Expectation Maximization (Contd.)

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Probabilistic Machine Learning (CS772A)

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$$\pi_k^{(t)} = \frac{N_k^{(t)}}{N}$$

The General EM Algorithm

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- Consider a latent variable model with joint distribution

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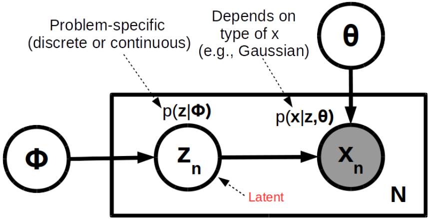

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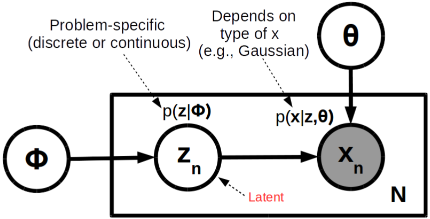

- Goal: Estimate the model parameters Θ via MLE/MAP (sometimes also the latent variales $\boldsymbol{z}_n$'s)

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- This procedure is basically the Expectation Maximization (EM) algorithm for latent variable models

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- Define $p_z = p(\mathbf{Z}|\mathbf{X}, \Theta)$. The identity below holds for any choice of the distribution q

$$\boxed{\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \mathrm{KL}(q||p_z)}$$

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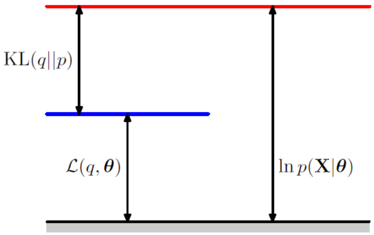

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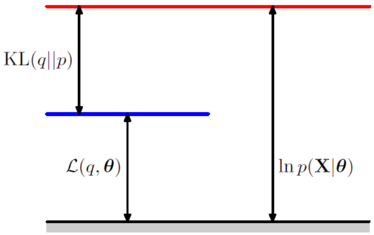

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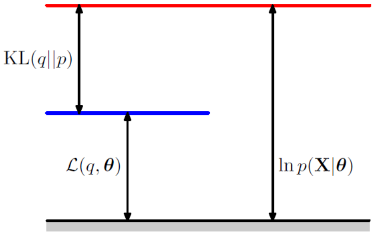

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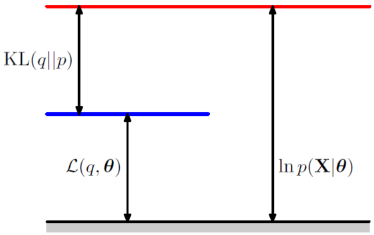

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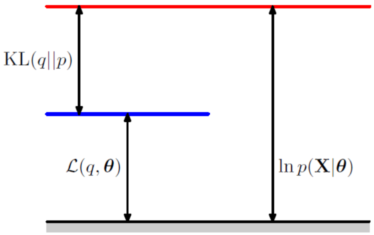

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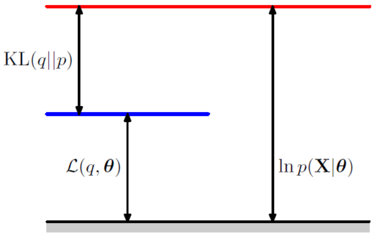

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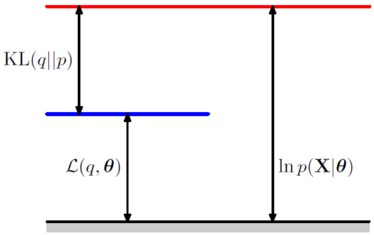
\mathcal{L}(q, \Theta) &= \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\Theta)}{q(\mathbf{Z})} \right\} \\
\text{KL}(q||p_z) &= -\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left\{ \frac{p(\mathbf{Z}|\mathbf{X}, \Theta)}{q(\mathbf{Z})} \right\}
\end{aligned}$$

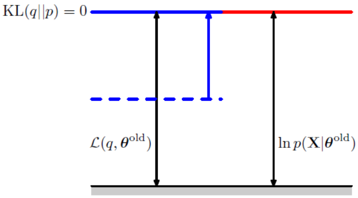
(Exercise: Verify the above identity)



- Since $\text{KL}(q||p_z) \geq 0$, $\mathcal{L}(q, \Theta)$ is a lower-bound on $\log p(\mathbf{X}|\Theta)$
  - **Consequence:** Maximizing $\mathcal{L}(q, \Theta)$ will also make $\log p(\mathbf{X}|\Theta)$ go up
- Therefore, to do MLE on $\log p(\mathbf{X}|\Theta)$, we can maximize $\mathcal{L}(q, \Theta)$ w.r.t. q and Θ
  - Maximizing $\mathcal{L}(q, \Theta)$ jointly w.r.t. q and Θ isn't possible, so we alternate between: (1) Given Θ, find the optimal q that maximizes $\mathcal{L}(q, \Theta)$, and (2) Given q, find the optimal Θ that maximizes $\mathcal{L}(q, \Theta)$

Given Θ, which q maximizes $\mathcal{L}(q, \Theta)$?

$$\boxed{\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \mathrm{KL}(q||p_z)}$$



- Since Θ (and thus $\log p(\mathbf{X}|\Theta)$) doesn't change in this step, the sum $\mathcal{L}(q, \Theta) + \mathrm{KL}(q||p_z)$ is fixed

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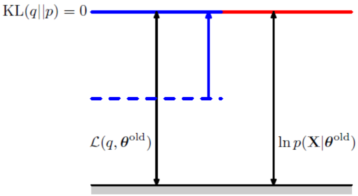

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- Therefore, with Θ fixed to Θ^{old}, maximizing the lower bound $\mathcal{L}(q, \Theta^{old})$ w.r.t. q, i.e.,

$$\boxed{\hat{q} = \arg\max_q \mathcal{L}(q, \Theta^{old})}$$

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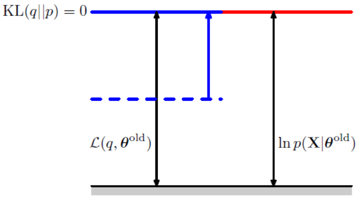

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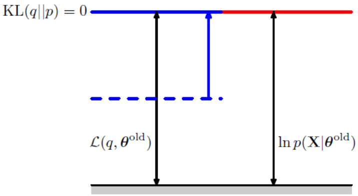

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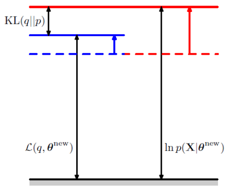
$$\boxed{\log p(\mathbf{X}|\Theta) = \mathcal{L}(q,\Theta) + \text{KL}(q||p_z)}$$

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



- With q fixed at $\hat{q} = p(\mathbf{Z}|\mathbf{X},\Theta^{old})$, we want to maximize $\mathcal{L}(\hat{q},\Theta)$ w.r.t. Θ, where

$$\mathcal{L}(\hat{q},\Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \log p(\mathbf{Z}|\mathbf{X},\Theta^{old})$$

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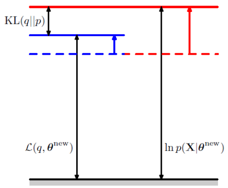

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$$\begin{aligned} \mathcal{L}(\hat{q},\Theta) &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \log p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \\ &= \mathcal{Q}(\Theta,\Theta^{old}) + \text{const} \end{aligned}$$

.. where $\mathcal{Q}(\Theta,\Theta^{old}) = \mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\Theta)]$ is the exp. complete data log-lik

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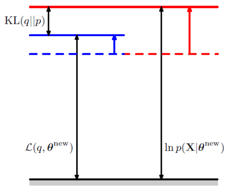

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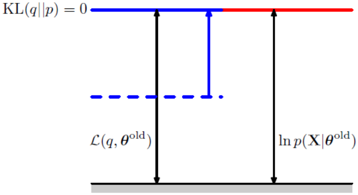
.. where $\mathcal{Q}(\Theta,\Theta^{old}) = \mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\Theta)]$ is the exp. complete data log-lik

- Therefore the optimal Θ is $\boxed{\Theta^{new} = \arg\max_{\Theta} \mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\Theta)]}$

EM Iterations never decrease $\log p(\mathbf{X}|\Theta)$

- Step 1: Setting $q = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$ makes KL zero, and $\mathcal{L}(q, \Theta^{old})$ becomes equal to $\log p(\mathbf{X}|\Theta^{old})$



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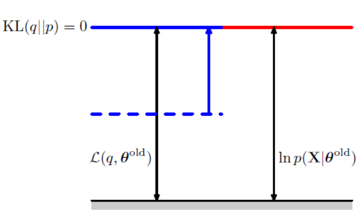

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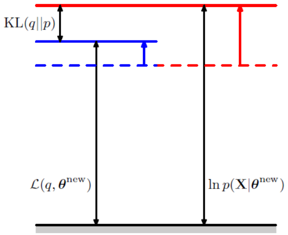

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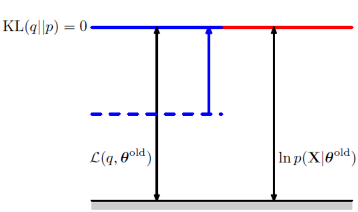

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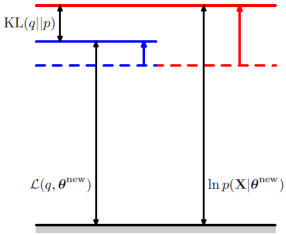

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- Step 2: Maximizing $\mathcal{L}(q, \Theta) = \mathcal{Q}(\Theta, \Theta^{old})$ w.r.t. Θ will lead to
  - $\mathcal{L}(q, \Theta)$ increasing, if not already at the optima

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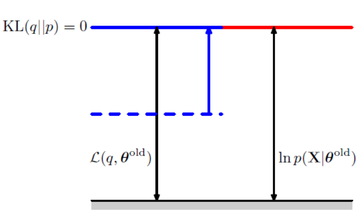

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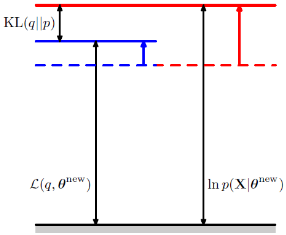

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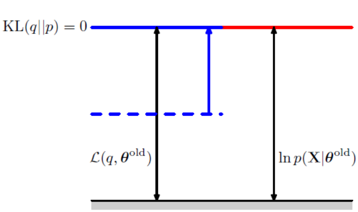

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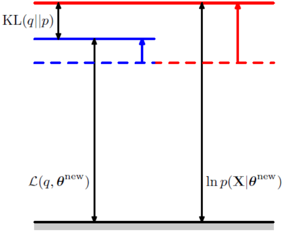

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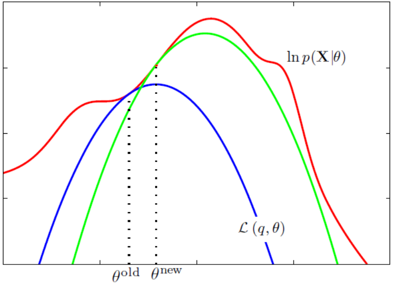
- Step 2: Maximizing $\mathcal{L}(q, \Theta) = \mathcal{Q}(\Theta, \Theta^{old})$ w.r.t. Θ will lead to
  - $\mathcal{L}(q, \Theta)$ increasing, if not already at the optima
  - $\mathrm{KL}(q||p_z) > 0$ again because $q \neq p(\mathbf{Z}|\mathbf{X}, \Theta^{new})$
  - As a result, ensures that $\log p(\mathbf{X}|\Theta^{new}) = \mathcal{L}(q, \Theta^{new}) + \mathrm{KL}(q||p_z) \geq \log p(\mathbf{X}|\Theta^{old})$

EM: A View in the Parameter (Θ) Space



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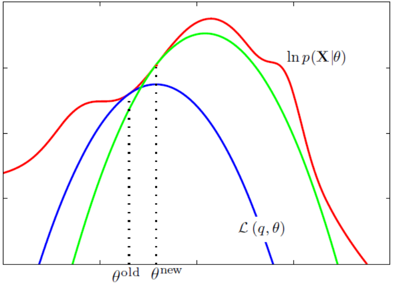

- E-step: Update of q makes the $\mathcal{L}(q, \Theta)$ curve touch the $\log p(\mathbf{X}|\Theta)$ curve at Θ^{old}

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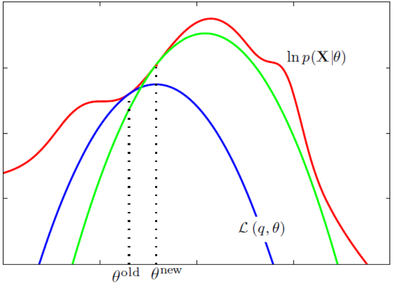

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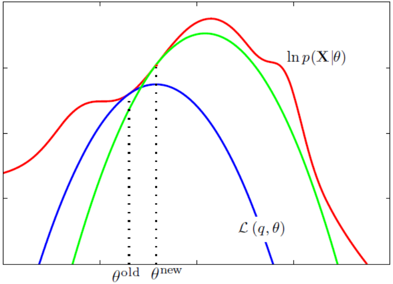

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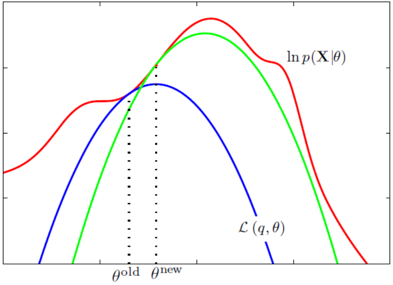

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- This continues until a local maxima of $\log p(\mathbf{X}|\Theta)$ is reached

An Alternate View of What EM Does

- Consider the ‘incomplete” data log likelihood

$$\log p(\mathbf{X}|\Theta) \quad = \quad \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta)$$

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- If we set $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta)$, the above inequality becomes equality.

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- If we <u>set</u> $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta)$, the above inequality becomes equality. To see this, note that

$$\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})}$$

An Alternate View of What EM Does

- Consider the 'incomplete" data log likelihood

$$\log p(\mathbf{X}|\Theta) = \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ can be any distribution)}$$

$$\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)\text{, if } \sum_i \lambda_i = 1)$$

$$\log p(\mathbf{X}|\Theta) \geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}$$

- If we set $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta)$, the above inequality becomes equality. To see this, note that

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- Thus ILL $\log p(\mathbf{X}|\Theta)$ is tightly lower-bounded by expected CLL $\mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\Theta)]$ which EM maximizes

The Expectation Maximization (EM) Algorithm

Initialize the parameters: Θ^{old}. Then alternate between these steps:

- **E (Expectation) step:**

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$$\mathcal{Q}(\Theta, \Theta^{old}) = \mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \Theta^{old})}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$$

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- If the incomplete log-lik $p(\mathbf{X}|\Theta)$ not yet converged then set $\Theta^{old} = \Theta^{new}$ and go to the E step.

EM: An Example of what “Expected CLL” looks like

- Already seen GMM. Let’s consider a latent factor model for dimensionality reduction (next class)

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

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- Note: The above is only a sketchy description of the procedure. I will provide a reference.

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