# Advanced probabilistic methods

## Lecture 5: Mixture models and EM

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February, 2018



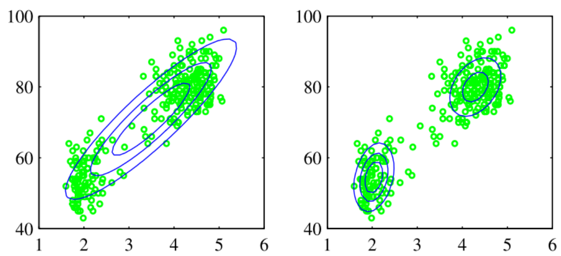
## Lecture 5 overview

- Gaussian mixture models (GMMs)
- EM algorithm
- EM for Gaussian mixture models
- Suggested reading: Bishop: *Pattern Recognition and Machine Learning*
  - p. 110-113 (2.3.9): Mixtures of Gaussians
  - *simple_example.pdf*
  - p. 430-443: EM for Gaussian mixtures



## Gaussian mixture models (motivation)

- Standard Gaussian model (left) gives bad fit to data with clusters
- Combination of two Gaussians (right) is much better



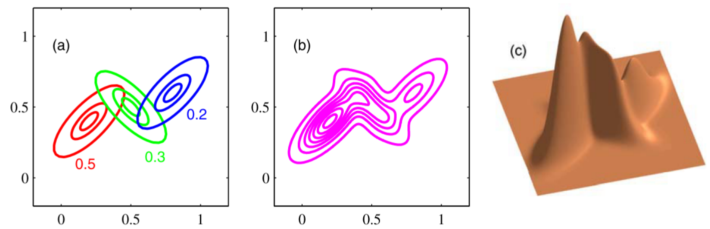



## Gaussian mixture models

- Gaussian mixture model with $K$ components has density

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k N(\mathbf{x}|\mu_k, \Sigma_k).$$

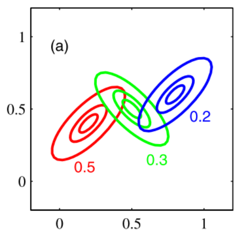
- $N(x|\mu_k, \Sigma_k)$ is a **component** with its own mean $\mu_k$ and covariance $\Sigma_k$.
- $\pi_k$ are the **mixing coefficients**, which satisfy $\sum_k \pi_k = 1$, $0 \leq \pi_k \leq 1$.

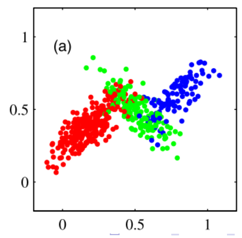


## GMMs, latent variable representation (1/2)

- Equivalent formulation is obtained by defining **latent variables** $\mathbf{z}_n = (z_{n1}, \ldots, z_{nK})$ which tell the component for observation $\mathbf{x}_n$
- In detail $\mathbf{z}_n$ is a vector with exactly one element equal to 1 and other elements equal to 0. $z_{nk} = 1$ means that the observation $\mathbf{x}_n$ belongs to component $k$.

$$\mathbf{z}_n = (0, \ldots, 0, \underbrace{1}_{k^{th}\text{ elem.}}, 0, \ldots, 0)^T$$






## GMMs, latent variable representation (2/2)

- Define

$$p(z_{nk} = 1) = \pi_k \quad \text{and} \quad p(\mathbf{x}_n | z_{nk} = 1) = N(\mathbf{x}_n | \mu_k, \Sigma_k),$$

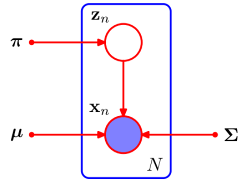
or equivalently

$$p(\mathbf{z}_n) = \prod_{k=1}^{K} \pi_k^{z_{nk}} \quad \text{and} \quad p(\mathbf{x}_n | \mathbf{z}_n) = \prod_{k=1}^{K} N(\mathbf{x}_n | \mu_k, \Sigma_k)^{z_{nk}}$$

- Then

$$p(\mathbf{x}_n) = \sum_{\mathbf{z}_n} p(\mathbf{z}_n) p(\mathbf{x}_n | \mathbf{z}_n) = \sum_k \pi_k N(\mathbf{x}_n | \mu_k, \Sigma_k)$$

$\rightarrow$ $\mathbf{x}_n$ has marginally the Gaussian mixture model distribution.






## GMM: responsibilities (1/2)

- Posterior probability $p(z_{nk} = 1 | \mathbf{x}_n)$ that observation $\mathbf{x}_n$ was generated by component $k$

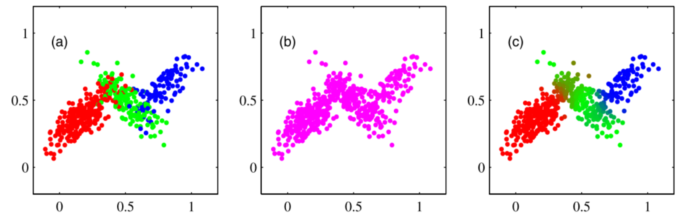
$$\gamma(z_{nk}) \equiv p(z_{nk} = 1 | \mathbf{x}_n) = \frac{p(z_{nk} = 1) p(\mathbf{x}_n | z_{nk} = 1)}{\sum_{j=1}^{K} p(z_{nj} = 1) p(\mathbf{x}_n | z_{nj} = 1)}$$
$$= \frac{\pi_k N(\mathbf{x}_n | \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j N(\mathbf{x}_n | \mu_j, \Sigma_j)}$$

- $\gamma(z_{nk})$ can be viewed as the **responsibility** that component $k$ takes for explaining the observation $\mathbf{x}_n$



## GMM: responsibilities (2/2)

- (left) samples from a joint distribution $p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$, showing both cluster labels $\mathbf{z}$ and observations $\mathbf{x}$ (**complete** data)
- (center) samples from the marginal distribution $p(\mathbf{x})$ (**incomplete** data)
- (right) **responsibilities** of the data points, computed using *known* parameters $\pi = (\pi_1, \ldots, \pi_K)$, $\mu = \mu_1, \ldots, \mu_K$, $\Sigma = (\Sigma_1, \ldots, \Sigma_K)$.
- Problem: in practice $\pi$, $\mu$, and $\Sigma$ are usually *unknown*.



## Idea of the EM algorithm (1/2)

- Let $X$ denote the observed data, and $\theta$ model parameters. The goal in maximum likelihood is to find $\widehat{\theta}$:

$$\widehat{\theta} = \arg\max_{\theta} \{\log p(X|\theta)\}$$

- If model contains latent variables $Z$, the log-likelihood is given by

$$\log p(X|\theta) = \log \left\{ \sum_{Z} p(X, Z|\theta) \right\},$$

  which may be difficult to maximize analytically
- Possible solutions: 1) numerical optimization, 2) the EM algorithm (expectation-maximization)



## Idea of the EM algorithm (2/2)

- $X$: **observed** data, $Z$: **unobserved** latent variables
- $\{X, Z\}$: **complete** data, $X$: **incomplete** data
- In EM algorithm, we assume that the complete data log-likelihood:

$$\log p(X, Z|\theta)$$

  is easy to maximize.
- Problem: $Z$ is not observed
- Solution: maximize

$$\begin{aligned} Q(\theta, \theta_0) &\equiv E_{Z|X,\theta_0}[\log p(X, Z|\theta)] \\ &= \sum_{Z} p(Z|X, \theta_0) \log p(X, Z|\theta) \end{aligned}$$

  where $p(Z|X, \theta_0)$ is the posterior distribution of the latent variables computed using the current parameter estimate $\theta_0$



## EM algorithm

**Goal**: maximize $\log p(X|\theta)$ w.r.t. $\theta$

1. Initialize $\theta_0$
2. **E-step** Evaluate $p(Z|X, \theta_0)$, and then compute

$$Q(\theta, \theta_0) = E_{Z|X,\theta_0}[\log p(X, Z|\theta)] = \sum_{Z} p(Z|X, \theta_0) \log p(X, Z|\theta)$$

3. **M-step** Evaluate $\theta^{new}$ using

$$\theta^{new} = \arg\max_{\theta} Q(\theta, \theta_0)$$

4. Repeat **E** and **M** steps until convergence



## EM algorithm, comments

- In general, $Z$ does not have to be discrete, just replace the summation in $Q(\theta, \theta_0)$ by integration.
- EM-algorithm can be used to compute the MAP (*maximum a posteriori*) estimate by maximizing in the M-step $Q(\theta, \theta_0) + \log p(\theta)$.
- In general, EM-algorithm is applicable when the observed data $X$ can be **augmented** into complete data $\{X, Z\}$ such that $\log p(X, Z|\theta)$ is easy to maximize; $Z$ does not have to be latent variables but can represent, for example, unobserved values of missing or censored observations.

## EM algorithm, simple example

- Consider $N$ independent observations $\mathbf{x} = (x_1, \ldots, x_N)$ from a two-component mixture of univariate Gaussians

$$p(x_n|\theta) = \frac{1}{2}N(x_n|0,1) + \frac{1}{2}N(x_n|\theta,1). \tag{1}$$

- One unknown parameter, $\theta$, the mean of the second component.
- **Goal**: estimate
$$\widehat{\theta} = \arg\max_{\theta} \{\log p(\mathbf{x}|\theta)\}.$$
- *simple_example.pdf* and *simple_em.m*



## EM algorithm for GMMs

$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k N(\mathbf{x}|\mu_k, \Sigma_k)$

1. Initialize parameter $\mu_k$, $\Sigma_k$ and mizing coefficients $\pi_k$. Repeat until convergence:
2. **E-step**: Evaluate the responsibilities using current parameter values
$$\gamma(z_{nk}) = \frac{\pi_k N(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_k N(\mathbf{x}_n|\mu_k, \Sigma_j)}$$
3. **M-step:** Re-estimate the parameters using the current responsibilities
$$\mu_k^{new} = \frac{1}{N_k}\sum_{n=1}^{N} \gamma(z_{nk})\mathbf{x}_n$$
$$\Sigma_k^{new} = \frac{1}{N_k}\sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \mu_k^{new})(\mathbf{x}_n - \mu_k^{new})^T$$
$$\pi_k^{new} = \frac{N_k}{N}$$

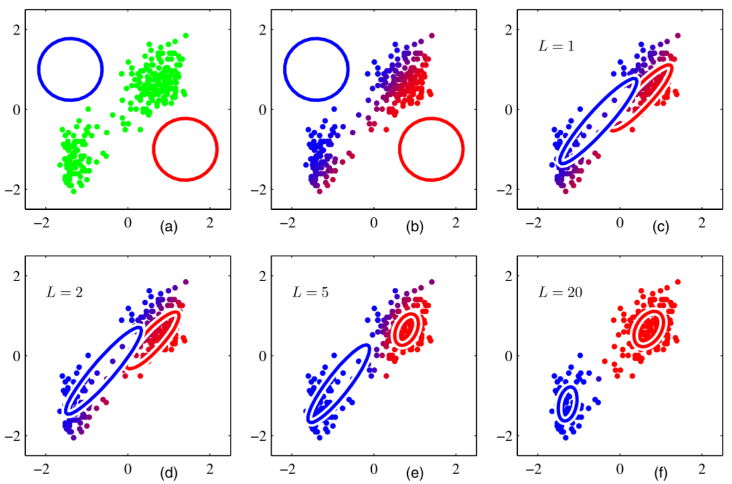


## Derivation of the EM algorithm for GMMs

- In the **M-step** the formulas for $\mu_k^{new}$ and $\Sigma_k^{new}$ are obtained by differentiating the expected complete data log-likelihood $Q(\theta, \theta_0)$ with respect to the particular parameters, and setting the derivatives to zero.
- The formula for $\pi_k^{new}$ can be derived by maximizing $Q(\theta, \theta_0)$ under the constraint $\sum_{k=}^{K} \pi_k = 1$. This can be done using the *Lagrange multipliers*.

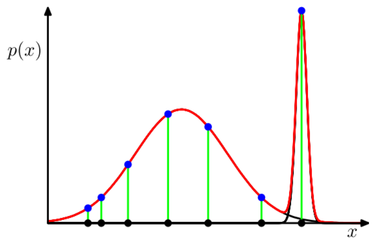


## Illustration of the EM algorithm for GMMs



## EM for GMM, caveats

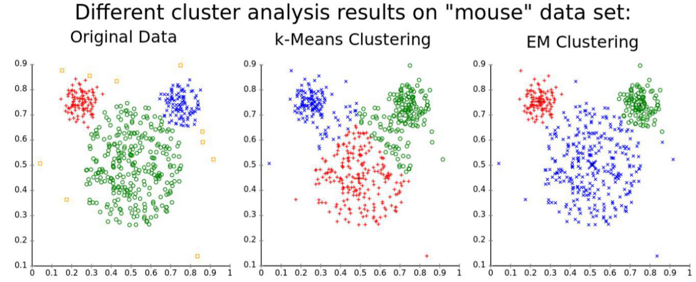
- EM converges to a local optimum. In fact, the ML estimation for GMMs is an ill-posed problem due to **singularities**: if $\sigma_k \to 0$ for components $k$ with a single data point, likelihood goes to infinity (fig). Remedy: prior on $\sigma_k$.
- **Label-switching**: non-identifiability due to the fact that cluster labels can be switched and likelihood remains the same.
- In practice it is recommended to initialize the EM for the GMM by k-means.






## GMM vs. k-means (1/2)

- "Why use GMMs and not just k-means?"




from Wikipedia

1. Clusters can be of different sizes and shapes
2. Probabilistic assignment of data items to clusters
3. Possibility to include prior knowledge (structure of the model/prior distributions on the parameters)



## Important points

- Definition of the Gaussian mixture model
- Representing the Gaussian mixture model using discrete latent variables, which specify the components (or clusters) of the observations
- ML-estimation of GMMs can be done using numerical optimization or the EM algorithm.
- The main idea of the EM algorithm is to maximize the expectation of the complete data log-likelihood, where the expectation is computed over the current posterior distribution of the latent variables.