Expectation Maximization (EM) Algorithm and Generative Models for Dim. Red.

Piyush Rai

Machine Learning (CS771A)

Sept 28, 2016

Recap: GMM

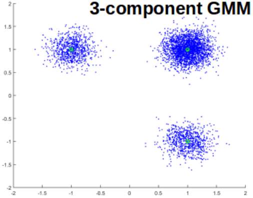
- The generative story for each $\boldsymbol{x}_n$, $n = 1, 2, \ldots, N$
  - First choose one of the K mixture components as

$$\boldsymbol{z}_n \sim \text{Multinomial}(\boldsymbol{z}_n|\pi) \qquad \text{(from the prior } p(\boldsymbol{z}) \text{ over } \boldsymbol{z}\text{)}$$

  - Suppose $\boldsymbol{z}_n = k$. Now generate $\boldsymbol{x}_n$ from the k-th Gaussian as

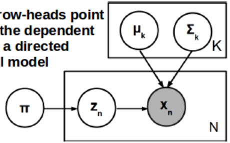
$$\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \text{(from the data distr. } p(\boldsymbol{x}|\boldsymbol{z})\text{)}$$

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

Recap: Learning GMM

- Initialize the parameters $\Theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ randomly, or using K-means

Recap: Learning GMM

- Initialize the parameters $\Theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ randomly, or using K-means
- Iterate until convergence (e.g., when $\log p(\boldsymbol{x}|\Theta)$ ceases to increase)

Recap: Learning GMM

- Initialize the parameters $\Theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ randomly, or using K-means
- Iterate until convergence (e.g., when $\log p(\boldsymbol{x}|\Theta)$ ceases to increase)
  - Given Θ, compute each expectation z_{nk} (post. prob. of $z_{nk} = 1$), $\forall n, k$

$$\gamma_{nk} = \mathbb{E}[z_{nk}] \propto \pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \text{(and re-normalize s.t. } \sum_{k=1}^K \gamma_{nk} = 1\text{)}$$

Recap: Learning GMM

- Initialize the parameters $\Theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ randomly, or using K-means
- Iterate until convergence (e.g., when $\log p(\boldsymbol{x}|\Theta)$ ceases to increase)
  - Given Θ, compute each expectation z_{nk} (post. prob. of $z_{nk} = 1$), $\forall n, k$

$$\gamma_{nk} = \mathbb{E}[z_{nk}] \propto \pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \text{(and re-normalize s.t. } \sum_{k=1}^K \gamma_{nk} = 1\text{)}$$

  - Given $\gamma_{nk} = \mathbb{E}[z_{nk}]$, and $N_k = \sum_{n=1}^N \gamma_{nk}$, update Θ as

$$\begin{aligned}
\boldsymbol{\mu}_k &= \frac{1}{N_k}\sum_{n=1}^N \gamma_{nk}\boldsymbol{x}_n \\
\boldsymbol{\Sigma}_k &= \frac{1}{N_k}\sum_{n=1}^N \gamma_{nk}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \\
\pi_k &= \frac{N_k}{N}
\end{aligned}$$

Recap: Learning GMM

- Initialize the parameters $\Theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ randomly, or using K-means
- Iterate until convergence (e.g., when $\log p(\boldsymbol{x}|\Theta)$ ceases to increase)
  - Given Θ, compute each expectation z_{nk} (post. prob. of $z_{nk} = 1$), $\forall n, k$

$$\gamma_{nk} = \mathbb{E}[z_{nk}] \propto \pi_k \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \text{(and re-normalize s.t. } \sum_{k=1}^K \gamma_{nk} = 1\text{)}$$

  - Given $\gamma_{nk} = \mathbb{E}[z_{nk}]$, and $N_k = \sum_{n=1}^N \gamma_{nk}$, update Θ as

$$\begin{aligned}
\boldsymbol{\mu}_k &= \frac{1}{N_k} \sum_{n=1}^N \gamma_{nk} \boldsymbol{x}_n \\
\boldsymbol{\Sigma}_k &= \frac{1}{N_k} \sum_{n=1}^N \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top \\
\pi_k &= \frac{N_k}{N}
\end{aligned}$$

(This algorithm is an instance of the more general Expectation Maximization (EM) algorithm which we will look at today)

Expectation Maximization (EM)

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ
- Goal: Estimate the model parameters Θ via MLE (or MAP)

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ
- Goal: Estimate the model parameters Θ via MLE (or MAP)

$$\hat{\Theta} = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta) \quad = \quad \arg\max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \qquad \text{(when } \mathbf{Z} \text{ is discrete)}$$

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X},\mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n,\boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ
- Goal: Estimate the model parameters Θ via MLE (or MAP)

$$\begin{aligned}\hat{\Theta} = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta) &= \arg\max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) \quad \text{(when } \mathbf{Z} \text{ is discrete)} \\ &= \arg\max_{\Theta} \log \int_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) d\mathbf{Z} \quad \text{(when } \mathbf{Z} \text{ is continuous)}\end{aligned}$$

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ
- Goal: Estimate the model parameters Θ via MLE (or MAP)

$$\hat{\Theta} = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta) = \arg\max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \quad \text{(when } \mathbf{Z} \text{ is discrete)}$$

$$= \arg\max_{\Theta} \log \int_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) d\mathbf{Z} \quad \text{(when } \mathbf{Z} \text{ is continuous)}$$

- Doing MLE in such models can be difficult because of the log-sum/integral

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ
- Goal: Estimate the model parameters Θ via MLE (or MAP)

$$
\begin{aligned}
\hat{\Theta} = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta) &= \arg\max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \quad \text{(when } \mathbf{Z} \text{ is discrete)} \\
&= \arg\max_{\Theta} \log \int_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) d\mathbf{Z} \quad \text{(when } \mathbf{Z} \text{ is continuous)}
\end{aligned}
$$

- Doing MLE in such models can be difficult because of the log-sum/integral
  - In general, can't do usual MLE/MAP to get closed form solution for Θ

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ
- Goal: Estimate the model parameters Θ via MLE (or MAP)

$$\begin{aligned}\hat{\Theta} = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta) &= \arg\max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \quad \text{(when } \mathbf{Z} \text{ is discrete)} \\ &= \arg\max_{\Theta} \log \int_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) d\mathbf{Z} \quad \text{(when } \mathbf{Z} \text{ is continuous)}\end{aligned}$$

- Doing MLE in such models can be difficult because of the log-sum/integral
  - In general, can't do usual MLE/MAP to get closed form solution for Θ
  - A reason: Even if $p(\mathbf{X}, \mathbf{Z}|\Theta)$ is in exponential family, $p(\mathbf{X}|\Theta)$ in general isn't

Parameter Estimation with Latent Variables

- Consider a generative model with joint distr. $p(\mathbf{X}, \mathbf{Z}|\Theta) = \prod_{n=1}^{N} p(\boldsymbol{x}_n, \boldsymbol{z}_n)$
  - Observed data: $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
  - Latent variables: $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^{N}$. All the model parameters: Θ
- Goal: Estimate the model parameters Θ via MLE (or MAP)

$$\hat{\Theta} = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta) = \arg\max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \quad \text{(when } \mathbf{Z} \text{ is discrete)}$$

$$= \arg\max_{\Theta} \log \int_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) d\mathbf{Z} \quad \text{(when } \mathbf{Z} \text{ is continuous)}$$

- Doing MLE in such models can be difficult because of the log-sum/integral
  - In general, can't do usual MLE/MAP to get closed form solution for Θ
  - A reason: Even if $p(\mathbf{X}, \mathbf{Z}|\Theta)$ is in exponential family, $p(\mathbf{X}|\Theta)$ in general isn't
  - Note: Exp. famil dist. are easy to work with when doing MLE/MAP on them (note that $\log \exp()$ would give simple expressions; easy to work with)

Exponential Family

- An exponential family distribution is defined as

$$p(x;\theta) = h(x)e^{\eta(\theta)T(x)-A(\theta)}$$

- θ is called the parameter of the family
- $h(x)$, $\eta(\theta)$, $T(x)$, and $A(\theta)$ are known functions
- $p(.)$ depends on x only through $T(x)$
- $T(x)$ is called the **sufficient statistics**: summarizes the entire $p(x;\theta)$
- Exponential family is the only family for which **conjugate priors** exist (often also in the exponential family)
- Many other nice properties (especially useful in Bayesian inference)

Many well-known distribution (Bernoulli, Binomial, categorical, beta, gamma, Gaussian, etc.) are exponential family distributions

https://en.wikipedia.org/wiki/Exponential_family

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
  - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
  - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random
  - Assume that MLE of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is easy to solve (e.g., will be the case if $p(\mathbf{Z})$ and $p(\mathbf{X}|\mathbf{Z})$ are in exponential family) than solving MLE of $\log p(\mathbf{X}|\Theta)$

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
  - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random
  - Assume that MLE of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is easy to solve (e.g., will be the case if $p(\mathbf{Z})$ and $p(\mathbf{X}|\mathbf{Z})$ are in exponential family) than solving MLE of $\log p(\mathbf{X}|\Theta)$
- **Two questions** to consider here:
  - How do we come up with our "guess" of $\mathbf{Z}$?

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
    - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random
    - Assume that MLE of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is easy to solve (e.g., will be the case if $p(\mathbf{Z})$ and $p(\mathbf{X}|\mathbf{Z})$ are in exponential family) than solving MLE of $\log p(\mathbf{X}|\Theta)$
- **Two questions** to consider here:
    - How do we come up with our "guess" of $\mathbf{Z}$?
    - Is MLE on $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ equivalent to MLE on $\log p(\mathbf{X}|\Theta)$?

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
  - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random
  - Assume that MLE of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is easy to solve (e.g., will be the case if $p(\mathbf{Z})$ and $p(\mathbf{X}|\mathbf{Z})$ are in exponential family) than solving MLE of $\log p(\mathbf{X}|\Theta)$
- **Two questions** to consider here:
  - How do we come up with our "guess" of $\mathbf{Z}$?
    - Given current estimate of $\Theta = \Theta^{old}$, guess $\mathbf{Z}$ using the posterior dist. of $\mathbf{Z}$

$$p(\mathbf{Z}|\Theta^{old}, \mathbf{X}) \propto p(\mathbf{Z})p(\mathbf{X}|\mathbf{Z}) \qquad \text{(but why this dist.? we will see shortly)}$$

  - Is MLE on $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ equivalent to MLE on $\log p(\mathbf{X}|\Theta)$?

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
  - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random
  - Assume that MLE of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is easy to solve (e.g., will be the case if $p(\mathbf{Z})$ and $p(\mathbf{X}|\mathbf{Z})$ are in exponential family) than solving MLE of $\log p(\mathbf{X}|\Theta)$
- **Two questions** to consider here:
  - How do we come up with our "guess" of $\mathbf{Z}$?
    - Given current estimate of $\Theta = \Theta^{old}$, guess $\mathbf{Z}$ using the posterior dist. of $\mathbf{Z}$

$$p(\mathbf{Z}|\Theta^{old}, \mathbf{X}) \propto p(\mathbf{Z})p(\mathbf{X}|\mathbf{Z}) \qquad \text{(but why this dist.? we will see shortly)}$$

  - Is MLE on $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ equivalent to MLE on $\log p(\mathbf{X}|\Theta)$?

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
  - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random
  - Assume that MLE of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is easy to solve (e.g., will be the case if $p(\mathbf{Z})$ and $p(\mathbf{X}|\mathbf{Z})$ are in exponential family) than solving MLE of $\log p(\mathbf{X}|\Theta)$
- **Two questions** to consider here:
  - How do we come up with our "guess" of $\mathbf{Z}$?
    - Given current estimate of $\Theta = \Theta^{old}$, guess $\mathbf{Z}$ using the posterior dist. of $\mathbf{Z}$

$$p(\mathbf{Z}|\Theta^{old}, \mathbf{X}) \propto p(\mathbf{Z})p(\mathbf{X}|\mathbf{Z}) \qquad \text{(but why this dist.? we will see shortly)}$$

  - Is MLE on $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ equivalent to MLE on $\log p(\mathbf{X}|\Theta)$?
    - (We will see that) $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is a tight lower-bound on $\log p(\mathbf{X}|\Theta)$

Parameter Estimation with Latent Variables

- Assume $\mathbf{Z}$ is known to us (somehow)
- Now do MLE on the joint p.d.f. $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$ instead of $\log p(\mathbf{X}|\Theta)$
  - .. actually MLE on the expected $\log p(\mathbf{X}, \mathbf{Z}|\Theta)$, since $\mathbf{Z}$ is random
  - Assume that MLE of $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is easy to solve (e.g., will be the case if $p(\mathbf{Z})$ and $p(\mathbf{X}|\mathbf{Z})$ are in exponential family) than solving MLE of $\log p(\mathbf{X}|\Theta)$
- **Two questions** to consider here:
  - How do we come up with our "guess" of $\mathbf{Z}$?
    - Given current estimate of $\Theta = \Theta^{old}$, guess $\mathbf{Z}$ using the posterior dist. of $\mathbf{Z}$

$$p(\mathbf{Z}|\Theta^{old}, \mathbf{X}) \propto p(\mathbf{Z})p(\mathbf{X}|\mathbf{Z}) \qquad \text{(but why this dist.? we will see shortly)}$$

  - Is MLE on $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ equivalent to MLE on $\log p(\mathbf{X}|\Theta)$?
    - (We will see that) $\mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)]$ is a tight lower-bound on $\log p(\mathbf{X}|\Theta)$
    - Maximizing this lower-bound iteratively will also improve $\log p(\mathbf{X}|\Theta)$

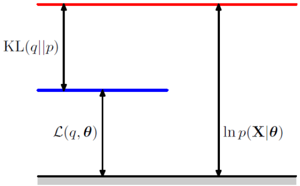
Justification

- The incomplete data log lik. can be written as a sum of two terms

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

where q is some distr. on $\mathbf{Z}$, $p_z = p(\mathbf{Z}|\mathbf{X},\Theta)$ is the posterior over $\mathbf{Z}$, and

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



(to verify, use $\log p(\mathbf{X},\mathbf{Z}|\Theta) = \log p(\mathbf{Z}|\mathbf{X},\Theta) + \log p(\mathbf{X}|\Theta)$ in the expression of $\mathcal{L}(q,\Theta)$)

Picture courtesy: PRML (Bishop, 2006)

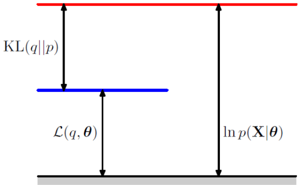
Justification

- The incomplete data log lik. can be written as a sum of two terms

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

where q is some distr. on $\mathbf{Z}$, $p_z = p(\mathbf{Z}|\mathbf{X},\Theta)$ is the posterior over $\mathbf{Z}$, and

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



(to verify, use $\log p(\mathbf{X},\mathbf{Z}|\Theta) = \log p(\mathbf{Z}|\mathbf{X},\Theta) + \log p(\mathbf{X}|\Theta)$ in the expression of $\mathcal{L}(q,\Theta)$)

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

Picture courtesy: PRML (Bishop, 2006)

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \mathrm{KL}(q||p_z)$. Consider the following scheme:

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \text{KL}(q||p_z)$. Consider the following scheme:

- With Θ fixed to Θ^{old}, maximize the "functional" $\mathcal{L}(q, \Theta^{old})$ w.r.t. q

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

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \text{KL}(q||p_z)$. Consider the following scheme:

- With Θ fixed to Θ^{old}, maximize the "functional" $\mathcal{L}(q, \Theta^{old})$ w.r.t. q

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

  which is equivalent to making $\text{KL}(q||p_z) = 0$ or setting $\hat{q} = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \mathrm{KL}(q||p_z)$. Consider the following scheme:

- With Θ fixed to Θ^{old}, maximize the "functional" $\mathcal{L}(q, \Theta^{old})$ w.r.t. q

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

  which is equivalent to making $\mathrm{KL}(q||p_z) = 0$ or setting $\hat{q} = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$

  (This step makes $\mathcal{L}(\hat{q}, \Theta^{old}) = \log p(\mathbf{X}|\Theta^{old})$; see next slide)

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \text{KL}(q||p_z)$. Consider the following scheme:

- With Θ fixed to Θ^{old}, maximize the "functional" $\mathcal{L}(q, \Theta^{old})$ w.r.t. q

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

  which is equivalent to making $\text{KL}(q||p_z) = 0$ or setting $\hat{q} = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$

  (This step makes $\mathcal{L}(\hat{q}, \Theta^{old}) = \log p(\mathbf{X}|\Theta^{old})$; see next slide)

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

$$\mathcal{L}(\hat{q}, \Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \log p(\mathbf{X}, \mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \log p(\mathbf{Z}|\mathbf{X}, \Theta^{old})}_{\text{constant w.r.t. } \Theta}$$

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q,\Theta) + \text{KL}(q||p_z)$. Consider the following scheme:

- With Θ fixed to Θ^{old}, maximize the "functional" $\mathcal{L}(q,\Theta^{old})$ w.r.t. q

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

  which is equivalent to making $\text{KL}(q||p_z) = 0$ or setting $\hat{q} = p(\mathbf{Z}|\mathbf{X},\Theta^{old})$

  (This step makes $\mathcal{L}(\hat{q},\Theta^{old}) = \log p(\mathbf{X}|\Theta^{old})$; see next slide)

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

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

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q,\Theta) + \text{KL}(q||p_z)$. Consider the following scheme:

- With Θ fixed to Θ^{old}, maximize the "functional" $\mathcal{L}(q,\Theta^{old})$ w.r.t. q

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

  which is equivalent to making $\text{KL}(q||p_z) = 0$ or setting $\hat{q} = p(\mathbf{Z}|\mathbf{X},\Theta^{old})$

  (This step makes $\mathcal{L}(\hat{q},\Theta^{old}) = \log p(\mathbf{X}|\Theta^{old})$; see next slide)

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

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

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

Justification (contd.)

Recall $\log p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + \text{KL}(q||p_z)$. Consider the following scheme:

- With Θ fixed to Θ^{old}, maximize the "functional" $\mathcal{L}(q, \Theta^{old})$ w.r.t. q

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

  which is equivalent to making $\text{KL}(q||p_z) = 0$ or setting $\hat{q} = p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$

  (This step makes $\mathcal{L}(\hat{q}, \Theta^{old}) = \log p(\mathbf{X}|\Theta^{old})$; see next slide)

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

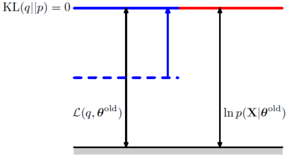
$$\begin{aligned}
\mathcal{L}(\hat{q}, \Theta) &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \log p(\mathbf{X}, \mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \log p(\mathbf{Z}|\mathbf{X}, \Theta^{old})}_{\text{constant w.r.t. } \Theta} \\
&= \mathcal{Q}(\Theta,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

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

  (This step ensures that $\log p(\mathbf{X}|\Theta^{new}) \geq \log p(\mathbf{X}|\Theta^{old})$; see next slide)

Justification (contd.)

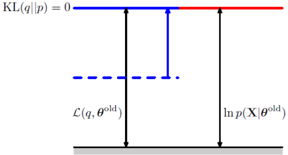
Step 1: Set $q = p(\mathbf{Z}|\mathbf{X}, \Theta)$, $\text{KL}(q||p_z)$ becomes 0, $\mathcal{L}(q, \Theta^{old})$ increases and becomes equal to $\log p(\mathbf{X}|\Theta^{old})$



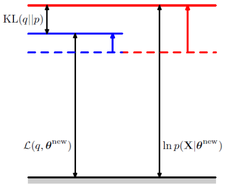
Picture courtesy: PRML (Bishop, 2006)

Justification (contd.)

Step 1: Set $q = p(\mathbf{Z}|\mathbf{X}, \Theta)$, $\text{KL}(q||p_z)$ becomes 0, $\mathcal{L}(q, \Theta^{old})$ increases and becomes equal to $\log p(\mathbf{X}|\Theta^{old})$



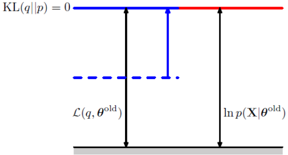
Step 2: Θ^{new} makes $\mathcal{L}(q, \Theta^{new})$ go further up, makes $\text{KL}(q||p_z) > 0$ again because $q \neq p(\mathbf{Z}|\mathbf{X}, \Theta^{new})$ and thus ensures that $\log p(\mathbf{X}|\Theta^{new}) \geq \log p(\mathbf{X}|\Theta^{old})$



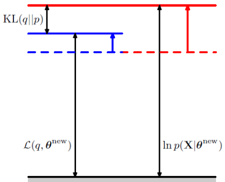
Picture courtesy: PRML (Bishop, 2006)

Justification (contd.)

Step 1: Set $q = p(\mathbf{Z}|\mathbf{X}, \Theta)$, $\text{KL}(q||p_z)$ becomes 0, $\mathcal{L}(q, \Theta^{old})$ increases and becomes equal to $\log p(\mathbf{X}|\Theta^{old})$



Step 2: Θ^{new} makes $\mathcal{L}(q, \Theta^{new})$ go further up, makes $\text{KL}(q||p_z) > 0$ again because $q \neq p(\mathbf{Z}|\mathbf{X}, \Theta^{new})$ and thus ensures that $\log p(\mathbf{X}|\Theta^{new}) \geq \log p(\mathbf{X}|\Theta^{old})$



These two steps never decrease $\log p(\mathbf{X}|\Theta)$. Thus it's a good way of doing MLE

Picture courtesy: PRML (Bishop, 2006)

An Alternate Justification

- Consider the 'incomplete" data log likelihood

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

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\log p(\mathbf{X}|\Theta) \quad = \quad \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X}, \mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)}$$

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\begin{aligned} \log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\ &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \end{aligned}$$

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\log p(\mathbf{X}|\Theta) = \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)}$$

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

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$
\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X}, \mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X}, \mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta}
\end{aligned}
$$

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$
\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}
$$

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \textstyle\sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}$$

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

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \textstyle\sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}$$

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

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

An Alternate Justification

- Consider the ‘incomplete” data log likelihood

$$\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}$$

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

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

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$
\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}
$$

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

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

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$
\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}
$$

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

$$
\begin{aligned}
\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log \frac{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}\, p(\mathbf{X}|\Theta)}{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}} = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log p(\mathbf{X}|\Theta) \\
&= \log p(\mathbf{X}|\Theta) \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta)
\end{aligned}
$$

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\log p(\mathbf{X}|\Theta) = \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)}$$

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

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

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

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

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

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$
\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}
$$

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

$$
\begin{aligned}
\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log \frac{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}\, p(\mathbf{X}|\Theta)}{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}} = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log p(\mathbf{X}|\Theta) \\
&= \log p(\mathbf{X}|\Theta) \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) = \log p(\mathbf{X}|\Theta)
\end{aligned}
$$

- Thus for $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta)$, we have

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}$$

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

$$\begin{aligned}
\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log \frac{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}\, p(\mathbf{X}|\Theta)}{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}} = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log p(\mathbf{X}|\Theta) \\
&= \log p(\mathbf{X}|\Theta) \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) = \log p(\mathbf{X}|\Theta)
\end{aligned}$$

- Thus for $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta)$, we have

$$\log p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}$$

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$
\begin{aligned}
\log p(\mathbf{X}|\Theta) &= \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(concave } f\text{, Jensen's Ineq.: } f(\textstyle\sum \lambda_i x_i) \geq \sum \lambda_i f(x_i)) \\
\log p(\mathbf{X}|\Theta) &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})}_{\text{doesn't depend on } \Theta} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.}
\end{aligned}
$$

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

$$
\begin{aligned}
\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log \frac{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}\, p(\mathbf{X}|\Theta)}{\cancel{p(\mathbf{Z}|\mathbf{X},\Theta)}} = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log p(\mathbf{X}|\Theta) \\
&= \log p(\mathbf{X}|\Theta) \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) = \log p(\mathbf{X}|\Theta)
\end{aligned}
$$

- Thus for $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta)$, we have

$$
\log p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.} = \mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\Theta)] + \text{const.}
$$

An Alternate Justification

- Consider the 'incomplete" data log likelihood

$$\log p(\mathbf{X}|\Theta) = \log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) = \log \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \quad \text{(where } q(\mathbf{Z}) \text{ is some dist.)}$$

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

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

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

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

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

- Thus for $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta)$, we have

$$\log p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta) \log p(\mathbf{X},\mathbf{Z}|\Theta) + \text{const.} = \mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\Theta)] + \text{const.}$$

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

The Expectation Maximization (EM) Algorithm

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

The Expectation Maximization (EM) Algorithm

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

- **E (Expectation) step:**

The Expectation Maximization (EM) Algorithm

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

- **E (Expectation) step:**
  - Compute the posterior $p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$ over latent variables $\mathbf{Z}$ using Θ^{old}

The Expectation Maximization (EM) Algorithm

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

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

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

The Expectation Maximization (EM) Algorithm

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

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

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

- **M (Maximization) step:**

The Expectation Maximization (EM) Algorithm

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

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

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

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

$$\begin{aligned} \Theta^{new} &= \arg\max_{\Theta} \mathcal{Q}(\Theta, \Theta^{old}) \quad \text{(if doing MLE)} \\ \Theta^{new} &= \arg\max_{\Theta} \{\mathcal{Q}(\Theta, \Theta^{old}) + \log p(\Theta)\} \quad \text{(if doing MAP)} \end{aligned}$$

The Expectation Maximization (EM) Algorithm

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

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

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

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

$$\begin{aligned} \Theta^{new} &= \arg\max_{\Theta} \mathcal{Q}(\Theta, \Theta^{old}) \quad \text{(if doing MLE)} \\ \Theta^{new} &= \arg\max_{\Theta} \{\mathcal{Q}(\Theta, \Theta^{old}) + \log p(\Theta)\} \quad \text{(if doing MAP)} \end{aligned}$$

- If the log-likelihood or the parameter values not converged then set $\Theta^{old} = \Theta^{new}$ and go to the E step.

The Expectation Maximization (EM) Algorithm

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

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

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

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

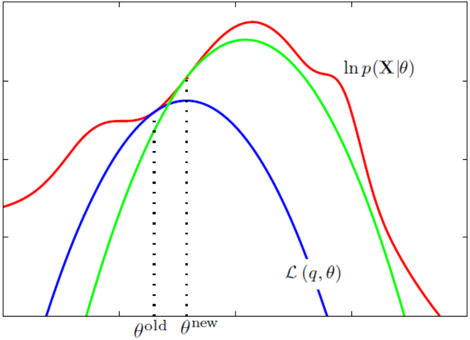
$$\begin{aligned} \Theta^{new} &= \arg\max_{\Theta} \mathcal{Q}(\Theta, \Theta^{old}) \quad \text{(if doing MLE)} \\ \Theta^{new} &= \arg\max_{\Theta} \{\mathcal{Q}(\Theta, \Theta^{old}) + \log p(\Theta)\} \quad \text{(if doing MAP)} \end{aligned}$$

- If the log-likelihood or the parameter values not converged then set $\Theta^{old} = \Theta^{new}$ and go to the E step.

The algorithm converges to a local maxima of $p(\mathbf{X}|\Theta)$ (as we saw)

EM: A View in the Parameter Space

- E-step: Update of q makes the $\mathcal{L}(q, \Theta)$ curve touch the $\log p(\mathbf{X}|\Theta)$ curve
- M-step gives the maxima Θ^{new} of $\mathcal{L}(q, \Theta)$
- Next E-step readjusts $\mathcal{L}(q, \Theta)$ curve (green) to meet $\log p(\mathbf{X}|\Theta)$ curve again
- This continues until a local maxima of $\log p(\mathbf{X}|\Theta)$ is reached



EM: Some Comments

- A general framework for parameter estimation in latent variable models

EM: Some Comments

- A general framework for parameter estimation in latent variable models
- Very widely used in problems with "missing data", e.g., missing features, or missing labels (semi-supervised learning)

EM: Some Comments

- A general framework for parameter estimation in latent variable models
- Very widely used in problems with "missing data", e.g., missing features, or missing labels (semi-supervised learning)
  - "Missing" parts can be treated as latent variables $\boldsymbol{z}$ and estimated using EM
- More advanced probabilistic inference algorithms are based on similar ideas

EM: Some Comments

- A general framework for parameter estimation in latent variable models
- Very widely used in problems with "missing data", e.g., missing features, or missing labels (semi-supervised learning)
  - "Missing" parts can be treated as latent variables $\boldsymbol{z}$ and estimated using EM
- More advanced probabilistic inference algorithms are based on similar ideas
  - E.g., variational Bayesian inference

EM: Some Comments

- A general framework for parameter estimation in latent variable models
- Very widely used in problems with "missing data", e.g., missing features, or missing labels (semi-supervised learning)
  - "Missing" parts can be treated as latent variables $\boldsymbol{z}$ and estimated using EM
- More advanced probabilistic inference algorithms are based on similar ideas
  - E.g., variational Bayesian inference
- Very easy to extend to online learning setting and gives SGD like algorithms (will post a reading on "Online EM" on the class webpage)

EM: Some Comments

- A general framework for parameter estimation in latent variable models
- Very widely used in problems with "missing data", e.g., missing features, or missing labels (semi-supervised learning)
  - "Missing" parts can be treated as latent variables $\boldsymbol{z}$ and estimated using EM
- More advanced probabilistic inference algorithms are based on similar ideas
  - E.g., variational Bayesian inference
- Very easy to extend to online learning setting and gives SGD like algorithms (will post a reading on "Online EM" on the class webpage)
- Note: The E and M steps may not always be possible to perform exactly (approximate inference methods may be needed in such cases)

Generative Models for Dimensionality Reduction

Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$

Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as

$$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$

Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as
$$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$
  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$

Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as
$$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$
  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, where $\mathbf{W}$ is a $D \times K$ matrix, $K \ll D$

Generative Model for Dimensionality Reduction

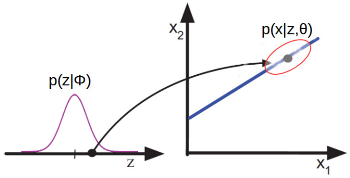
- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as
  $$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$
  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, where $\mathbf{W}$ is a $D \times K$ matrix, $K \ll D$ and Gaussian noise $\epsilon_n \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_D)$

Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as
$$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$
  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, where $\mathbf{W}$ is a $D \times K$ matrix, $K \ll D$ and Gaussian noise $\epsilon_n \sim \mathcal{N}(0, \sigma^2\mathbf{I}_D)$. Equivalent to saying
$$\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{x}|\mathbf{W}\boldsymbol{z}_n, \sigma^2\mathbf{I}_D)$$

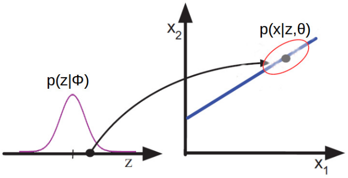
Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as
$$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$
  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, where $\mathbf{W}$ is a $D \times K$ matrix, $K \ll D$ and Gaussian noise $\epsilon_n \sim \mathcal{N}(0, \sigma^2\mathbf{I}_D)$. Equivalent to saying
$$\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{x}|\mathbf{W}\boldsymbol{z}_n, \sigma^2\mathbf{I}_D)$$



Generative Model for Dimensionality Reduction

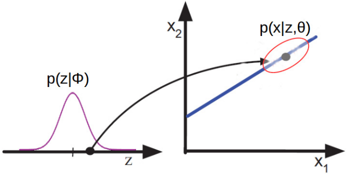
- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as
  $$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$
  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, where $\mathbf{W}$ is a $D \times K$ matrix, $K \ll D$ and Gaussian noise $\epsilon_n \sim \mathcal{N}(0, \sigma^2\mathbf{I}_D)$. Equivalent to saying
  $$\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{x}|\mathbf{W}\boldsymbol{z}_n, \sigma^2\mathbf{I}_D)$$



- This defines a probabilistic PCA (PPCA) generative model

Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as
  $$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$
  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, where $\mathbf{W}$ is a $D \times K$ matrix, $K \ll D$ and Gaussian noise $\epsilon_n \sim \mathcal{N}(0, \sigma^2\mathbf{I}_D)$. Equivalent to saying
  $$\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{x}|\mathbf{W}\boldsymbol{z}_n, \sigma^2\mathbf{I}_D)$$



- This defines a probabilistic PCA (PPCA) generative model
- When Gaussian noise has diag. instead of spherical covar: Factor Analysis

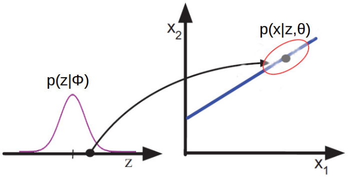
Generative Model for Dimensionality Reduction

- Assume the following generative model for each $\boldsymbol{x}_n \in \mathbb{R}^D$
  - First draw a latent variable (latent factors or latent features) $\boldsymbol{z}_n \in \mathbb{R}^K$ as

$$\boldsymbol{z}_n \sim \mathcal{N}(\boldsymbol{z}|0, \mathbf{I}_K)$$

  - Now draw $\boldsymbol{x}_n$ by transforming $\boldsymbol{z}_n$ as $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, where $\mathbf{W}$ is a $D \times K$ matrix, $K \ll D$ and Gaussian noise $\epsilon_n \sim \mathcal{N}(0, \sigma^2\mathbf{I}_D)$. Equivalent to saying

$$\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{x}|\mathbf{W}\boldsymbol{z}_n, \sigma^2\mathbf{I}_D)$$



- This defines a probabilistic PCA (PPCA) generative model
- When Gaussian noise has diag. instead of spherical covar: Factor Analysis
- Given observations $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^N$, we want to learn params $\Theta = \{\mathbf{W}, \sigma^2\}$ and latent variables $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^N$. EM gives a nice and efficient way of doing this.

Generative Model for Dimensionality Reduction

- The model for each observation $\boldsymbol{x}_n$

$$\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$$

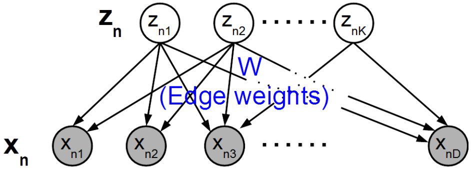
- Note: We'll assume data to be centered, otherwise $\boldsymbol{x}_n = \boldsymbol{\mu} + \mathbf{W}\boldsymbol{z}_n + \epsilon_n$

Generative Model for Dimensionality Reduction

- The model for each observation $\boldsymbol{x}_n$

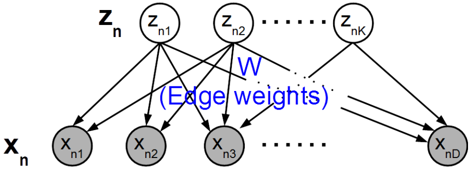
$$\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$$

- Note: We'll assume data to be centered, otherwise $\boldsymbol{x}_n = \boldsymbol{\mu} + \mathbf{W}\boldsymbol{z}_n + \epsilon_n$
- Zooming in at the relationship between each $\boldsymbol{x}_n$ and each $\boldsymbol{z}_n$



Generative Model for Dimensionality Reduction

- The model for each observation $\boldsymbol{x}_n$
$$\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$$
- Note: We'll assume data to be centered, otherwise $\boldsymbol{x}_n = \boldsymbol{\mu} + \mathbf{W}\boldsymbol{z}_n + \epsilon_n$
- Zooming in at the relationship between each $\boldsymbol{x}_n$ and each $\boldsymbol{z}_n$



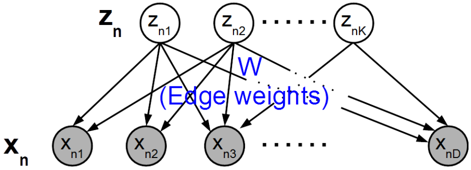
- A directed graphical model linking $\boldsymbol{z}_n$ and $\boldsymbol{x}_n$ via "edge weights" $\mathbf{W}$

Generative Model for Dimensionality Reduction

- The model for each observation $\boldsymbol{x}_n$

$$\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$$

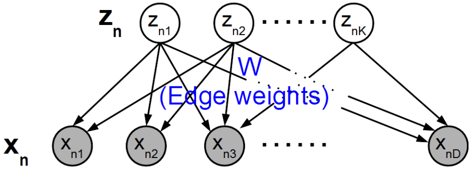
- Note: We'll assume data to be centered, otherwise $\boldsymbol{x}_n = \boldsymbol{\mu} + \mathbf{W}\boldsymbol{z}_n + \epsilon_n$
- Zooming in at the relationship between each $\boldsymbol{x}_n$ and each $\boldsymbol{z}_n$



- A directed graphical model linking $\boldsymbol{z}_n$ and $\boldsymbol{x}_n$ via "edge weights" $\mathbf{W}$
- The $D \times K$ matrix $\mathbf{W}$ is also called the factor loading matrix

Generative Model for Dimensionality Reduction

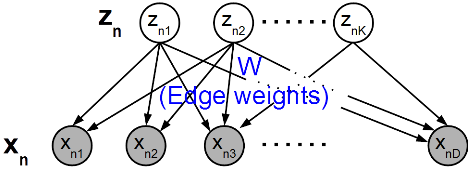
- The model for each observation $\boldsymbol{x}_n$
$$\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$$
- Note: We'll assume data to be centered, otherwise $\boldsymbol{x}_n = \boldsymbol{\mu} + \mathbf{W}\boldsymbol{z}_n + \epsilon_n$
- Zooming in at the relationship between each $\boldsymbol{x}_n$ and each $\boldsymbol{z}_n$



- A directed graphical model linking $\boldsymbol{z}_n$ and $\boldsymbol{x}_n$ via "edge weights" $\mathbf{W}$
- The $D \times K$ matrix $\mathbf{W}$ is also called the factor loading matrix
  - Can think of each column of $\mathbf{W}$ as a basis (but not mutually orthogonal)

Generative Model for Dimensionality Reduction

- The model for each observation $\boldsymbol{x}_n$
$$\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$$
- Note: We'll assume data to be centered, otherwise $\boldsymbol{x}_n = \boldsymbol{\mu} + \mathbf{W}\boldsymbol{z}_n + \epsilon_n$
- Zooming in at the relationship between each $\boldsymbol{x}_n$ and each $\boldsymbol{z}_n$



- A directed graphical model linking $\boldsymbol{z}_n$ and $\boldsymbol{x}_n$ via "edge weights" $\mathbf{W}$
- The $D \times K$ matrix $\mathbf{W}$ is also called the factor loading matrix
  - Can think of each column of $\mathbf{W}$ as a basis (but not mutually orthogonal)
  - $\mathbf{W}$ can be used to interpret the relationship of b/w the K latent features and D observed features of each observation $\boldsymbol{x}_n$

Some Nice Aspects about PPCA/FA

- Can also be seen as modeling data using a low-rank Gaussian

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

Some Nice Aspects about PPCA/FA

- Can also be seen as modeling data using a low-rank Gaussian

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

- PPCA reduces to PCA as the noise variance σ^2 tends to zero

Some Nice Aspects about PPCA/FA

- Can also be seen as modeling data using a low-rank Gaussian

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

- PPCA reduces to PCA as the noise variance σ^2 tends to zero
- Can use EM to estimate the model parameters (which can be more efficient than standard PCA based on eigen-decomposition)

Some Nice Aspects about PPCA/FA

- Can also be seen as modeling data using a low-rank Gaussian

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

- PPCA reduces to PCA as the noise variance σ^2 tends to zero
- Can use EM to estimate the model parameters (which can be more efficient than standard PCA based on eigen-decomposition)
- Gaussian assumption of $\boldsymbol{x}_n$ and $\boldsymbol{z}_n$ can be removed to model other data types

Some Nice Aspects about PPCA/FA

- Can also be seen as modeling data using a low-rank Gaussian

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

- PPCA reduces to PCA as the noise variance σ^2 tends to zero
- Can use EM to estimate the model parameters (which can be more efficient than standard PCA based on eigen-decomposition)
- Gaussian assumption of $\boldsymbol{x}_n$ and $\boldsymbol{z}_n$ can be removed to model other data types
- Can extend this basic model to dynamic settings, e.g., by changing the prior

$$p(\boldsymbol{z}_n) = \mathcal{N}(\boldsymbol{z}_n | \boldsymbol{z}_{n-1}, \mathbf{I}_K)$$

Some Nice Aspects about PPCA/FA

- Can also be seen as modeling data using a low-rank Gaussian

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

- PPCA reduces to PCA as the noise variance σ^2 tends to zero
- Can use EM to estimate the model parameters (which can be more efficient than standard PCA based on eigen-decomposition)
- Gaussian assumption of $\boldsymbol{x}_n$ and $\boldsymbol{z}_n$ can be removed to model other data types
- Can extend this basic model to dynamic settings, e.g., by changing the prior

$$p(\boldsymbol{z}_n) = \mathcal{N}(\boldsymbol{z}_n | \boldsymbol{z}_{n-1}, \mathbf{I}_K)$$

- Can model data using a mixture of PPCA or mixture of FA models

Next Class

- Talk in more detail about PPCA, Factor Analysis, and extensions
- EM algorithm for parameter estimation in these models
- Finish off the discussion of generative models and unsupervised learning and move on to "Assorted Topics"