Generative Models for Clustering, GMM, and Intro to EM

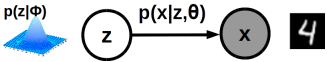
Piyush Rai

Machine Learning (CS771A)

Sept 26, 2016

Generative Models

- A probabilistic way to think about the data generation process



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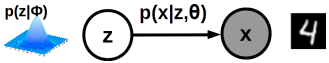

- Idea: First generate a random latent variable $\boldsymbol{z}$ from a prior distr. $p(\boldsymbol{z}|\phi)$ and then generate $\boldsymbol{x}$ conditioned on $\boldsymbol{z}$ from the data distr. $p(\boldsymbol{x}|\boldsymbol{z}, \theta)$

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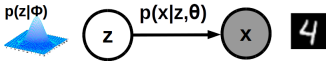

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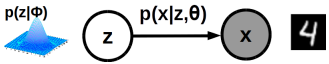

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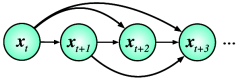

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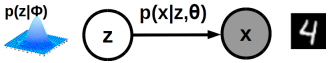

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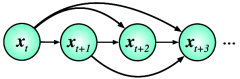

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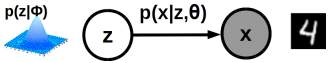

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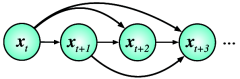

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Generative Models for Clustering

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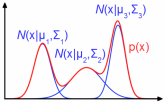
- A generative model for data clustering
- Data assumed generated from a mixture of K Gaussians



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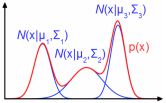

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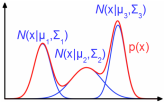

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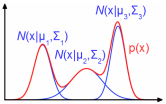

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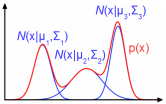

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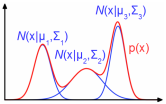

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- Note: The prior $p(\boldsymbol{z}|\pi)$ on each $\boldsymbol{z}_n$ is a multinomial, i.e., $p(\boldsymbol{z}_n|\pi) = \prod_{k=1}^{K} \pi_k^{z_{nk}}$

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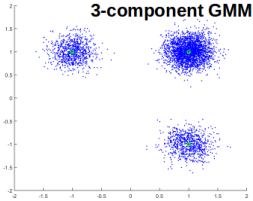
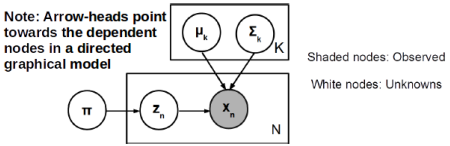
Some simulated data from a 3-component GMM



Directed Graphical Model for a K-component GMM



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- Multivariate Gaussian in D dimensions

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- Note: The "trace trick" simplifies the derivative calculations

$$\underbrace{\boldsymbol{x}^\top \Sigma^{-1}\boldsymbol{x}}_{\text{a scalar}} = \text{trace}(\boldsymbol{x}^\top \Sigma^{-1}\boldsymbol{x}) = \text{trace}(\Sigma^{-1}\boldsymbol{x}\boldsymbol{x}^\top)$$

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- To learn the GMM parameters Θ, we have to do MLE on $p(\boldsymbol{x})$
- In general, it is not an easy problem due to the difficult form of $p(\boldsymbol{x})$ (for "why", see the next slide)

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- Note: For problems where $\boldsymbol{z}_n$ is continuous or comes from a combinatorially large space (e.g., it's a binary vector), doing MLE will be even harder!

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Learning GMM: The Difficulty

- Given N observations $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$, the log-likelihood will be

$$\mathcal{L} = \log \prod_{n=1}^{N} p(\boldsymbol{x}_n) = \sum_{n=1}^{N} \log p(\boldsymbol{x}_n) = \sum_{n=1}^{N} \log \underbrace{\sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\text{params get coupled!}}$$

- Due to the coupling of parameters, MLE by simply taking derivatives of $\mathcal{L}$ and setting to zero won't give a closed form solution of $\Theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$
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  In such cases, something like EM becomes even more important

Learning GMM by Making Guesses!

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  - A more formal view of this iterative procedure is given by the Expectation Maximization (EM) algorithm (next lecture)

Learning GMM

- The complete data log-likelihood over the N obs.

$$\sum_{n=1}^{N} \log p(\boldsymbol{x}_n, \boldsymbol{z}_n) = \sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\boldsymbol{z}_n)p(\boldsymbol{z}_n) = \sum_{n=1}^{N} \log \underbrace{\prod_{k=1}^{K} [p(\boldsymbol{x}_n|\boldsymbol{z}_n = k)p(\boldsymbol{z}_n = k)]^{z_{nk}}}_{\text{(note that, for each } n\text{, only one } z_{nk} \text{ will be 1)}}$$

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  - In such cases, we can use the posterior expectations of the z_{nk}'s (which are basically posterior probabilities of cluster assignments of points to clusters)

Learning GMM: Cluster Assignment Probabilities

- Posterior expectations $\mathbb{E}[z_{nk}]$ can be computed using current estimates of Θ

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.. and do MLE for the parameters Θ using this as the objective function

Learning GMM: Component Parameters

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

Learning GMM: Component Parameters

- 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.

$$\mathcal{L} = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} [\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]$$

- Taking derivatives w.r.t. $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$, $\forall k = 1, \ldots, K$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = \frac{\partial}{\partial \boldsymbol{\mu}_k} \sum_{n=1}^{N} \gamma_{nk} \log \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = 0 \qquad \text{(note: constants w.r.t. } \mu_k \text{ can be ignored)}$$

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- For each k, it's a "weighted" version of the MLE problem for the multivariate Gaussian $\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, given observations $\{\boldsymbol{x}_n\}_{n=1}^N$ with weights $\{\gamma_{nk}\}_{n=1}^N$
- Can also solve for π_k likewise (subject to contraint $\sum_{k=1}^{K} \pi_k = 1$)
- Derivations are a bit tedious (but straightforward). I will provide a note.

GMM Parameter Update Equations

- The final expressions for updates of $\{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$

$$\begin{aligned}
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- Also note that each point $\boldsymbol{x}_n$ contributes to each $\{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ but fractionally (based on the values of γ_{nk})

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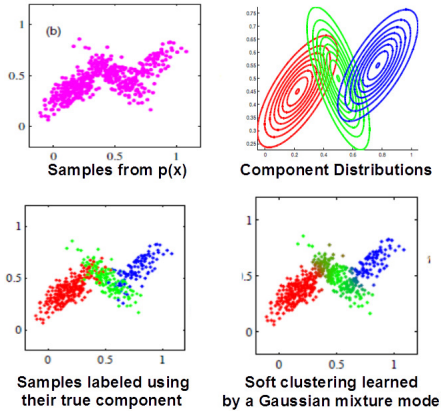
(It's basically an Expectation Maximization (EM) algorithm for learning GMM. We will look at EM more formally in the next class.)

Illustration of GMM Clustering



Notice the "mixed" colored points in the overlapping regions in the final clustering

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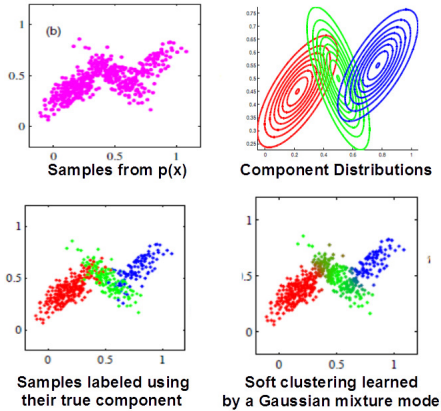

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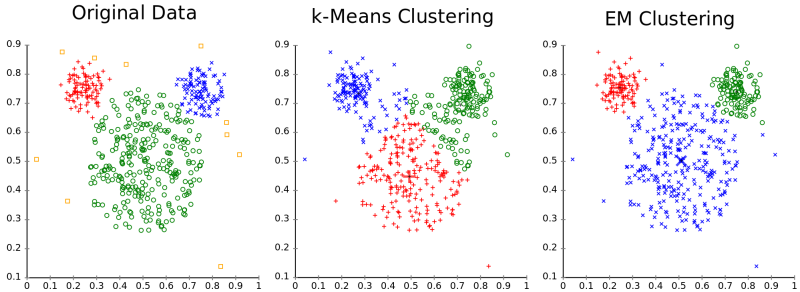
Also check out this demo of GMM: `https://www.youtube.com/watch?v=B36fzChfyGU`

GMM vs K-means

For the GMM clustering (rightmost figure), the most probable cluster for each point has been labeled



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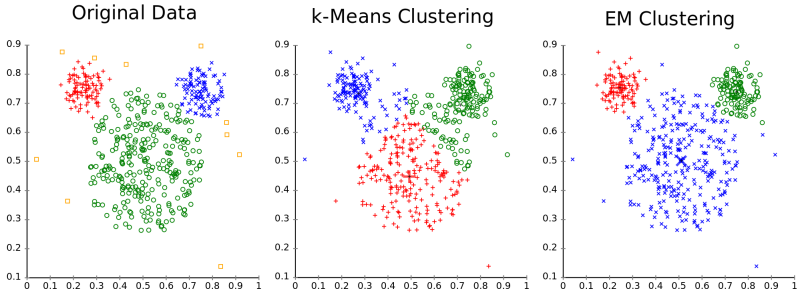

Note that K-means, unlike GMM, tends to learn equi-sized clusters.

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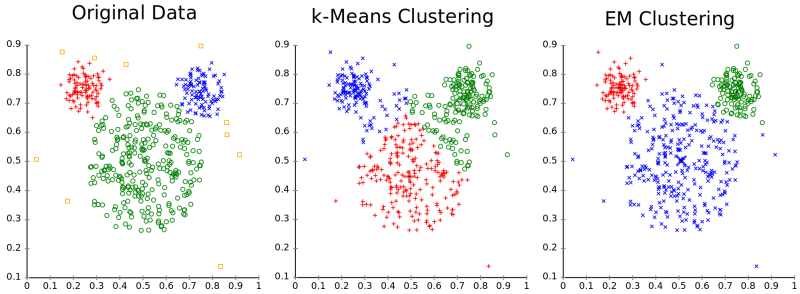

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GMM with $\Sigma_k = \mathbf{I}$ and $\pi_k = 1/K$, and soft assignments converted to hard assign. (setting the largest prob. to 1, rest to 0), is equivalent to K-means.

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  $p(y = k)$ and $p(\boldsymbol{x}|\boldsymbol{z} = k)$ can be efficiently estimated using training data
- Number of clusters (K) in a mixture model can be learned from data using nonparametric Bayesian methods (e.g., "infinite" mixture models)

Next Class

- The general Expectation Maximization (EM) algorithm
- Generative models for dimensionality reduction
  - Factor Analysis and Probabilistic PCA (and extensions)
  - EM based parameter estimation for these models