Latent Variable Models and Expectation Maximization

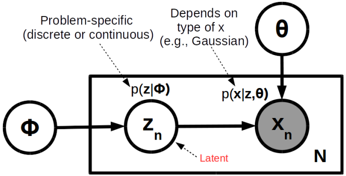
Piyush Rai

Introduction to Machine Learning (CS771A)

September 27, 2018

Recap: Latent Variable Models

- Assume each observation $\boldsymbol{x}_n$ to be associated with a "local" latent variable $\boldsymbol{z}_n$



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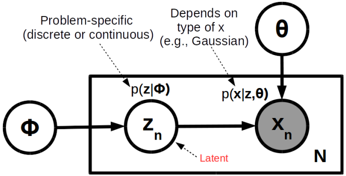

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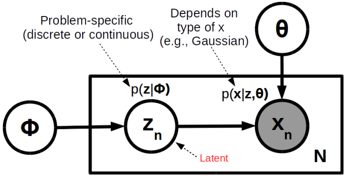

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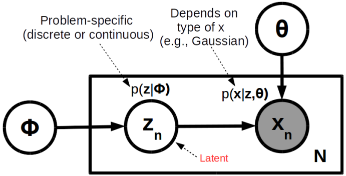

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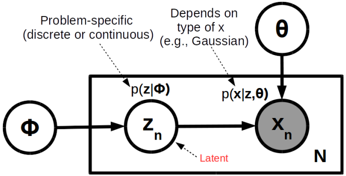

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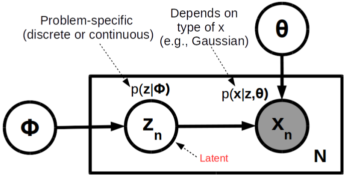

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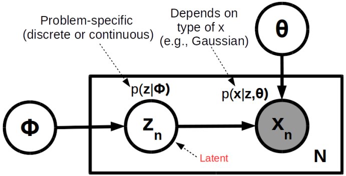

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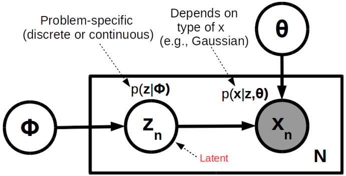

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- Given data $\mathbf{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, the goal is to estimate the parameters Θ or latent variable $\mathbf{Z}$ or both (note: we can usually estimate Θ given $\mathbf{Z}$, and vice-versa)

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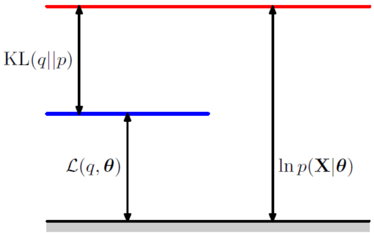

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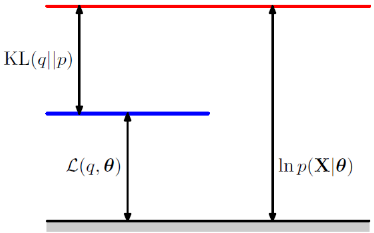

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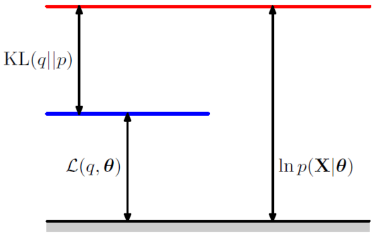

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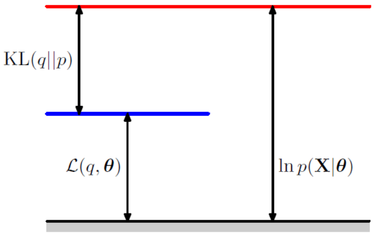

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- Maximizing $\mathcal{L}(q, \Theta)$ will also improve $\log p(\mathbf{X}|\Theta)$

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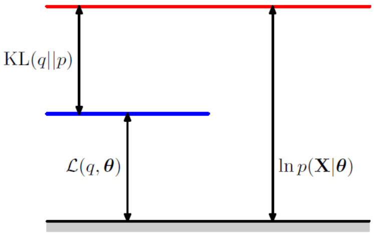
$$\mathcal{L}(q,\Theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log\left\{\frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})}\right\}$$

$$\text{KL}(q||p_z) = -\sum_{\mathbf{Z}} q(\mathbf{Z}) \log\left\{\frac{p(\mathbf{Z}|\mathbf{X},\Theta)}{q(\mathbf{Z})}\right\}$$

(Exercise: Verify the above identity)



- Since $\text{KL}(q||p_z) \geq 0$, $\mathcal{L}(q,\Theta)$ is a lower-bound on $\log p(\mathbf{X}|\Theta)$

$$\log p(\mathbf{X}|\Theta) \geq \mathcal{L}(q,\Theta)$$

- Maximizing $\mathcal{L}(q,\Theta)$ will also improve $\log p(\mathbf{X}|\Theta)$. Also, as we'll see, it's easier to maximize $\mathcal{L}(q,\Theta)$

Maximizing $\mathcal{L}(q, \Theta)$

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- $\mathcal{Q}(\Theta, \Theta^{old}) = \mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \Theta^{old})}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is known as expected complete data log-likelihood (CLL)

What's Going On: A Visual Illustration..

- Step 1: We set $\hat{q} = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$, $\mathcal{L}(\hat{q}, \Theta)$ touches $\log p(\mathbf{X}|\Theta)$ at Θ^{old}
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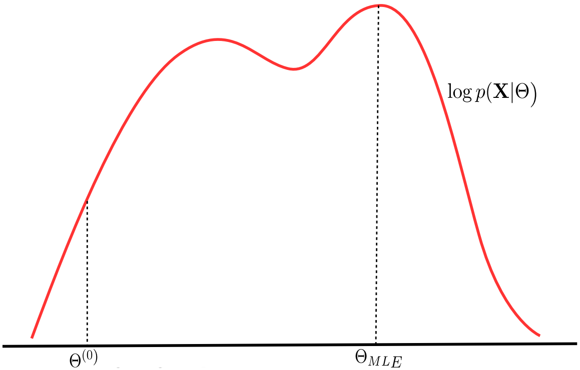

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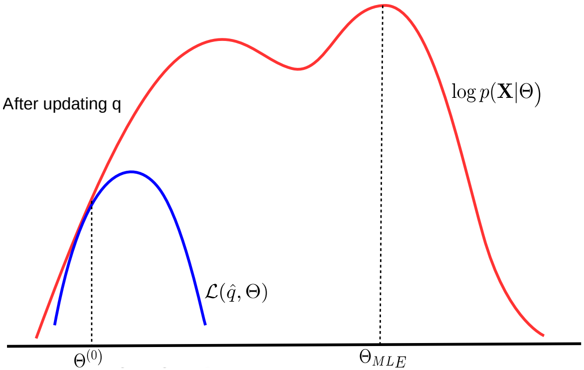

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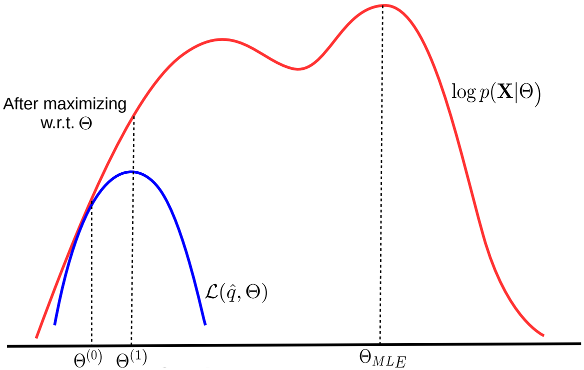

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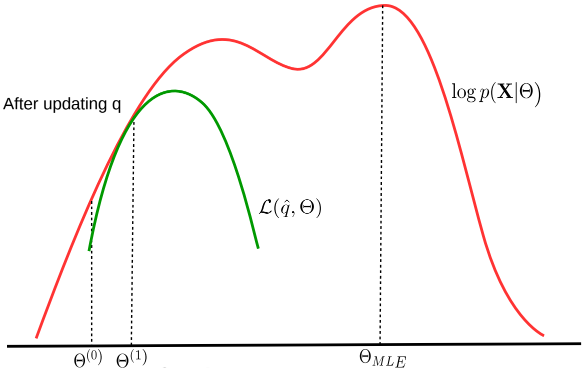

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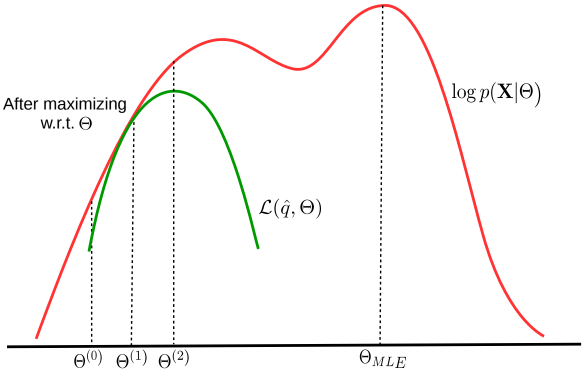

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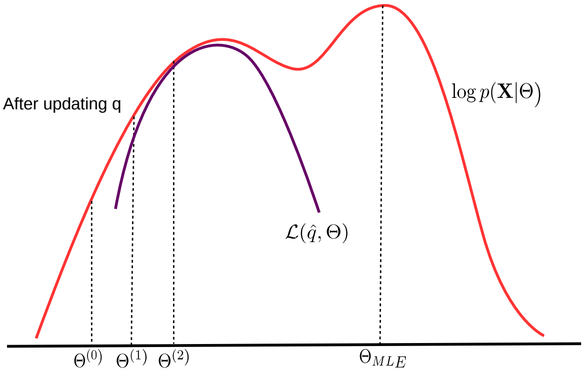

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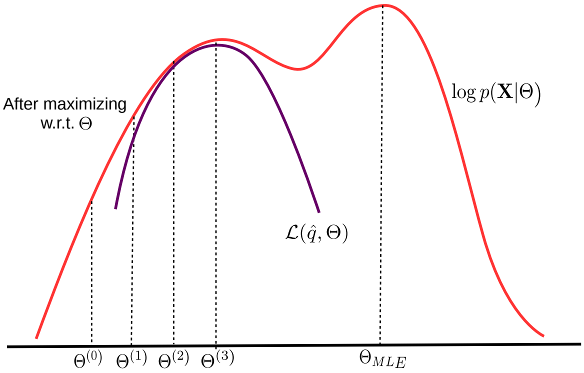

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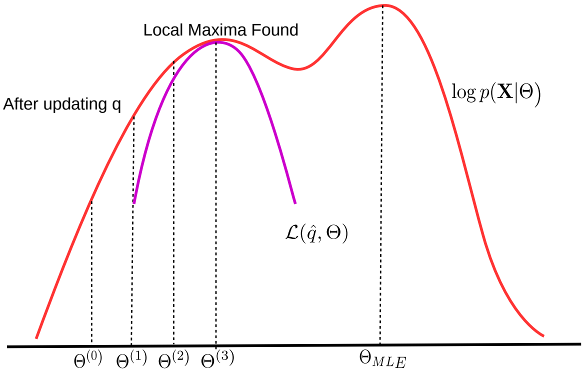

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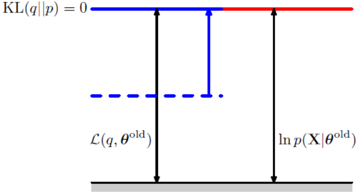
- The two-step alternating optimzation scheme we saw can never decrease $p(\mathbf{X}|\Theta)$ (good thing)
- To see this consider both steps: (1) Optimize q given $\Theta = \Theta^{old}$; (2) Optimize Θ given this q



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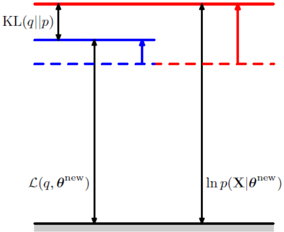

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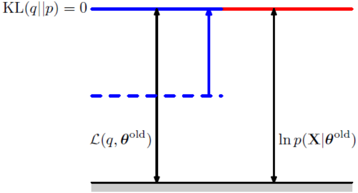

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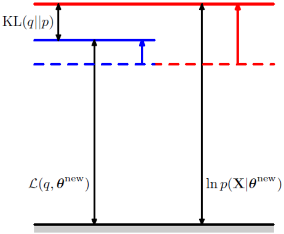

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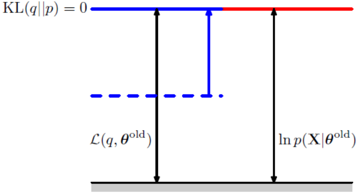

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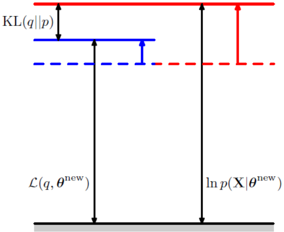

(Step 2)

- Step 1 keeps Θ fixed, so $p(\mathbf{X}|\Theta)$ obviously can't decrease (stays unchanged in this step)
- Step 2 maximizes the lower bound $\mathcal{L}(q, \Theta)$ w.r.t Θ. Thus $p(\mathbf{X}|\Theta)$ can't decrease!

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The ALT-OPT of $\mathcal{L}(q, \Theta)$ that we saw leads to the EM algorithm (Dempster, Laird, Rubin, 1977)

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4. If not yet converged, set $t = t + 1$ and go to step 2.

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$$p(\boldsymbol{z}_n^{(t)}|\boldsymbol{x}_n, \Theta^{(t-1)}) = \frac{p(\boldsymbol{z}_n^{(t)}|\Theta^{(t-1)})p(\boldsymbol{x}_n|\boldsymbol{z}_n^{(t)}, \Theta^{(t-1)})}{p(\boldsymbol{x}_n|\Theta^{(t-1)})} \propto \text{prior} \times \text{likelihood}$$

3. Step 2: Now maximize the expected complete data log-likelihood w.r.t. Θ

$$\Theta^{(t)} = \arg\max_{\Theta} \mathcal{Q}(\Theta, \Theta^{(t-1)}) = \arg\max_{\Theta} \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n^{(t)}|\boldsymbol{x}_n, \Theta^{(t-1)})}[\log p(\boldsymbol{x}_n, \boldsymbol{z}_n^{(t)}|\Theta)]$$

4. If not yet converged, set $t = t + 1$ and go to step 2.

Note: If we can take the MAP estimate $\hat{\boldsymbol{z}}_n$ of $\boldsymbol{z}_n$ (not full posterior) in Step 1 and maximize the CLL in Step 2 using that estimate, i.e., do $\arg\max_{\Theta} \sum_{n=1}^{N} \log p(\boldsymbol{x}_n, \hat{\boldsymbol{z}}_n^{(t)}|\Theta)$, this will be identical to ALT-OPT

Writing Down the Expected CLL

- Deriving the EM algorithm for any model requires finding the expression of the expected CLL

$$\mathcal{Q}(\Theta, \Theta^{old}) = \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\Theta^{old})}[\log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta)]$$

$$= \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\Theta^{old})}[\log p(\boldsymbol{x}_n|\boldsymbol{z}_n, \Theta) + \log p(\boldsymbol{z}_n|\Theta)]$$

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    - .. and so on..
- The expected CLL may not always be computable and may need to be approximated

EM for Gaussian Mixture Model

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- Let's first look at the CLL. Similar to generative classification with Gaussian class-conditionals

$$\log p(\mathbf{X}, \mathbf{Z}|\Theta) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}[\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)] \qquad \text{(we've seen how we get this)}$$

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.. where the expectation is w.r.t. the current posterior of $\boldsymbol{z}_n$, i.e., $p(\boldsymbol{z}_n|\boldsymbol{x}_n, \Theta^{old})$

- In this case, we only need $\mathbb{E}[z_{nk}]$ which can be computed as

$$\mathbb{E}[z_{nk}] = \gamma_{nk} \quad = \quad 0 \times p(z_{nk} = 0|\boldsymbol{x}_n, \Theta^{old}) + 1 \times p(z_{nk} = 1|\boldsymbol{x}_n, \Theta^{old}) = p(z_{nk} = 1|\boldsymbol{x}_n)$$

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&\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)}
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- 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 $\sum_{k=1}^{K} \mathbb{E}[z_{nk}] = 1$

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3. Given "responsibilities" $\gamma_{nk} = \mathbb{E}[z_{nk}]$, and $N_k = \sum_{n=1}^N \gamma_{nk}$, re-estimate Θ via MLE

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

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4. Set $t = t + 1$ and go to step 2 if not yet converged

Another Example: (Probabilistic) Dimensionality Reduction

- Let's consider a latent factor model for dimensionality reduction (will revisit this later)

$$p(\boldsymbol{x}_n|\boldsymbol{z}_n, \mathbf{W}, \sigma^2) = \mathcal{N}(\mathbf{W}\boldsymbol{z}_n, \sigma^2\mathbf{I}_D) \qquad p(\boldsymbol{z}_n) = \mathcal{N}(\mathbf{0}, \mathbf{I}_K)$$

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