Gaussian Mixture Models

- Fuzzy C-Means is “OK” as a non-crisp clustering alg. but (as K-Means) favors spherical clusters → better approaches

- Example: Gaussian Mixture Models (GMM)
  - Linear combination of Gaussians
    \[ p(x) = \sum_{k=1}^{K} \pi_k N(x|\mu_k, \Sigma_k) \quad \text{where} \quad \sum_{k=1}^{K} \pi_k = 1, \ 0 \leq \pi_k \leq 1 \]
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\[6\]
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    \[ p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \Sigma_k) \] where \( \sum_{k=1}^{K} \pi_k = 1, \ 0 \leq \pi_k \leq 1 \)

  ![Graph showing Gaussian Mixture Models](image)

  Parameters to be estimated

  This is usually written as \( p(x|\Theta) \) denoting the dependency on the parameters \( \Theta = \{\pi_k, \mu_k, \Sigma_k\}_k \). Writing this as a conditional probability makes sense in connection with Bayesian Machine Learning (see [8]).
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this is usually written as \( p(x|\theta) \) denoting the dependency on the parameters \( \theta = \{\pi_k, \mu_k, \Sigma_k\}_{k \in \{1, 2, \ldots, K\}} \)

Writing this as a conditional probability makes sense in connection with Bayesian Machine Learning (see [8])

For a distribution \( p(x|\theta) \) parametrized by a set of parameters \( \theta \) and iid data \( X = \{x_1, x_2, \ldots, x_N\} \), simple machine learning corresponds to finding the \( \theta \) that best explains the data

- iid: „identically independently drawn“ \( \Rightarrow p(X|\theta) = \prod_i p(x_i|\theta) \)

- \( p(X|\theta) \) is called likelihood

- „finding the \( \theta \) that best explains the data“:
  Maximum Likelihood: \( \theta_{ML} = \arg \max_{\theta} p(X|\theta) \) \( \Rightarrow \nabla_{\theta} p(X|\theta) = 0 \)

- convenient: use \( \log p(X|\theta) \) instead of \( p(X|\theta) \)
  \( \Rightarrow \log p(X|\theta) = \sum_i \log p(x_i|\theta) \)
For a distribution \( p(x|\theta) \) parametrized by a set of parameters \( \theta \) and iid data \( X = \{x_1, x_2, \ldots, x_N\} \), simple machine learning corresponds to finding the \( \hat{\theta} \) that best explains the data.

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**Maximum Likelihood**: \( \hat{\theta}_{ML} = \arg \max_\theta p(X|\theta) \Rightarrow \forall \theta \ p(X|\theta) \leq p(X|\hat{\theta}_{ML}) \)

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For a distribution \( p(x|\theta) \) parametrized by a set of parameters \( \theta \) and iid data \( X = \{x_1, x_2, ..., x_N\} \), simple machine learning corresponds to finding the \( \theta \) that best explains the data.

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\[
\log p(X|\theta) = \sum_i \log p(x_i|\theta)
\]

Example: \( x \in \mathbb{R}^n \) and \( p(x|\theta) \) is one multivariate Gaussian

\[
p(x|\theta) = \mathcal{N}(x|\mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^D|\Sigma|^{1/2}}} \exp \left\{ -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right\}
\]

\( \log \text{likelihood:} \quad (\text{see base e}) \)

\[
\ln p(X|\theta) = \ln p(X|\mu, \Sigma) = -\frac{ND}{2} \ln(2\pi) - \frac{N}{2} \ln |\Sigma| - \frac{1}{2} \sum_{n=1}^{N} (x_n - \mu)^T \Sigma^{-1} (x_n - \mu)
\]

Maximum log likelihood:

\[
\theta_{ML} = \text{argmax}_\theta \log p(X|\theta) \Rightarrow \nabla_\theta \left( \sum_i \log p(x_i|\theta) \right) = 0
\]

\[
\mu_{ML} = \frac{1}{N} \sum x_n
\]

\[
\Sigma_{ML} = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{ML})(x_n - \mu_{ML})^T
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$$p(x|\theta) = \mathcal{N}(x|\mu, \Sigma) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right\}$$

- **Log likelihood:** \( \log p(X|\theta) = \ln p(X|\mu, \Sigma) = -\frac{ND}{2} \ln(2\pi) - \frac{N}{2} \ln |\Sigma| - \frac{1}{2} \sum_{n=1}^{N} (x_n - \mu)^T \Sigma^{-1} (x_n - \mu) \)

- **Maximum log likelihood:**
  \[ \Theta_{ML} = \arg\max_{\Theta} \log p(X|\Theta) \Rightarrow \forall_{\Theta} \left( \sum_{i} \log p(x_i|\theta) \right) = 0 \]
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- Maximum log likelihood:

$$\Theta_{ML} = \arg \max_{\theta} \log p(X|\theta) \Rightarrow \forall_{\theta} \left( \sum_i \log p(x_i|\theta) \right) = 0$$

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GMM: $p(x|\theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k), \quad 0 \leq \pi_k \leq 1, \quad \sum_{k=1}^{K} \pi_k = 1$
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**1 of K representation**

- \( K \)-dimensional binary random variable \( z \)
- \( z_k \in \{0, 1\} \) and \( \sum_k z_k = 1 \)
- \( p(z_k = 1) = \pi_k \)
- \( p(z) = \prod_{k=1}^{K} \pi_k^z_k \)

**conditional probability**

\[
p(x|z_k = 1) = \mathcal{N}(x|\mu_k, \Sigma_k) \quad p(x|z) = \prod_{k=1}^{K} \mathcal{N}(x|\mu_k, \Sigma_k)^{z_k}
\]

\[
p(x) = \sum_z p(z)p(x|z) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)
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GMM-Basics

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- **GMM-Basics**

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1 of k representation

- \( K \)-dimensional binary random variable \( z \)
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- \( p(z) = \prod_{k=1}^{K} \pi_k^z_k \)

Remark:
If we have several observations \( x_1, \ldots, x_N \), then, because we have represented the marginal distribution in the form \( p(x) = \sum_z p(x|z)p(z) \), it follows that for every observed data point \( x_n \) there is a corresponding latent variable \( z_n \).

\[ p(x) = \sum_z p(x|z)p(z) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \]

Example:

Responsibilities

\[ \gamma(z_k) \equiv p(z_k = 1|x) = \frac{p(z_k = 1)p(x|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(x|z_j = 1)} \]
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Example

GMM: \[ p(x | \theta) = p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k). \quad 0 \leq \pi_k \leq 1 \quad \sum_{k=1}^{K} \pi_k = 1 \]

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remark: If we have several observations \( x_1, \ldots, x_N \), then, because we have represented the marginal distribution in the form \( p(x) = \sum_{x} p(x,z) \), it follows that for every observed data point \( x_n \) there is a corresponding latent variable \( z_n \).
\[ p(x) = \sum_{x} p(x|z)p(x|z) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \]
\[ p(x,z) \]
GMM-Basics

Maximum likelihood (GMM)

\[ \ln p(X | \pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k N(x_n | \mu_k, \Sigma_k) \right\} \]

- \( \text{Vector of } K \text{-dim. means } \mu_k \)
- \( \text{Vector of } K \text{-DxD covariances } \Sigma_k \)

- \( \text{maximizing w.r.t } \pi, \mu \text{ and } \Sigma \rightarrow \)
  \[ \mu_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) x_n \]
  \[ \Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(x_n - \mu_k)(x_n - \mu_k)^T \]
  \[ (N_k = \sum_{n=1}^{N} \gamma(z_{nk})) \]
  \[ \pi_k = \frac{N_k}{N} \]

\[ \gamma(z_k) = p(z_k = 1 | x) = \frac{p(z_k = 1)p(x | z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(x | z_j = 1)} = \frac{\pi_k N(x | \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j N(x | \mu_j, \Sigma_j)} \]

Example

(a) (b) (c)
Maximum likelihood (GMM)

\[
\ln p(X|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k N(x_n|\mu_k, \Sigma_k) \right\}
\]

- Vector of \( K \) D-dim. means \( \mu_k \)
- Vector of \( K \) DxD covariances \( \Sigma_k \)

- maximizing w.r.t. \( \pi, \mu \) and \( \Sigma \) \( \rightarrow \)

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\left( N_k = \sum_{n=1}^{N} \gamma(z_{nk}) \right) \\
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Example

![Example plots](image)

Maximum likelihood (GMM)

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Maximaler Likelihood (GMM)

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so what?! \( \Rightarrow \) Problem: Expr. depend on \( \gamma(z_{nk}) \) which depends on \( \pi, \mu, \Sigma \) which depends on \( \gamma(z_{nk}) \) which depends on ....

Idea: Alternating approach (EM-algorithm):

Step t: Evaluate \( \gamma(z_{nk})_{(t)} \) using \((\pi, \mu, \Sigma)_{(t-1)}\)
Evaluate \((\pi, \mu, \Sigma)_{(t)}\) using \(\gamma(z_{nk})_{(t-1)}\)

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GMM-Basics

Maximum likelihood (GMM)

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$$\mu_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) x_n$$

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• so what?! ⇒ Problem: Expr. depend on $\gamma(z_{nk})$ which depends on $\pi, \mu, \Sigma$ which depends on $\gamma(z_{nk})$ which depends on .....

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1. Step t: Evaluate $\gamma(z_{nk})_{(t)}$ using $(\pi, \mu, \Sigma)_{(t-1)}$
2. Evaluate $(\pi, \mu, \Sigma)_{(t)}$ using $\gamma(z_{nk})_{(t)}$

GMM-Basics

Maximum likelihood (GMM)

[Diagrams showing different distributions and likelihoods]
EM for Gaussian Mixtures

Given a Gaussian mixture model, the goal is to maximize the likelihood function with respect to the parameters (comprising the means and covariances of the components and the mixing coefficients).

1. Initialize the means $\mu_k$, covariances $\Sigma_k$ and mixing coefficients $\pi_k$, and evaluate the initial value of the log likelihood.

2. E step. Evaluate the responsibilities using the current parameter values

$$
\gamma(z_{nk}) = \frac{\pi_k N(x_n | \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j N(x_n | \mu_j, \Sigma_j)} \quad (9.23)
$$

Having latent variables $Z$, ML becomes

$$
\ln p(X|\theta) = \ln \left( \sum_z p(X, Z|\theta) \right)
$$

Summation inside $\ln \rightarrow$ Problems!

If we knew the complete dataset $\{X, Z\}$ (and thus the distribution $p(X, Z|\theta)$), we could use ML to solve for $\theta$ with $p(X, Z|\theta)$ directly (which is easy, as we will see, because $p(X, Z|\theta)$ is of exponential family (the functional form is known!!))

We only know $p(Z|X, \theta) \rightarrow$ responsibilities, as we will see $\rightarrow$ compute expectation of (unknown) quantity $p(X, Z|\theta)$ or even better of the quantity $\ln p(X, Z|\theta)$
EM-algorithm: General View

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- We only know $p(Z|X, \theta)$ (⇒ responsibilities, as we will see) → compute expectation of (unknown) quantity $p(X, Z|\theta)$ or even better of the quantity $\ln p(X, Z|\theta)$

GMM-Basics

Maximum likelihood (GMM)

**EM for Gaussian Mixtures**

Given a Gaussian mixture model, the goal is to maximize the likelihood function with respect to the parameters (comprising the means and covariances of the components and the mixing coefficients).

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2. **E step.** Evaluate the responsibilities using the current parameter values

$$
\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_n|\mu_j, \Sigma_j)}.
$$

$$(9.23)$$

- **Example**

- Responsibilities

$$
\gamma(z_k) \equiv p(z_k = 1|x) = \frac{p(z_k = 1)p(x|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(x|z_j = 1)}
$$

$$
= \frac{\pi_k \mathcal{N}(x|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x|\mu_j, \Sigma_j)}.
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EM-algorithm: General View

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EM: Relation to K-Means

- If we use \(k\) Gaussians with \(\Sigma = \sigma I\):

\[
p(x|\mu_k, \Sigma_k) = \frac{1}{(2\pi\sigma)^{1/2}} \exp \left\{ -\frac{1}{2\sigma} ||x - \mu_k||^2 \right\}
\]

- we get for the responsibilities:

\[
\gamma(z_{nk}) = \frac{\pi_k}{\sum_j \pi_j \exp \left\{ -\frac{1}{2\sigma} ||x_n - \mu_j||^2 / 2\sigma \right\}}
\]

- Letting \(\sigma \rightarrow 0\) and Taylor-Expansion:

\[
E_Z[\ln p(X, Z|\mu, \Sigma, \pi)] \rightarrow -\frac{1}{2} \sum_{n=1}^N \sum_{k=1}^K r_{nk} ||x_n - \mu_k||^2 + \text{const}
\]

→ same as on slide 18
If we use 
\[ p(x|\mu_k, \Sigma_k) = \frac{1}{(2\pi)^d/2} \exp \left\{ -\frac{1}{2\epsilon} \|x - \mu_k\|^2 \right\} \]
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Information Networks / Knowledge NW

**Most studied examples:** citation NW (tree), the WWW;

**Example findings:**
- $p(k)$ of author having $k$ papers: $p(k) \sim k^{-\alpha}$: power law
- distribution of in or out degrees of WWW pages (also for citation NW): $p(k) \sim k^{-\alpha}$

**Other examples:**
- bipartite preference networks: 
  - recommender systems == link prediction on these NW; 
  - example: collaborative filtering
- ontologies, semantic NW
- word networks
- tripartite tag/author/item networks 
  - Folksonomies

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- the Internet,
- electric power grids,
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- biochemical pathways, gene-protein and protein-protein interaction NW
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Mean Average Path Length

- "Small World Effect": \( l(n) \sim \text{small} \Rightarrow l(n) \in O(\log(n)) \)
- undirected graph:

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\ell = \frac{1}{2} n(n+1) \sum_{i \geq j} d_{ij}.
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formula also counts 0 distances from i to i: \( \frac{1}{2} n(n+1) = \frac{1}{2} n(n-1) + n \)
- Expression allowing for disconnected components (where \( d_{ij} = \infty \) can occur): harmonic mean:

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Transitivity / Clustering Coefficient

- Clustering coefficient (whole graph):
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