Mixture Models and GMM (Contd.)

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Probabilistic Machine Learning (CS772A)

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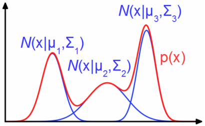
Recap: Gaussian Mixture Model

- A model for data clustering and density estimation
- Assumes data generated from a mixture of K Gaussians with mixing proportions $\pi_1, \ldots, \pi_K$



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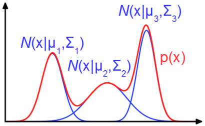

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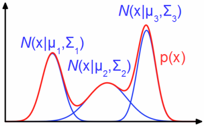

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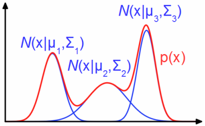

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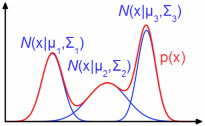

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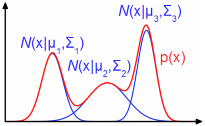

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$$p(\boldsymbol{x}_n|\boldsymbol{z}_n = k) = \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)$$

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- Doing MLE on this objective is tricky due to the "$\log \sum$" term
  - Parameters get coupled; no closed form solution (iterative methods needed, slow convergence)
- An alternating "guess, re-estimate, and repeat until converge" algorithm helps solve such problems in a clean, simple, and efficient way; basically, the Expectation Maximization (EM) algorithm

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\text{Thus} \quad \mathbb{E}[z_{nk}] &\propto \pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \text{(Posterior prob. that } \boldsymbol{x}_n \text{ is generated by } k\text{-th Gaussian)}
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$$\begin{aligned} \mathbb{E}[z_{nk}] &= 0 \times p(z_{nk} = 0|\boldsymbol{x}_n) + 1 \times p(z_{nk} = 1|\boldsymbol{x}_n) \\ &= p(z_{nk} = 1|\boldsymbol{x}_n) \\ &\propto p(z_{nk} = 1)p(\boldsymbol{x}_n|z_{nk} = 1) \qquad \text{(from Bayes Rule)} \\ \text{Thus} \quad \mathbb{E}[z_{nk}] &\propto \pi_k\mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \text{(Posterior prob. that } \boldsymbol{x}_n \text{ is generated by } k\text{-th Gaussian)} \end{aligned}$$

- Note: We can finally normalize $\mathbb{E}[z_{nk}]$ as $\mathbb{E}[z_{nk}] = \frac{\pi_k\mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_{\ell=1}^{K}\pi_\ell\mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_\ell,\boldsymbol{\Sigma}_\ell)}$ since $\sum_{k=1}^{K}\mathbb{E}[z_{nk}] = 1$

GMM Parameter Estimation

- The CLL gets further simplified to

$$\text{CLL}(\Theta) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} \log p(\boldsymbol{z}_n = k) p(\boldsymbol{x}_n | \boldsymbol{z}_n = k) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} [\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]$$

- Simple algebraic form. MLE easy by taking (partial) derivatives w.r.t. each parameter
- However, to do so, we need the z_{nk}'s (each a binary r.v.). This is where we'll make a guess.
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- **Wait!** Computing $\mathbb{E}[z_{nk}]$ requires knowing $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^{K}$ (chicken-and-egg problem ☹)

GMM Parameter Estimation: The Alternating Approach

Can solve the chicken-and-egg problem by taking an alternating approach

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$$\mathbb{E}[z_{nk}]$$

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.. this will give ML estimates for parameters $\Theta = \{\pi_k, \mu_k, \Sigma_k\}$. Details on the next slides.

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The algorithm alternates between step 1 and 2 until convergence

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This is an example of the more general **Expectation Maximization** (EM) algorithm.

GMM Parameter Estimation: The Alternating Approach

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The algorithm alternates between step 1 and 2 until convergence

This is an example of the more general **Expectation Maximization** (EM) algorithm. EM can be used for MLE/MAP in probabilistic models **that contain latent variables** making standard MLE/MAP hard

GMM Parameter Estimation

- Given $\mathbb{E}[z_{nk}] = \gamma_{nk} = \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_{\ell=1}^{K} \pi_\ell \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_\ell,\boldsymbol{\Sigma}_\ell)}$, the expected complete data log-lik.

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- For each k, it's a "weighted" version of the MLE for the multivar. Gaussian $\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

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- Can also solve for π_k likewise (subject to contraint $\sum_{k=1}^{K}\pi_k = 1$)

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- Derivations are a bit tedious (but straightforward). I will provide a note.

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- Suppose $N_k = \sum_{n=1}^{N} \gamma_{nk}$

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$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma_{nk} \boldsymbol{x}_n$$

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$$
\begin{aligned}
\boldsymbol{\mu}_k &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma_{nk} \boldsymbol{x}_n \\
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\pi_k &= \frac{N_k}{N}
\end{aligned}
$$

- Note that μ_k, Σ_k updates are similar to multivar. Gaussian MLE equations
- Each $\boldsymbol{x}_n, n = 1, \ldots, N$ contributes to each $\{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$ update but fractionally (based on γ_{nk})

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$$\gamma_{nk} = \mathbb{E}[z_{nk}] \propto \pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \text{(and re-normalize s.t. } \sum_{k=1}^K \gamma_{nk} = 1\text{)}$$

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Summary: EM for Learning GMM

- Initialize the parameters $\Theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ randomly, or using K-means
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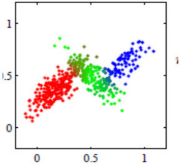
$$\begin{aligned}
\boldsymbol{\mu}_k &= \frac{1}{N_k}\sum_{n=1}^N \gamma_{nk}\boldsymbol{x}_n \\
\boldsymbol{\Sigma}_k &= \frac{1}{N_k}\sum_{n=1}^N \gamma_{nk}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \\
\pi_k &= \frac{N_k}{N}
\end{aligned}$$

GMM: Some Important Aspects

- GMM learns a probabilitic ("soft") clustering as opposed to hard clustering (e.g., K-means)



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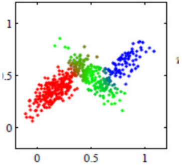
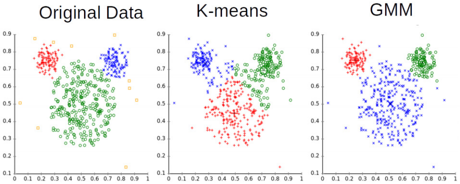


Soft clustering learned by a Gaussian mixture model

- GMM doesn't assume the clusters to be spherical and equi-sized as opposed to K-means (recall that each Gaussian has a specific covariance which can control the shape of that cluster)



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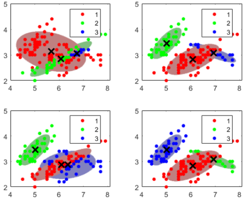

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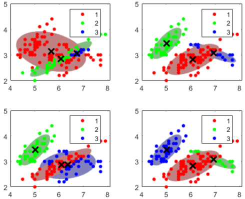

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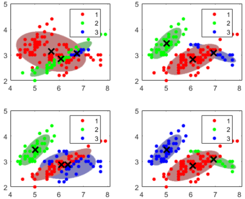

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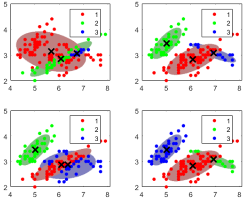

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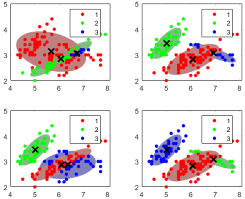

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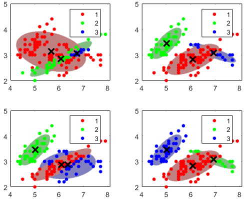

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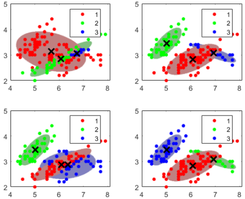

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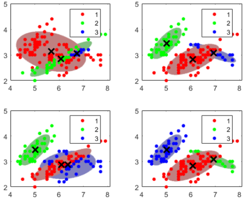

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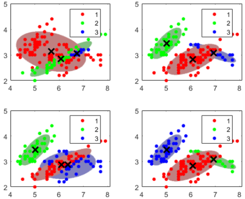

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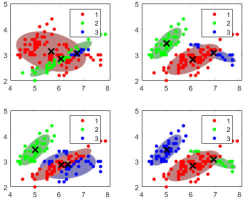

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  - Use low-rank Gaussians for each mixture component (mixture of factor analyzers)

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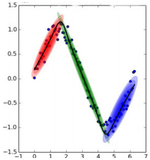
- Mixture of Experts: Each "expert" is a probabilistic supervised learning model $p(y|\boldsymbol{x}, \theta_k)$
  - Overall model is a convex combination of the experts

$$p(y|\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k(\boldsymbol{x}) p(y|\boldsymbol{x}, \theta_k)$$

  - Enables learning rich models (e.g., nonlinear reg.) from simpler models (e.g., linear reg.)



Next Class: The General EM Algorithm