Generative Models for Clustering, GMM, and Intro to EM

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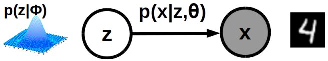
Machine Learning (CS771A)

Sept 26, 2016

Generative Models

- A probabilistic way to think about the data generation process



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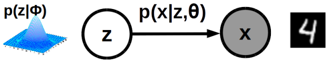

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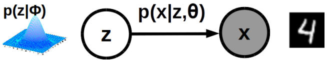

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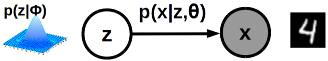

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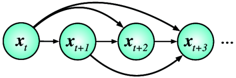

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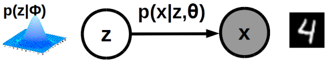

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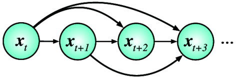

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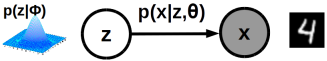

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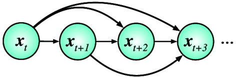

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Generative Models for Clustering

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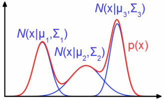
- A generative model for data clustering
- Data assumed generated from a mixture of K Gaussians



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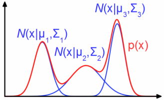

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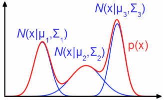

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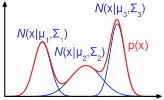

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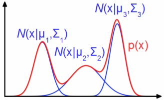

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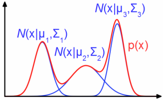

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- Note: The prior $p(\boldsymbol{z}|\pi)$ on each $\boldsymbol{z}_n$ is a multinomial, i.e., $p(\boldsymbol{z}_n|\pi) = \prod_{k=1}^{K} \pi_k^{z_{nk}}$

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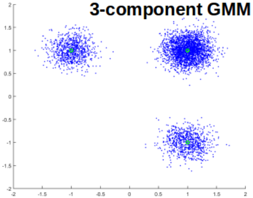
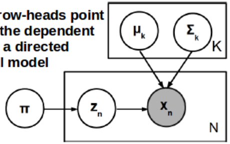
Some simulated data from a 3-component GMM



Directed Graphical Model for a K-component GMM

Note: Arrow-heads point towards the dependent nodes in a directed graphical model



Shaded nodes: Observed

White nodes: Unknowns

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

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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!

$$\mathcal{L} = \sum_{n=1}^{N} \log \underbrace{\int_{\boldsymbol{z}_n} p(\boldsymbol{x}_n | \boldsymbol{z}_n) p(\boldsymbol{z}_n) d\boldsymbol{z}_n}_{\text{Ouch! Intractable integral!!!}}$$

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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!

$$\mathcal{L} = \sum_{n=1}^{N} \log \underbrace{\int_{\boldsymbol{z}_n} p(\boldsymbol{x}_n | \boldsymbol{z}_n) p(\boldsymbol{z}_n) d\boldsymbol{z}_n}_{\text{Ouch! Intractable integral!!!}}$$

In such cases, something like EM becomes even more important

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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.

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- What if we don't have a *deterministic* guess for z_{nk}?
  - 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

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

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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 $\{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$

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\boldsymbol{\mu}_k &= \frac{1}{N_k}\sum_{n=1}^{N} \gamma_{nk}\boldsymbol{x}_n \\
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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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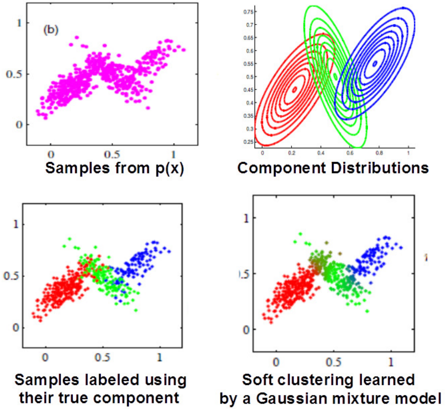
(It's basically an Expectation Maximization (EM) algorithm for learning GMM. We will look at EM more formally in the next class.)

Illustration of GMM Clustering



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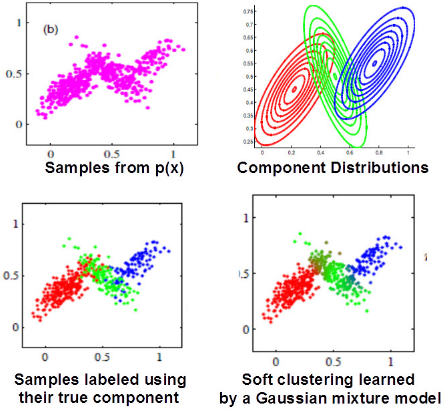

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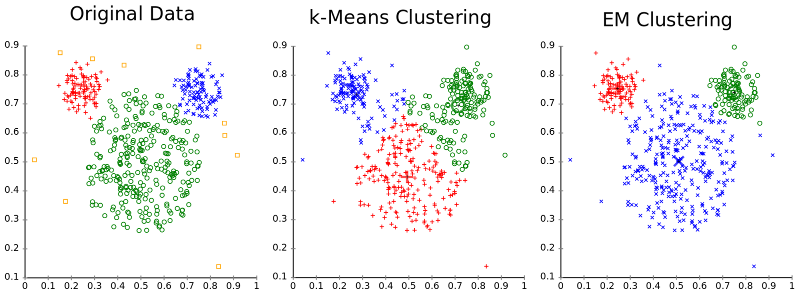
Also check out this demo of GMM: `https://www.youtube.com/watch?v=B36fzChfyGU`

GMM vs K-means

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



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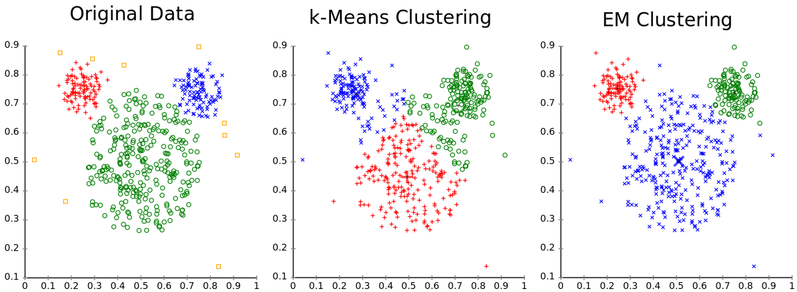

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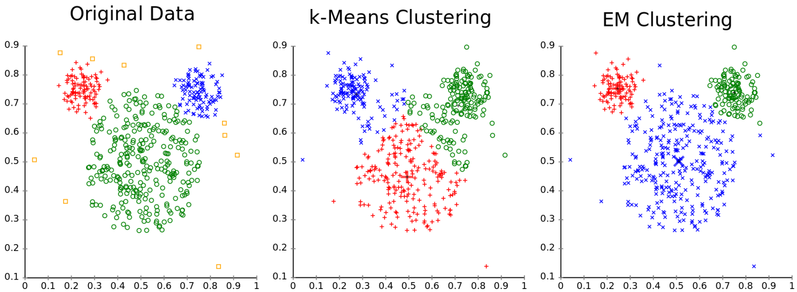

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GMM with $\Sigma_k = \mathbf{I}$ and $\pi_k = 1/K$, and soft assignments converted to hard assign. (setting the largest prob. to 1, rest to 0), is equivalent to K-means.

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- 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