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

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Machine Learning (CS771A)

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Recap: GMM

- The generative story for each x_n , n = 1, 2, ..., N
 - First choose one of the K mixture components as

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

• Suppose $z_n = k$. Now generate x_n from the k-th Gaussian as

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

Some simulated data from a 3-component GMM

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

White nodes: Unknowns

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

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 - 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

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

- $oldsymbol{ heta}$ 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

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 - Maximizing this lower-bound iteratively will also improve $\log p(\mathbf{X}|\Theta)$



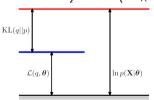
Justification

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

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

where q is some distr. on \mathbf{Z} , $p_{\mathbf{Z}} = p(\mathbf{Z}|\mathbf{X},\Theta)$ is the posterior over \mathbf{Z} , and $\mathcal{L}(q,\Theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left\{ \frac{p(\mathbf{X},\mathbf{Z}|\Theta)}{q(\mathbf{Z})} \right\}$

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



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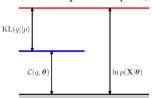
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• Since $KL(q||p_z) \ge 0$, $\mathcal{L}(q,\Theta)$ is a lower-bound on $\log p(\mathbf{X}|\Theta)$ for any q

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$$= \mathcal{O}(\Theta, \Theta^{old}) + \text{const}$$

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

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which is equivalent to making $KL(q||p_z) = 0$ 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

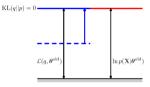
$$\mathcal{L}(\hat{q}, \Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \log p(\mathbf{X}, \mathbf{Z}|\Theta) - \underbrace{\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \log p(\mathbf{Z}|\mathbf{X}, \Theta^{old})}_{\text{constant w.r.t. }\Theta}$$

 $= \mathcal{Q}(\Theta, \Theta^{old}) + const$

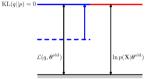
$$\Theta^{\textit{new}} = \arg\max_{\Theta} \mathcal{Q}(\Theta, \Theta^{\textit{old}}) \qquad (\text{where } \mathcal{Q}(\Theta, \Theta^{\textit{old}}) = \mathbb{E}[\log p(\mathbf{X}, \mathbf{Z}|\Theta)])$$

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

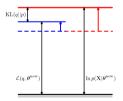
Step 1: Set $q = p(\mathbf{Z}|\mathbf{X}, \Theta)$, $\mathsf{KL}(q||p_z)$ becomes 0, $\mathcal{L}(q, \Theta^{old})$ increases and becomes equal to $\log p(\mathbf{X}|\Theta^{old})$



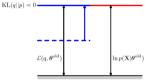
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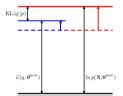
Step 2: Θ^{new} makes $\mathcal{L}(q, \Theta^{new})$ go further up, makes $\mathsf{KL}(q||p_z) > 0$ again because $q \neq p(\mathbf{Z}|\mathbf{X}, \Theta^{new})$ and thus ensures that $\log p(\mathbf{X}|\Theta^{new}) \geq \log p(\mathbf{X}|\Theta^{old})$



Step 1: Set $q = p(\mathbf{Z}|\mathbf{X}, \Theta)$, $\mathsf{KL}(q||p_z)$ 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 $\mathsf{KL}(q||p_z) > 0$ 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

Machine Learning (CS771A)

• Consider the 'incomplete" data log likelihood

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

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

• Consider the 'incomplete" data log likelihood

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

Consider the 'incomplete" data log likelihood

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

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

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

Consider the 'incomplete" data log likelihood

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

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

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

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

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

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

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

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

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

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



Consider the 'incomplete" data log likelihood

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

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

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



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

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



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

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 - 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

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

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E (Expectation) step:

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M (Maximization) step:

Maximize the expected complete data log-likelihood w.r.t. Θ

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

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E (Expectation) step:

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

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

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

M (Maximization) step:

Maximize the expected complete data log-likelihood w.r.t. Θ

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

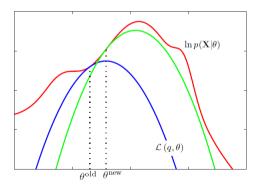
• If the log-likelihood or the parameter values not converged then set $\Theta^{old} = \Theta^{new}$ and go to the E step.

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



EM: A View in the Parameter Space

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



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EM: Some Comments

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- 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)

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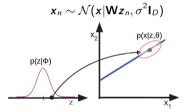
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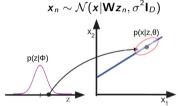
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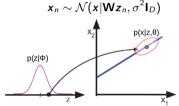


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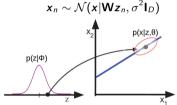


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- When Gaussian noise has diag. instead of spherical covar: Factor Analysis
- Given observations $\mathbf{X} = \{\mathbf{x}_n\}_{n=1}^N$, we want to learn params $\Theta = \{\mathbf{W}, \sigma^2\}$ and latent variables $\mathbf{Z} = \{\mathbf{z}_n\}_{n=1}^N$.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

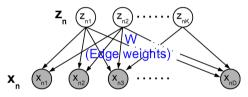
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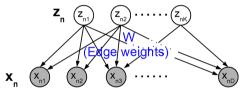
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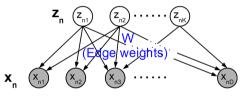
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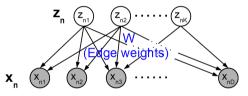
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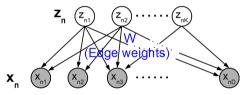
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 - W can be used to interpret the relationship of b/w the K latent features and D observed features of each observation x_n

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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"