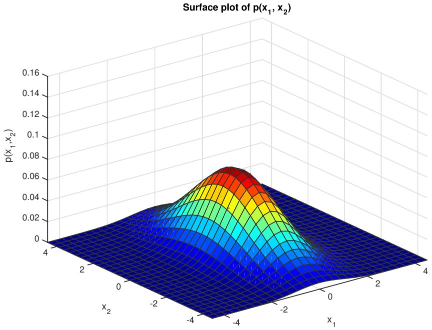
Spherical Gaussian

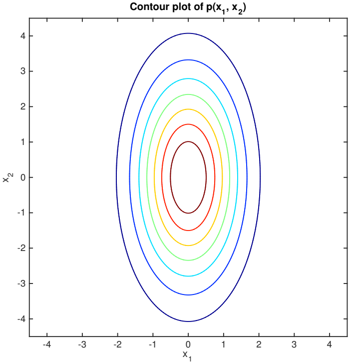


$$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \rho_{12} = 0$$

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

Diagonal Covariance Gaussian

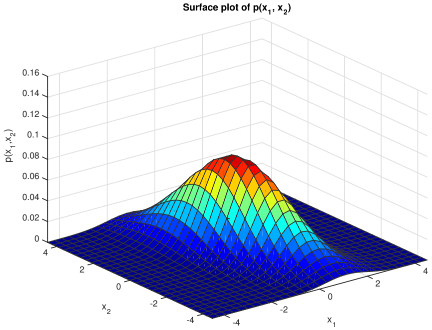


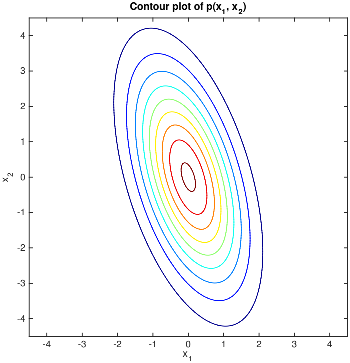


$$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix} \qquad \rho_{12} = 0$$

NB: Correlation coefficient $\rho_{ij} = \dfrac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}} \quad (-1 \leq \rho_{ij} \leq 1)$

Full covariance Gaussian





$$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & -1 \\ -1 & 4 \end{pmatrix} \qquad \rho_{12} = -0.5$$

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

Parameter estimation of a multivariate Gaussian distribution

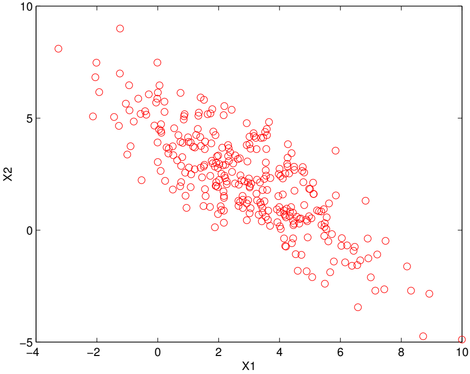
- It is possible to show that the mean vector $\hat{\boldsymbol{\mu}}$ and covariance matrix $\hat{\boldsymbol{\Sigma}}$ that maximise the likelihood of the training data are given by:

$$\hat{\boldsymbol{\mu}} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n$$

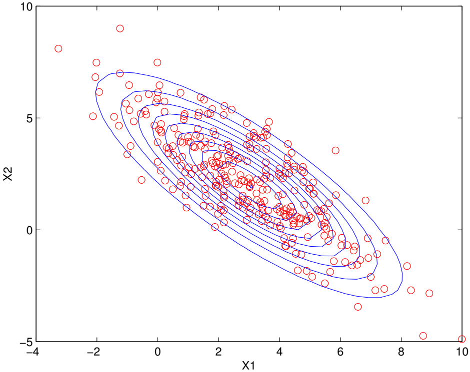
$$\hat{\boldsymbol{\Sigma}} = \frac{1}{N}\sum_{n=1}^{N} (\boldsymbol{x}_n - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_n - \hat{\boldsymbol{\mu}})^T$$

where $\boldsymbol{x}_n = (x_{n,1}, \ldots, x_{n,D})^T$.

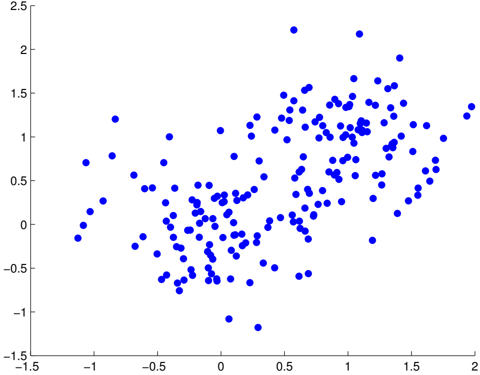
Example data



Maximum likelihood fit to a Gaussian

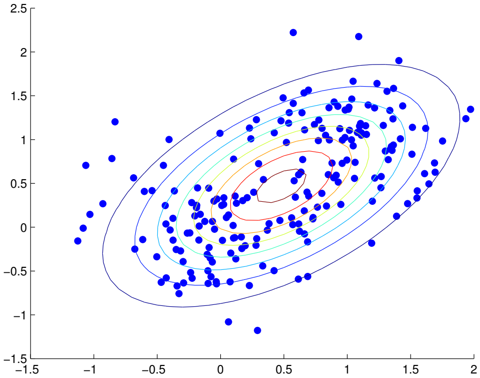


Data in clusters (example 1)



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

Example 1 fit by a Gaussian



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

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
  1. 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 $p(\mathrm{x} | C = m)$

  The component C is not observed
- We can calculate the probability density of x as

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

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

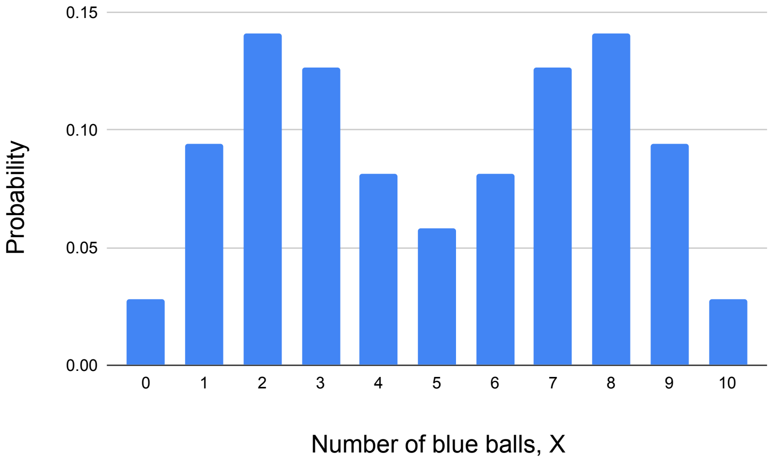
Simple example

- 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 α_1, α_2 are the proportions of blue balls in the respective bags

Simple example



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

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

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_{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 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 nth 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:

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

$$\hat{\boldsymbol{\Sigma}}_m = \frac{\sum_n z_{mn} (\mathbf{x}_n - \hat{\boldsymbol{\mu}}_m)(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_m)^T}{N_m}$$

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

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 $P(m|\mathrm{x})$, 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

$$\sum_m P(m|x;\lambda_0) \log P(x, m\,;\lambda)$$

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

(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 $P(m \mid x_n)$:

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

- We can imagine this as assigning data points to component m weighted by the component occupation probability $P(m \mid x_n)$
- In the bag example: imagine estimating which bag has been chosen at the nth 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:

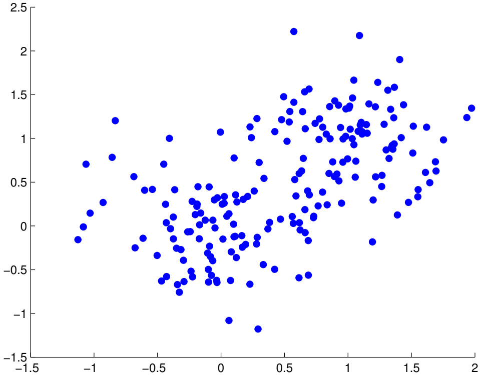
$$\hat{\boldsymbol{\mu}}_m = \frac{\sum_n P(m \mid \boldsymbol{x}_n)\boldsymbol{x}_n}{\sum_n P(m \mid \boldsymbol{x}_n)} = \frac{\sum_n P(m \mid \boldsymbol{x}_n)\boldsymbol{x}_n}{N_m^*}$$

$$\hat{\boldsymbol{\Sigma}}_m = \frac{\sum_n P(m \mid \boldsymbol{x}_n)(\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_m)(\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_m)^T}{\sum_n P(m \mid \boldsymbol{x}_n)}$$

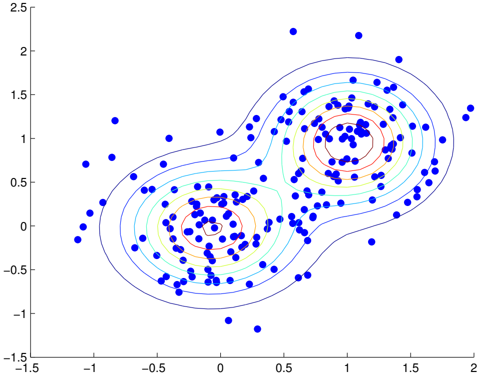
$$= \frac{\sum_n P(m \mid \boldsymbol{x}_n)(\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_m)(\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_m)^T}{N_m^*}$$

$$\hat{P}(m) = \frac{1}{N}\sum_n P(m \mid \boldsymbol{x}_n) = \frac{N_m^*}{N}$$

Example 1 fit using a GMM

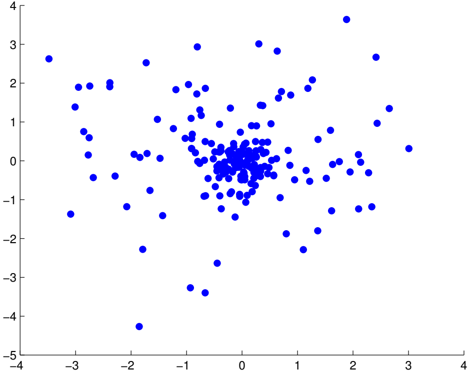


Example 1 fit using a GMM



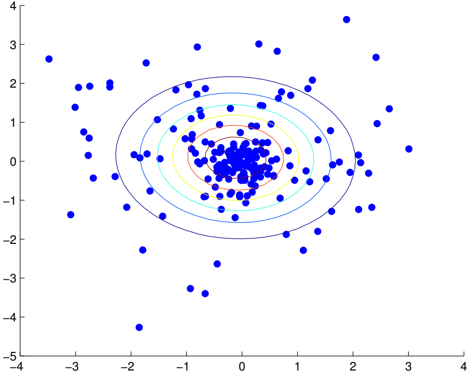
Fitted with a two component GMM using EM

Peakily distributed data (Example 2)



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

Example 2 fit by a Gaussian



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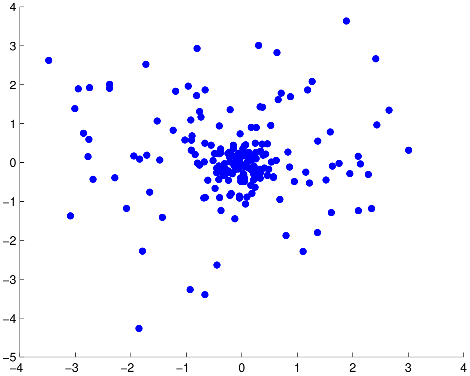
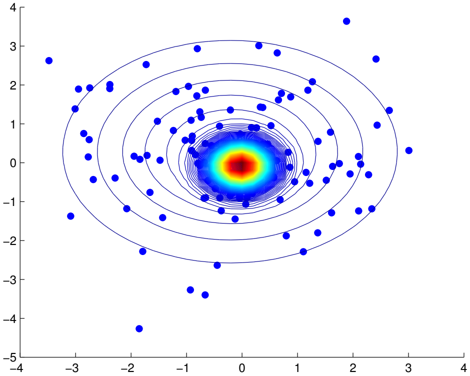
Example 2 fit by a GMM

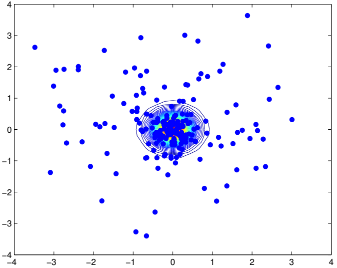


Example 2 fit by a GMM

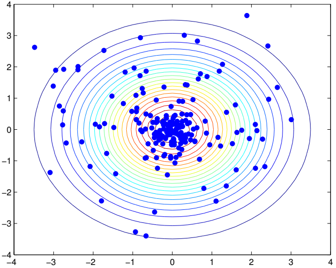


Fitted with a two component GMM using EM

Example 2: component Gaussians



$P(\mathrm{x} \mid m=1)$



$P(\mathrm{x} \mid m=2)$

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 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:

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

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

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

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:

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

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

  ($\xi_{tm}(j)$ in Jurafsky and Martin's SLP)

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

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

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

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

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

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.