# Latent Variable Models

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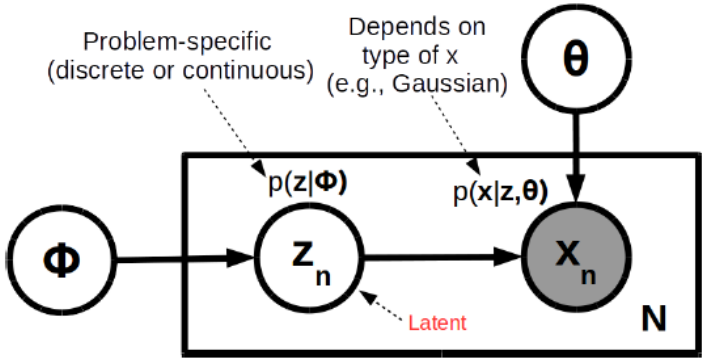



- Variables that cannot be observed (both in training and testing)

Advantages:

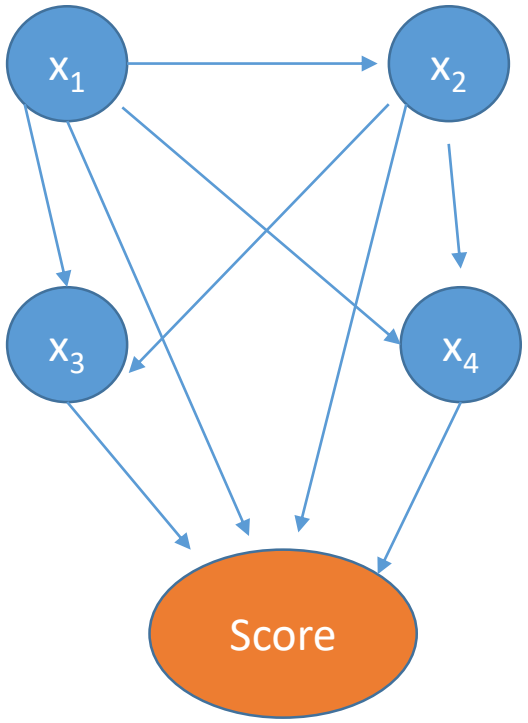
- Augment model to simplify inference (logistic regression)
- Latent features/properties of data (clusters, topics, representation)

# Example of Latent Variable

- Team Selection for a Sports Meet

| Height ($x_1$) (m) | Weight ($x_2$) (kg) | Daily exercise ($x_3$) (kCal) | Hours of sleep ($x_4$) (hrs) | Performance Score |
|---|---|---|---|---|
| 1.64 | 85 | 2300 | 8 | 60 |
| 1.83 | 80 | 2700 | 7 | 90 |
| 1.52 | 70 | 2200 | 6 | 70 |

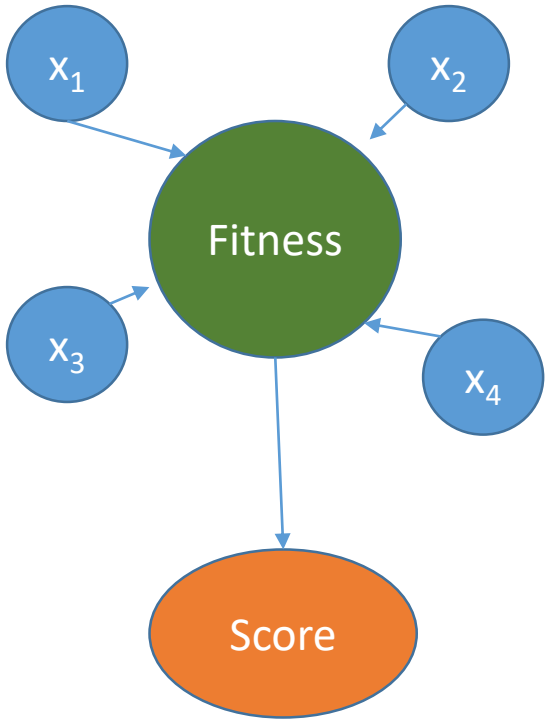
# Probabilistic Inference




$p(score|x_1, x_2, x_3, x_4)$

Large number possible combinations of the variables.

# Probabilistic Inference




$p(\text{score}|\text{fitness})p(\text{fitness}|x_1)p(\text{fitness}|x_2)p(\text{fitness}|x_3)p(\text{fitness}|x_4)$

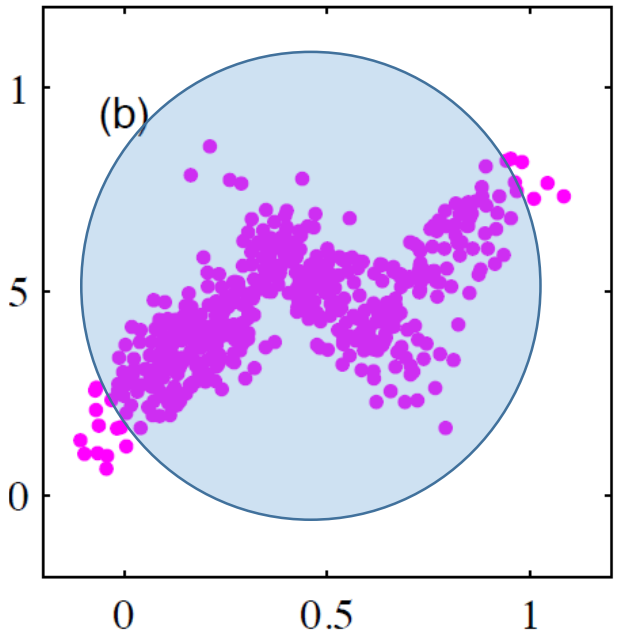
Reduction in number of model parameters

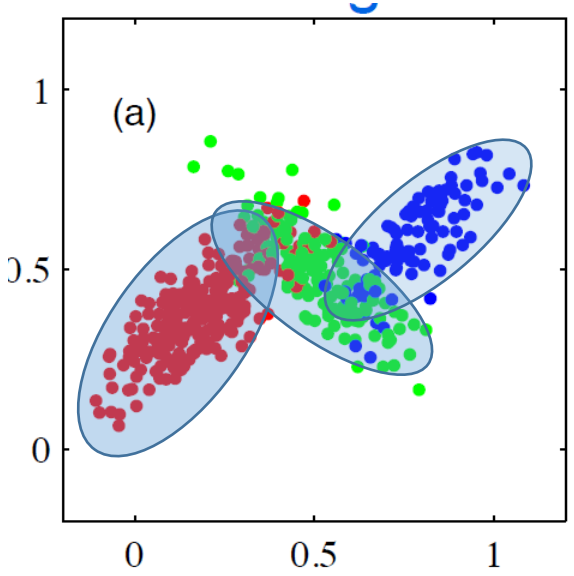
Fitness – latent variable

# Parameters vs Latent Variables

- Parameters are global, Latent Variables are observation specific/local
- Computationally difficult to do posterior inference for all the variables
- Hybrid inference
  - Estimate Posterior for latent/local variable
  - Point estimate (e.g., MLE) for parameters/global variables

# Example: Gaussian Mixture Model (GMM)



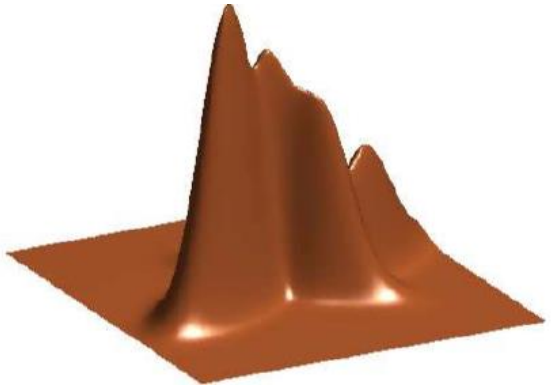
# Mixture of Gaussian

- A Gaussian mixture model represents a **distribution** as

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

with $\pi_k$ the mixing coefficients, where:

$$\sum_{k=1}^{K} \pi_k = 1 \quad \text{and} \quad \pi_k \geq 0 \quad \forall k$$



- GMMs are **universal approximators of densities**

# Latent Variable View of GMM

- We could introduce a hidden (latent) variable $z$ which would represent which Gaussian generated our observation $\mathbf{x}$, with some probability
- Let $z \sim \text{Categorical}(\boldsymbol{\pi})$ (where $\pi_k \geq 0, \quad \sum_k \pi_k = 1$)
- Then:

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(\mathbf{x}, z = k)$$

$$= \sum_{k=1}^{K} \underbrace{p(z = k)}_{\pi_k} \underbrace{p(\mathbf{x}|z = k)}_{\mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}$$

# Parameter Estimation of GMM

- Maximum likelihood maximizes

$$\ln p(\mathbf{X}|\pi,\mu,\Sigma) = \sum_{n=1}^{N} \ln \left( \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k,\Sigma_k) \right)$$

w.r.t $\Theta = \{\pi_k, \mu_k, \Sigma_k\}$

- How would you optimize this?
- Can we have a closed form update?
- Don't forget to satisfy the constraints on $\pi_k$

# Parameter Estimation in GMM

- A Gaussian mixture distribution:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

- We had: $z \sim \text{Categorical}(\boldsymbol{\pi})$ (where $\pi_k \geq 0, \quad \sum_k \pi_k = 1$)
- Joint distribution: $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$
- Log-likelihood:

$$\ell(\boldsymbol{\pi}, \mu, \Sigma) = \ln p(\mathbf{X}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(\mathbf{x}^{(n)}|\pi, \mu, \Sigma)$$

$$= \sum_{n=1}^{N} \ln \sum_{z^{(n)}=1}^{K} p(\mathbf{x}^{(n)}|\, z^{(n)}; \mu, \Sigma) p(z^{(n)}|\, \boldsymbol{\pi})$$

- Note: We have a hidden variable $z^{(n)}$ for every observation
- General problem: sum inside the log

# Learning Parameters

- **If we knew** $z^{(n)}$ for every $x^{(n)}$, the maximum likelihood problem is easy:

$$\ell(\boldsymbol{\pi}, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(x^{(n)}, z^{(n)} | \pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(\mathbf{x}^{(n)} | \, z^{(n)}; \mu, \Sigma) + \ln p(z^{(n)} | \, \boldsymbol{\pi})$$

$$\begin{aligned}
\mu_k &= \frac{\sum_{n=1}^{N} 1_{[z^{(n)}=k]} \, \mathbf{x}^{(n)}}{\sum_{n=1}^{N} 1_{[z^{(n)}=k]}} \\
\Sigma_k &= \frac{\sum_{n=1}^{N} 1_{[z^{(n)}=k]} \, (\mathbf{x}^{(n)} - \mu_k)(\mathbf{x}^{(n)} - \mu_k)^T}{\sum_{n=1}^{N} 1_{[z^{(n)}=k]}} \\
\pi_k &= \frac{1}{N} \sum_{n=1}^{N} 1_{[z^{(n)}=k]}
\end{aligned}$$

# Learning Parameters

- Similarly if we knew the parameters $\pi$, $\mu$, $\Sigma$
  - Estimating the latent variable is easy

- Chicken and Egg Problem!

# Expectation Maximization Algorithm

- Optimization uses the Expectation Maximization algorithm, which alternates between two steps:
  1. E-step: Compute the posterior probability that each Gaussian generates each datapoint (as this is unknown to us)
  2. M-step: Assuming that the data really was generated this way, change the parameters of each Gaussian to maximize the probability that it would generate the data it is currently responsible for.

# EM Algorithm

- Elegant and powerful method for finding maximum likelihood solutions for models with latent variables
  1. E-step:
     - In order to adjust the parameters, we must first solve the inference problem: Which Gaussian generated each datapoint?
     - We cannot be sure, so it's a distribution over all possibilities.

$$\gamma_k^{(n)} = p(z^{(n)} = k|\mathbf{x}^{(n)}; \pi, \mu, \Sigma)$$

  2. M-step:
     - Each Gaussian gets a certain amount of posterior probability for each datapoint.
     - At the optimum we shall satisfy

$$\frac{\partial \ln p(\mathbf{X}|\pi, \mu, \Sigma)}{\partial \Theta} = 0$$

     - We can derive closed form updates for all parameters

# E Step

- Conditional probability (using Bayes rule) of $\mathbf{z}$ given $\mathbf{x}$

$$\begin{aligned}
\gamma_k = p(z=k|\mathbf{x}) &= \frac{p(z=k)p(\mathbf{x}|z=k)}{p(\mathbf{x})} \\
&= \frac{p(z=k)p(\mathbf{x}|z=k)}{\sum_{j=1}^{K} p(z=j)p(\mathbf{x}|z=j)} \\
&= \frac{\pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\mu_j, \Sigma_j)}
\end{aligned}$$

# M Step

- Log-likelihood:

$$\ln p(\mathbf{X}|\pi,\mu,\Sigma) = \sum_{n=1}^{N} \ln \left( \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k,\Sigma_k) \right)$$

- Set derivatives to 0:

$$\frac{\partial \ln p(\mathbf{X}|\pi,\mu,\Sigma)}{\partial \mu_k} = 0 = \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k,\Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\mu_j,\Sigma_j)} \Sigma_k (\mathbf{x}^{(n)} - \mu_k)$$

- We used:

$$\mathcal{N}(\mathbf{x}|\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\left( -\frac{1}{2} (\mathbf{x}-\mu)^T \Sigma^{-1} (\mathbf{x}-\mu) \right)$$

  and:

$$\frac{\partial (\mathbf{x}^T A \mathbf{x})}{\partial \mathbf{x}} = \mathbf{x}^T (A + A^T)$$

# M Step

$$\frac{\partial \ln p(\mathbf{X}|\pi,\mu,\Sigma)}{\partial \mu_k} = 0 = \sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k,\Sigma_k)}{\sum_{j=1}^{K}\pi_j \mathcal{N}(\mathbf{x}|\mu_j,\Sigma_j)}}_{\gamma_k^{(n)}} \Sigma_k(\mathbf{x}^{(n)} - \mu_k)$$

- This gives

$$\mu_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma_k^{(n)}\mathbf{x}^{(n)}$$

with $N_k$ the effective number of points in cluster $k$

$$N_k = \sum_{n=1}^{N}\gamma_k^{(n)}$$

# M Step

- We can get similarly expression for the variance

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} (\mathbf{x}^{(n)} - \mu_k)(\mathbf{x}^{(n)} - \mu_k)^T$$

- We can also minimize w.r.t the mixing coefficients

$$\pi_k = \frac{N_k}{N}, \quad \text{with} \quad N_k = \sum_{n=1}^{N} \gamma_k^{(n)}$$

- The optimal mixing proportion to use (given these posterior probabilities) is just the fraction of the data that the Gaussian gets responsibility for.
- Note that this is not a closed form solution of the parameters, as they depend on the responsibilities $\gamma_k^{(n)}$, which are complex functions of the parameters
- But we have a simple iterative scheme to optimize

# Summary of GMM

- Initialize the means $\mu_k$, covariances $\Sigma_k$ and mixing coefficients $\pi_k$
- Iterate until convergence:
  - E-step: Evaluate the responsibilities given current parameters

$$\gamma_k^{(n)} = p(z^{(n)}|\mathbf{x}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}^{(n)}|\mu_j, \Sigma_j)}$$

  - M-step: Re-estimate the parameters given current responsibilities

$$\begin{aligned}
\mu_k &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} \mathbf{x}^{(n)} \\
\Sigma_k &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} (\mathbf{x}^{(n)} - \mu_k)(\mathbf{x}^{(n)} - \mu_k)^T \\
\pi_k &= \frac{N_k}{N} \quad \text{with} \quad N_k = \sum_{n=1}^{N} \gamma_k^{(n)}
\end{aligned}$$

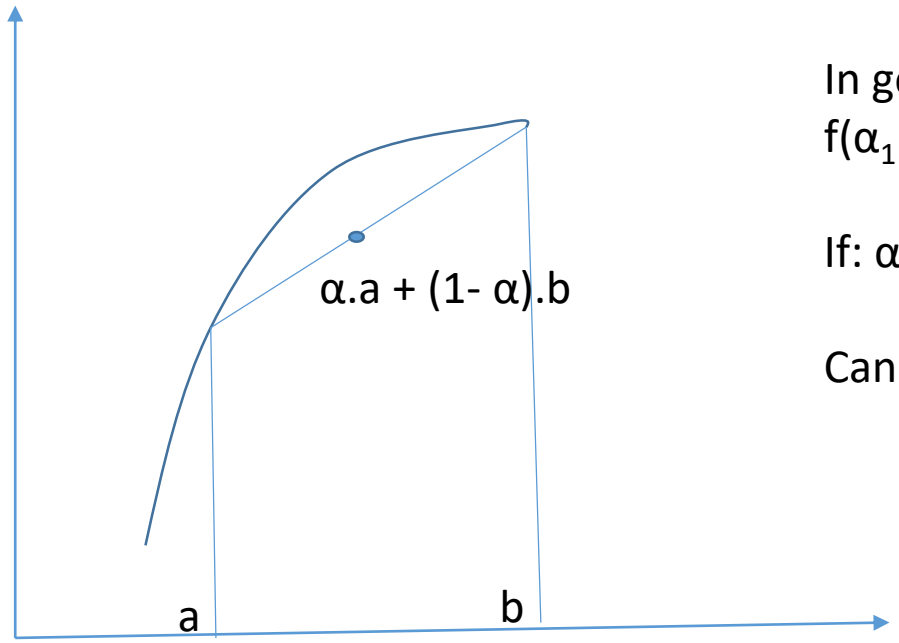
  - Evaluate log likelihood and check for convergence

$$\ln p(\mathbf{X}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left( \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k) \right)$$

# Generalized Expectation Maximization

# Generalized EM Algorithm

$$f(\alpha.a + (1- \alpha).b) \geq \alpha.f(a) + (1- \alpha).f(b)$$




Concave function

In general:

$$f(\alpha_1.a_1 + \alpha_2.a_2 + \alpha_3.a_3) \geq \alpha_1.f(a_1) + \alpha_2.f(a_2) + \alpha_3.f(a_3)$$

If: $\alpha_1 + \alpha_2 + \alpha_3 = 1$

Can think of α's as probabilities.

Logarithm is an example of concave function

# Jensen Inequality

**Theorem.** Let $f$ be a convex function, and let $X$ be a random variable. Then:

$$\mathrm{E}[f(X)] \geq f(\mathrm{E}X).$$

Reverse holds for concave functions.

If f is concave, -f is convex

# Kullback-Leibler Divergence

- Measures similarity between two distributions

$$D_{KL}(p||q) = \int_x p(x) log \frac{p(x)}{q(x)} dx$$

- The value is greater than or equal to zero.
- The value is zero when two distributions are identical.

# MLE in LVM

- Suppose we want to estimate parameters $\Theta$ via MLE. If we knew both $\boldsymbol{x}_n$ and $\boldsymbol{z}_n$ then we could do

$$\Theta_{MLE} = \arg\max_{\Theta} \sum_{n=1}^{N} \log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta) = \arg\max_{\Theta} \sum_{n=1}^{N} [\log p(\boldsymbol{z}_n|\phi) + \log p(\boldsymbol{x}_n|\boldsymbol{z}_n, \theta)]$$

- Simple to solve (usually closed form) if $p(\boldsymbol{z}_n|\phi)$ and $p(\boldsymbol{x}_n|\boldsymbol{z}_n, \theta)$ are "simple" (e.g., exp-fam. dist.)
- However, in LVMs where $\boldsymbol{z}_n$ is "hidden", the MLE problem will be the following

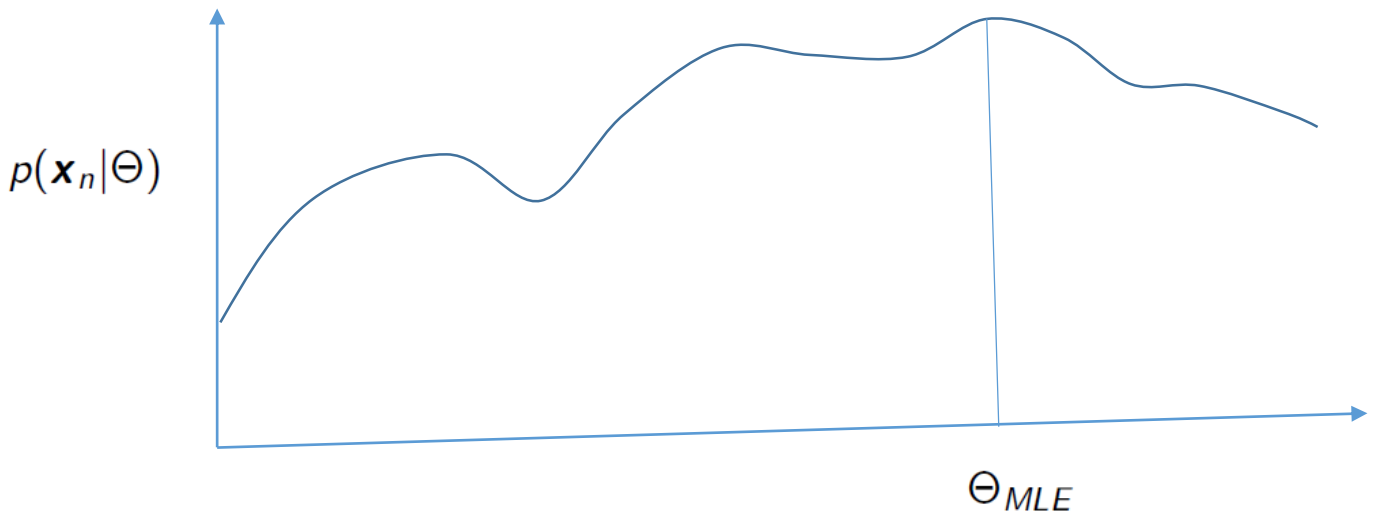
$$\Theta_{MLE} = \arg\max_{\Theta} \sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\Theta) = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta)$$

- The form of $p(\boldsymbol{x}_n|\Theta)$ may not be simple since we need to sum over unknown $\boldsymbol{z}_n$'s possible values

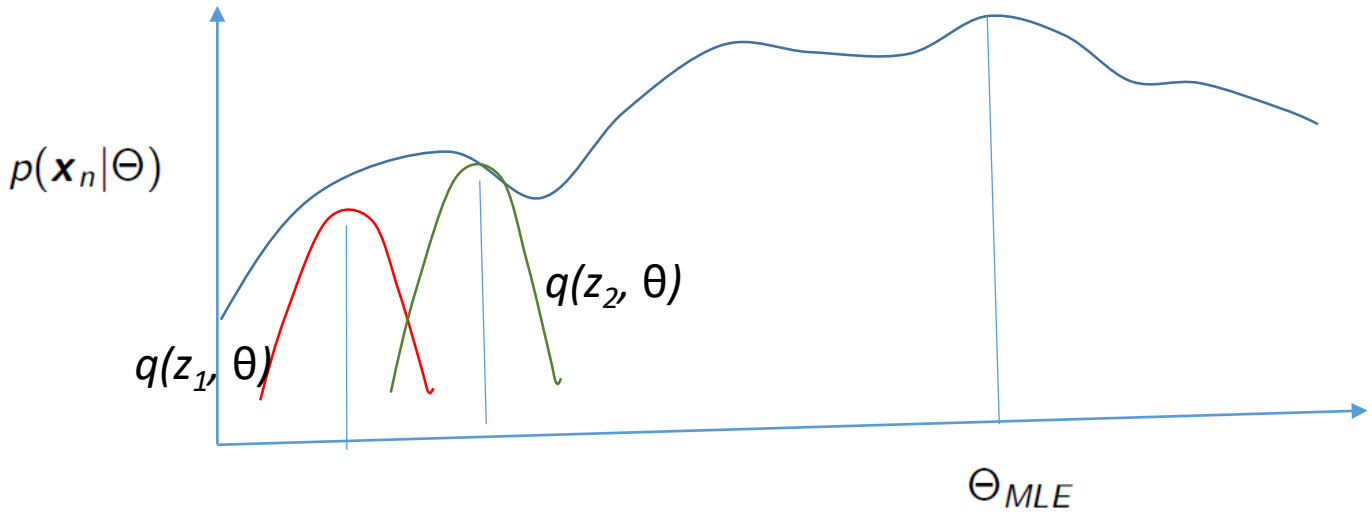
$$p(\boldsymbol{x}_n|\Theta) = \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta) \qquad \text{or if } \boldsymbol{z}_n \text{ is continuous: } \quad p(\boldsymbol{x}_n|\Theta) = \int p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta) d\boldsymbol{z}_n$$

# MLE in LVM: Optimization Problem

- The summation/integral may lead to complex expressions for the likelihood



# Optimizing a Lower Bound




$p(\boldsymbol{x}_n|\Theta) \geq q(z, \theta)$

$q$ – variational distribution, changes with z

Depends on both latent variable and parameter
Easy to maximise

# Two Step Iterative Optimization (for MLE)

- Step 1: Obtain the variational distribution lower bound with lowest gap
- Step 2: Obtain the maximum point for that variational distribution as candidate solution for $\theta_{MLE}$
- Repeat

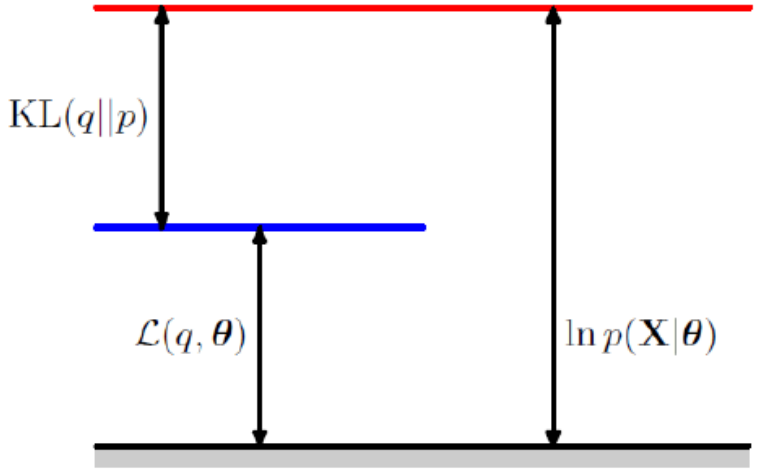
# Lower Bound on the Likelihood

- Define $p_z = p(\mathbf{Z}|\mathbf{X}, \Theta)$ and let $q(\mathbf{Z})$ be some distribution over $\mathbf{Z}$
- Assume discrete $\mathbf{Z}$, the identity below holds for any choice of the distribution $q(\mathbf{Z})$

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

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

(Exercise: Verify the above identity)




- Since $\mathrm{KL}(q||p_z) \geq 0$, $\mathcal{L}(q, \Theta)$ 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 $\log p(\mathbf{X}|\Theta)$

# Maximising $\mathcal{L}$

- First recall the identity we had: $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \mathrm{KL}(q||p_z)$ with

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

- Maximize $\mathcal{L}$ w.r.t. $q$ with $\Theta$ fixed at $\Theta^{old}$: Since $\log p(\mathbf{X}|\Theta)$ will be a constant in this case,

$$\hat{q} = \arg\max_{q} \mathcal{L}(q, \Theta^{old}) = \arg\min_{q} \mathrm{KL}(q||p_z) = p_z = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$$

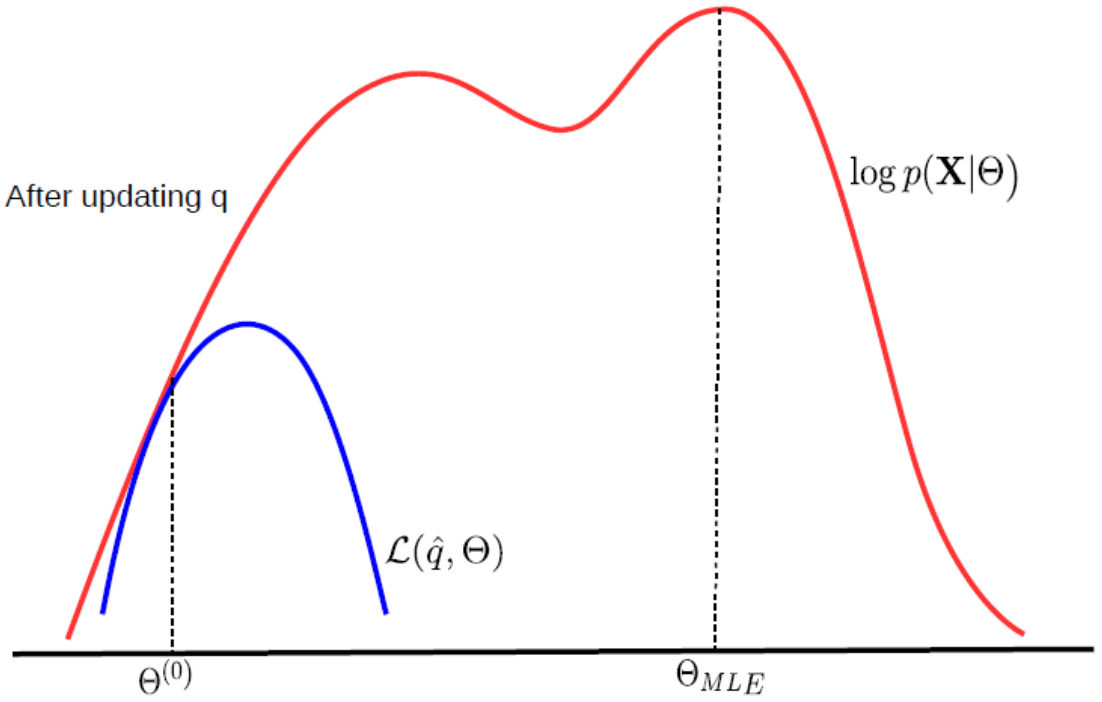
- Maximize $\mathcal{L}$ w.r.t. $\Theta$ with $q$ fixed at $\hat{q} = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$

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

.. therefore, $\boxed{\Theta^{new} = \arg\max_{\theta} \mathcal{Q}(\Theta, \Theta^{old})}$ where $\mathcal{Q}(\Theta, \Theta^{old}) = \mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \Theta^{old})}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$

# Visualization

- 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 $\Theta^{old}$
- Step 2: We maximize $\mathcal{L}(\hat{q}, \Theta)$ w.r.t. $\Theta$ (equivalent to maximizing $\mathcal{Q}(\Theta, \Theta^{old})$)



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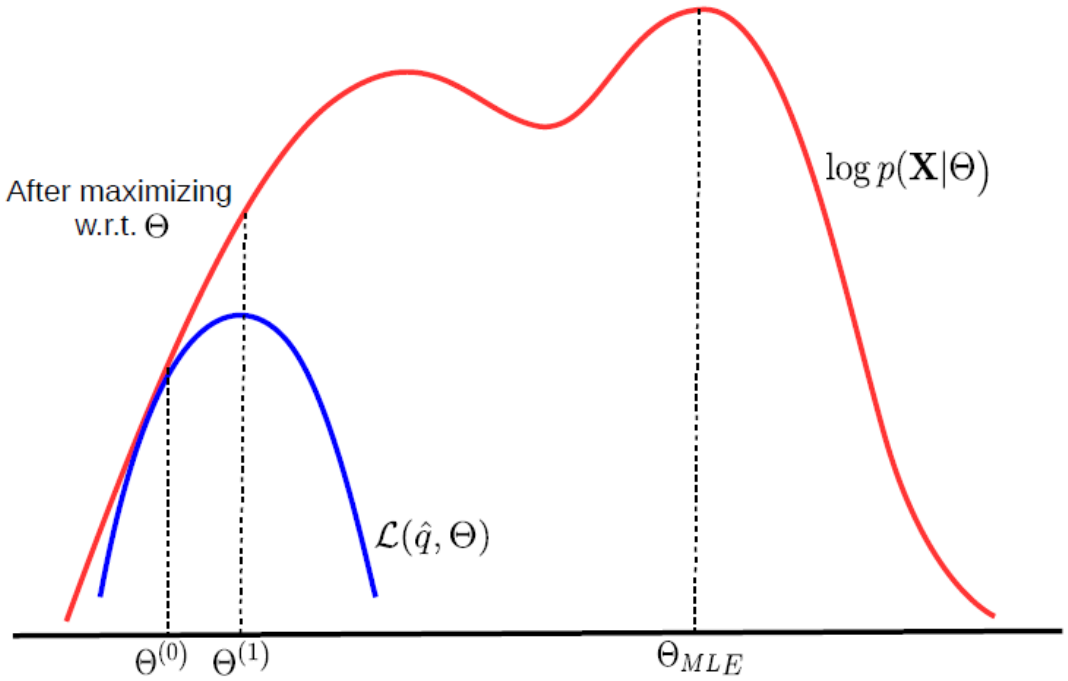

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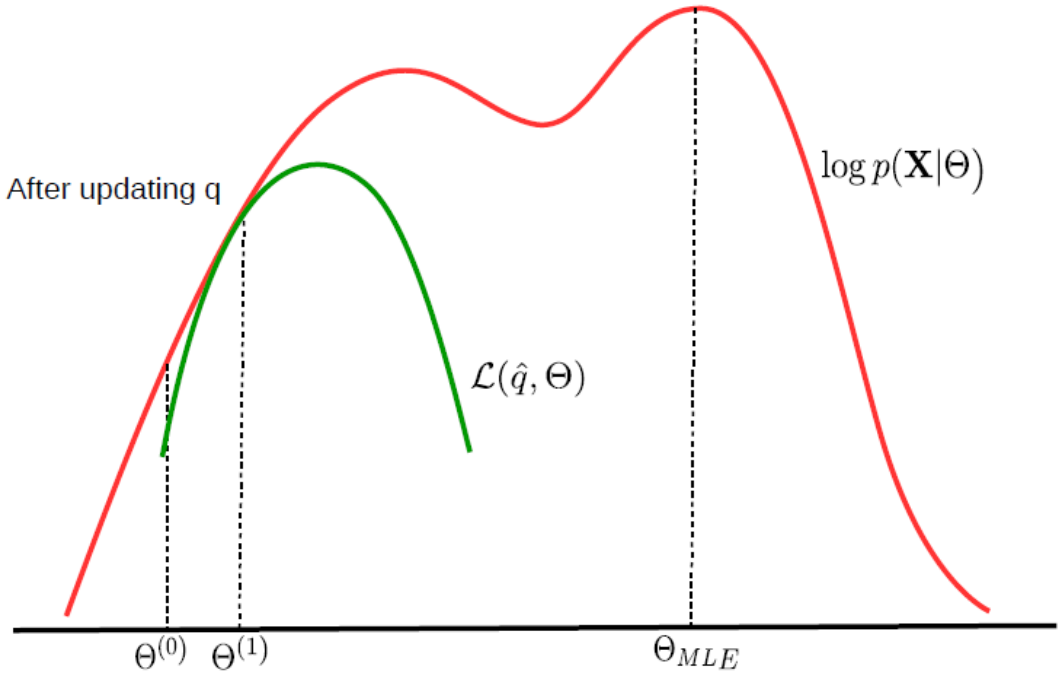

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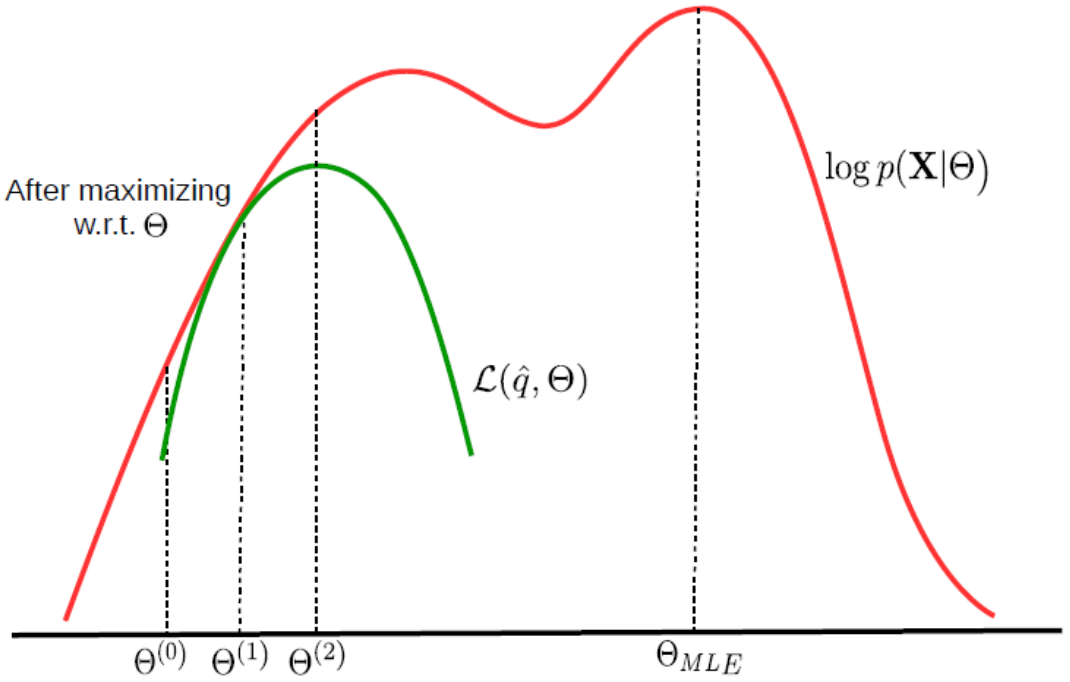

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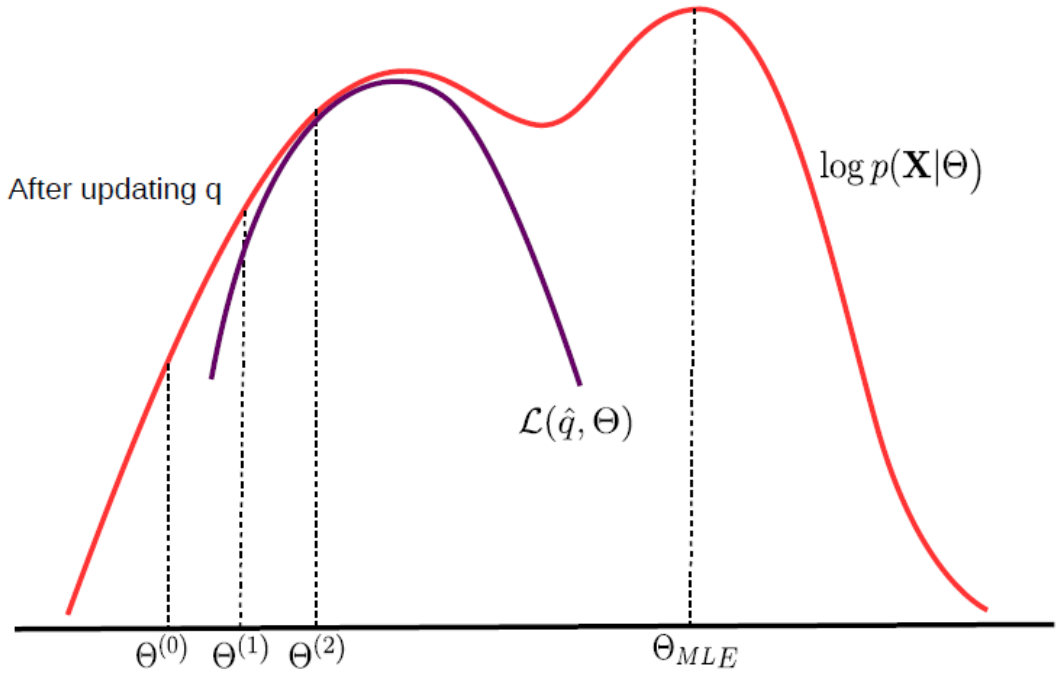

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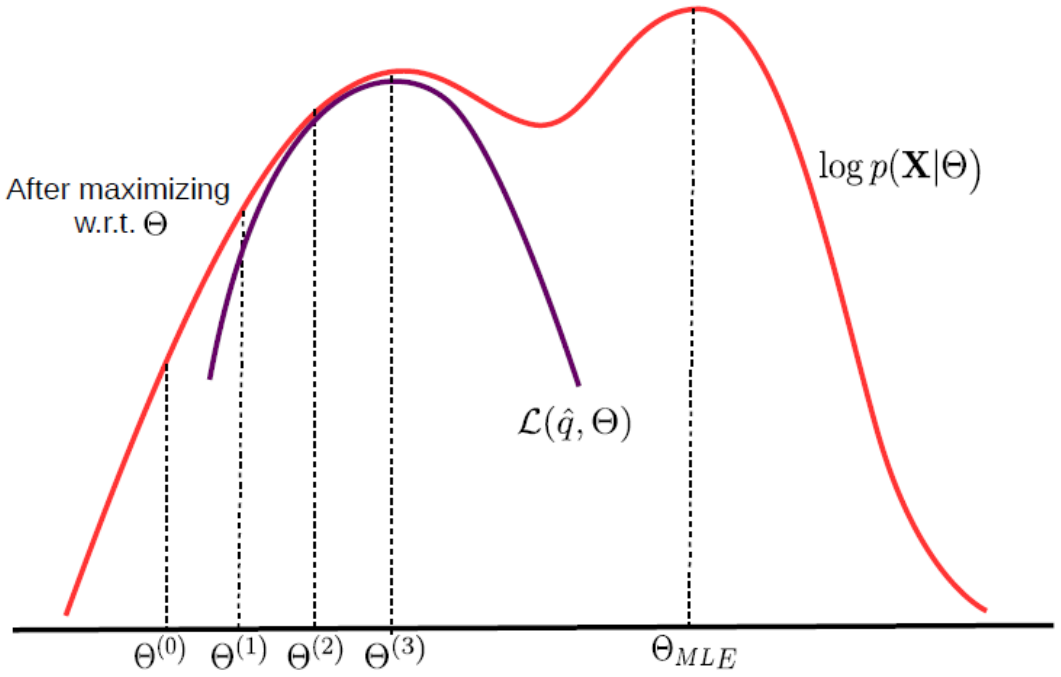
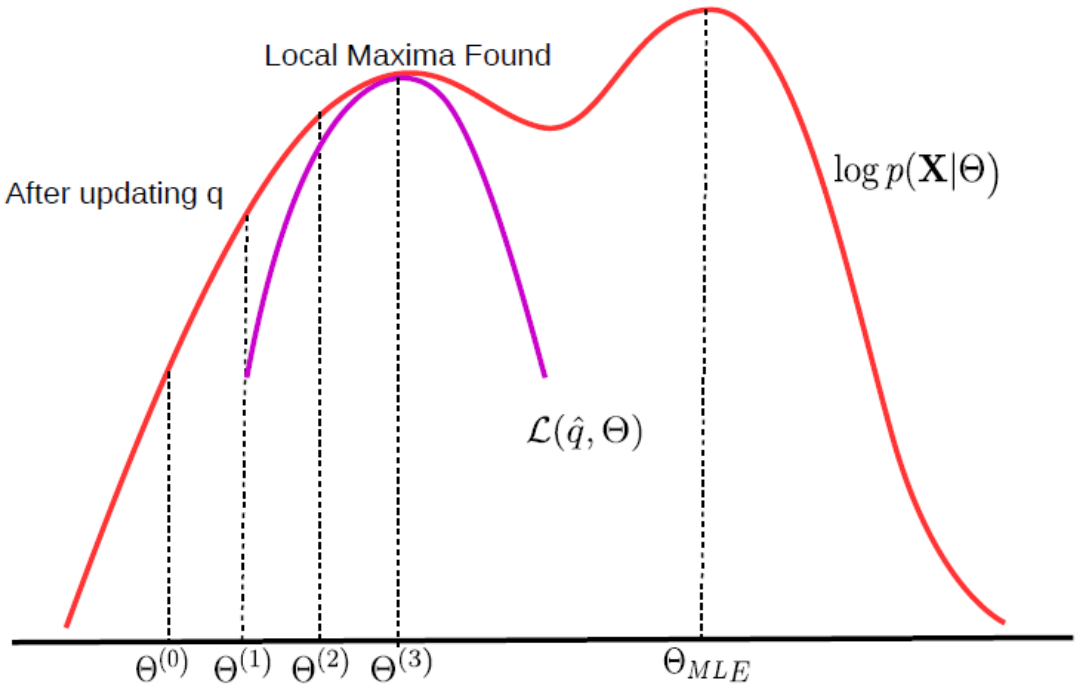


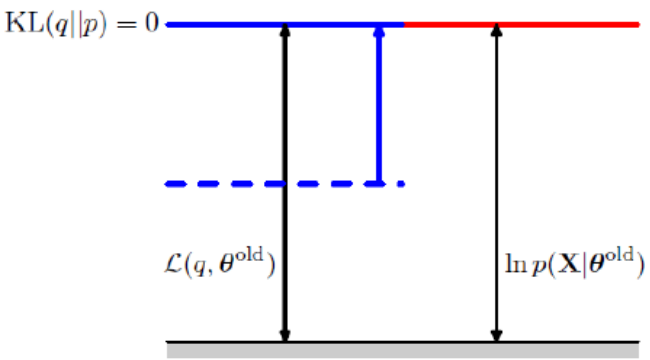
# Visualization

- 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 $\Theta^{old}$
- Step 2: We maximize $\mathcal{L}(\hat{q}, \Theta)$ w.r.t. $\Theta$ (equivalent to maximizing $\mathcal{Q}(\Theta, \Theta^{old})$)

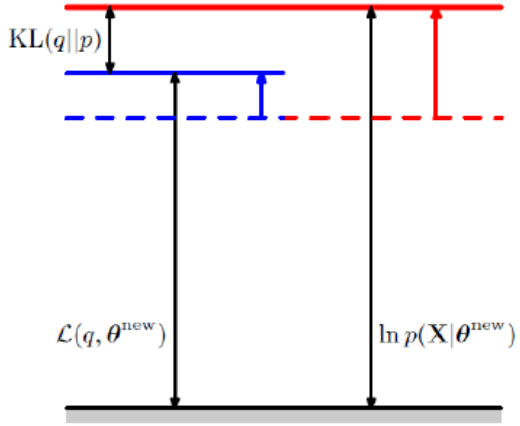


# Monotonicity

- 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 $\Theta$ given this $q$




(Step 1)




(Step 2)

- Step 1 keeps $\Theta$ 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 $\Theta$. Thus $p(\mathbf{X}|\Theta)$ can't decrease!

# The EM Algorithm

Initialize the parameters: $\Theta^{old}$. Then alternate between these steps:

- **E (Expectation) step:**
  - Compute the posterior distribution $p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$ over latent variables $\mathbf{Z}$ using $\Theta^{old}$
  - Compute the expected complete data log-likelihood w.r.t. *this* posterior distribution

$$\begin{aligned} \mathcal{Q}(\Theta, \Theta^{old}) &= \mathbb{E}_{p(\mathbf{Z}|\mathbf{X},\Theta^{old})}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)] = \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\Theta^{old})}[\log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta)] \\ &= \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\Theta^{old})}[\log p(\boldsymbol{x}_n|\boldsymbol{z}_n, \Theta) + \log p(\boldsymbol{z}_n|\Theta)] \end{aligned}$$

- **M (Maximization) step:**
  - Maximize the expected complete data log-likelihood w.r.t. $\Theta$

$$\Theta^{new} = \arg\max_{\Theta} \mathcal{Q}(\Theta, \Theta^{old})$$

Continue till log-likelihood does not converge!

# Pseudocode

## The EM Algorithm

- Initialize $\Theta$ as $\Theta^{(0)}$, set $t = 1$
- Step 1: Compute conditional posterior of latent vars given current params $\Theta^{(t-1)}$

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

- Step 2: Now maximize the expected complete data log-likelihood w.r.t. $\Theta$

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

- If not yet converged, set $t = t + 1$ and go to Step 1.

# Applications of EM

- Mixture of (multivariate) Gaussians/Bernoullis,multinoullis, Mixture of experts models
- Problems with missing labels/features (treat these as latent variables)
- Note that EM not only gives estimates of the parameters $\Theta$ but also infers latent variables $\mathbf{Z}$
- Hyperparameter estimation in probabilistic models (an alternative to MLE-II)
  - We've already seen MLE-II where we did MLE on marginal likelihood, e.g., for linear regression

$$p(\boldsymbol{y}|\mathbf{X}, \lambda, \beta) = \int p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}, \beta) p(\boldsymbol{w}|\lambda) d\boldsymbol{w}$$

  - As an alternative, can treat $\boldsymbol{w}$ as a latent variable and $\beta, \lambda$ as parameters and use EM to learn these