# DSC291: Machine Learning with Few Labels

## Supervised/Unsupervised Learning

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# Recap: KL Divergence

- Kullback-Leibler (KL) divergence: measures the closeness of two distributions $p(\boldsymbol{x})$ and $q(\boldsymbol{x})$

$$\mathrm{KL}(q(\boldsymbol{x}) \,||\, p(\boldsymbol{x})) = \sum_{\boldsymbol{x}} q(\boldsymbol{x}) \log \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}$$

  - a.k.a. Relative entropy
  - KL >= 0  (Jensen's inequality)
  - Intuitively:
    - If $q$ is high and $p$ is high, then we are happy (i.e. low KL divergence)
    - If $q$ is high and $p$ is low then we pay a price (i.e. high KL divergence).
    - If $q$ is low then we don't care (i.e. also low KL divergence, regardless of $p$)
  - not a true "distance":
    - not commutative (symmetric) $\mathrm{KL(p||q)} \mathrel{!}= \mathrm{KL(q||p)}$
    - doesn't satisfy triangle inequality

# Recap: Supervised Learning

- Model to be learned $p_\theta(\boldsymbol{x})$
- Observe **full** data $\mathcal{D} = \{ \boldsymbol{x}_i \}_{i=1}^N$
  - e.g., $\boldsymbol{x}_i$ includes both input (e.g., image) and output (e.g., image label)
  - $\mathcal{D}$ defines an empirical data distribution $\tilde{p}(\boldsymbol{x})$
    - $\boldsymbol{x} \sim \mathcal{D} \quad \Leftrightarrow \quad \boldsymbol{x} \sim \tilde{p}(\boldsymbol{x})$

- Maximum Likelihood Estimation (MLE)
  - The most classical learning algorithm

$$\min_\theta - \mathbb{E}_{x\sim\tilde{p}(\boldsymbol{x})} \Big[ \quad \log p_\theta(\boldsymbol{x}) \quad \Big]$$

- **Question:** Show that MLE is minimizing the KL divergence between the empirical data distribution and the model distribution

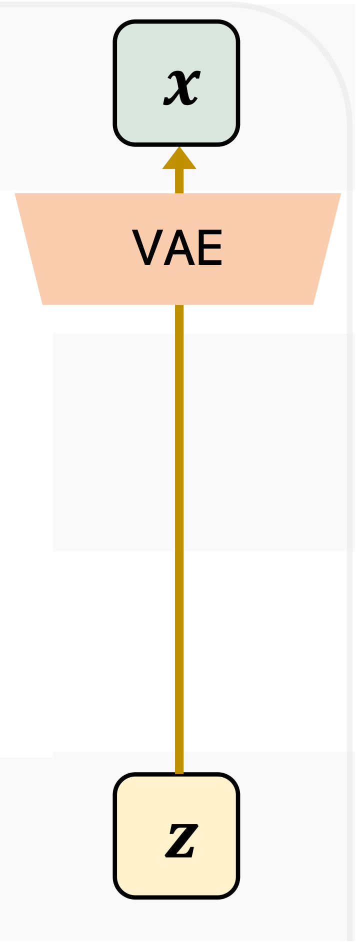
$$\mathrm{KL}(\tilde{p}(\boldsymbol{x}) \,||\, p_\theta(\boldsymbol{x})) = -\mathbb{E}_{\tilde{p}(\boldsymbol{x})}[\log p_\theta(\boldsymbol{x})] + H(\tilde{p}(\boldsymbol{x}))$$

↓

Cross entropy

# Unsupervised Learning

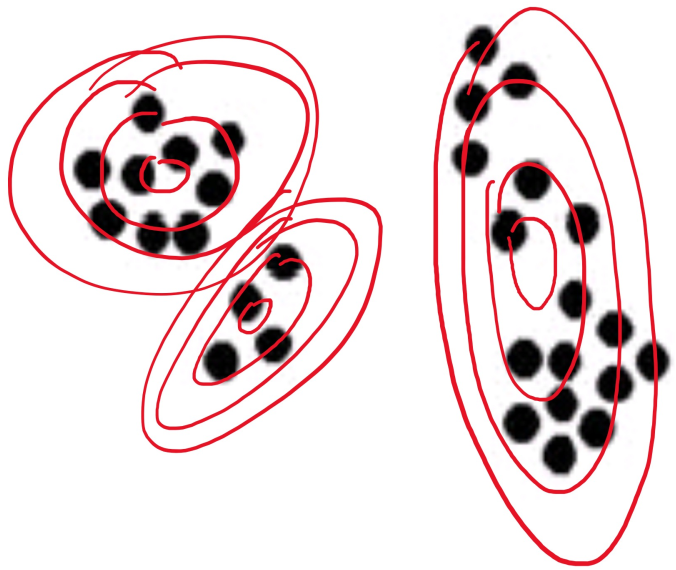
- Each data instance is partitioned into two parts:
  - observed variables $\boldsymbol{x}$
  - latent (unobserved) variables $\boldsymbol{z}$
- Want to learn a model $p_\theta(\boldsymbol{x}, \boldsymbol{z})$




[Content adapted from CMU 10-708]

# Latent (unobserved) variables

- A variable can be unobserved (latent) because:
  - imaginary quantity: meant to provide some simplified and abstractive view of the data generation process
    - e.g., speech recognition models, mixture models, …



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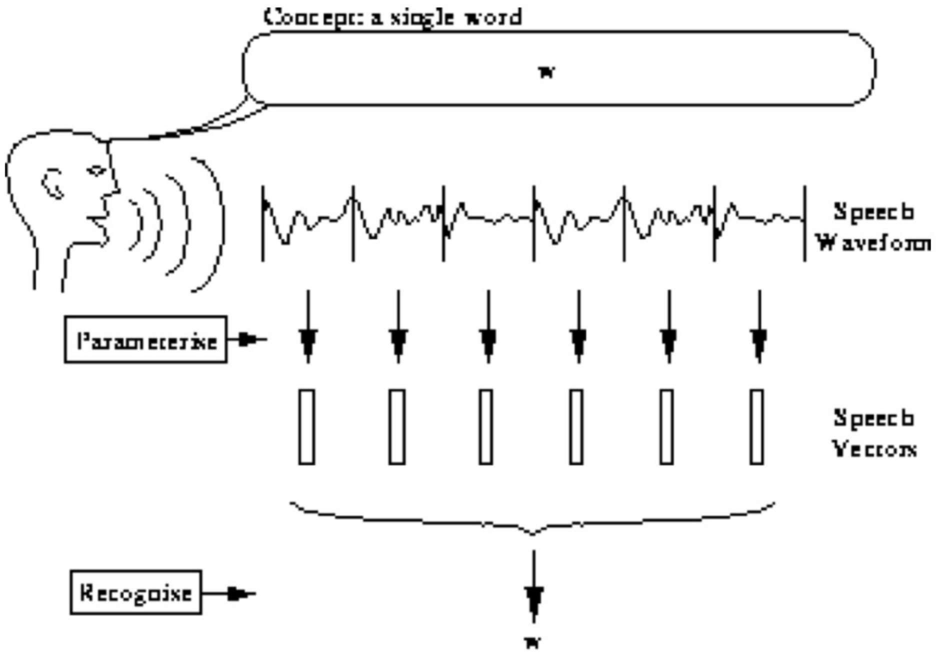
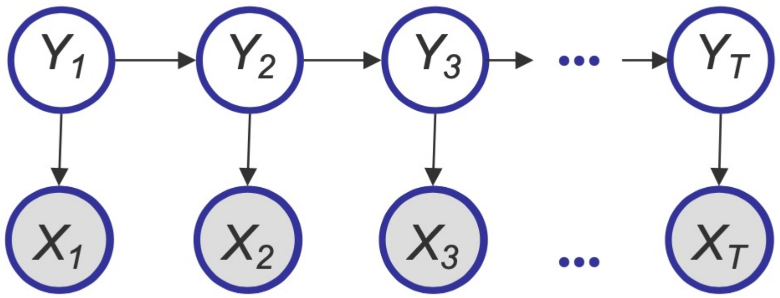



Fig. 1.2 Isolated Word Problem



# Latent (unobserved) variables

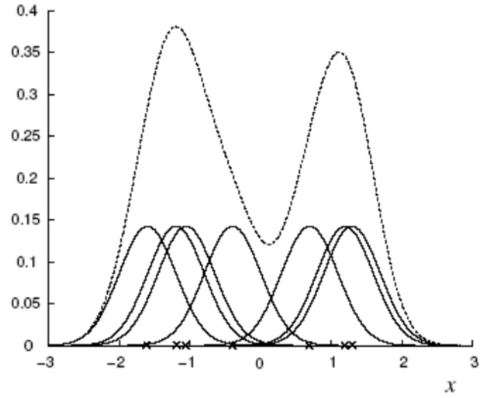
- A variable can be unobserved (latent) because:
  - imaginary quantity: meant to provide some simplified and abstractive view of the data generation process
    - e.g., speech recognition models, mixture models, …
  - a real-world object (and/or phenomena), but difficult or impossible to measure
    - e.g., the temperature of a star, causes of a disease, evolutionary ancestors …
  - a real-world object (and/or phenomena), but sometimes wasn't measured, because of faulty sensors, etc.
- Discrete latent variables can be used to partition/cluster data into sub-groups
- Continuous latent variables (factors) can be used for dimensionality reduction (e.g., factor analysis, etc.)

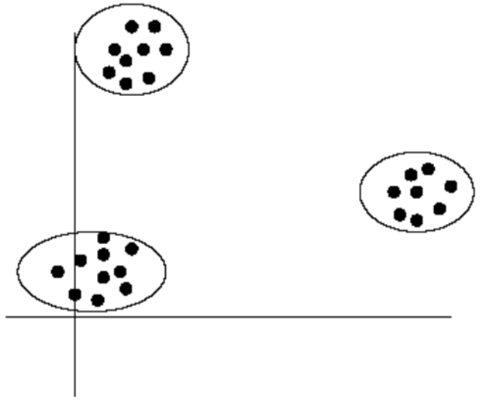
# Example: Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components:

$$p(x_n|\mu,\Sigma) = \sum_k \pi_k N(x_n|\mu_k,\Sigma_k)$$

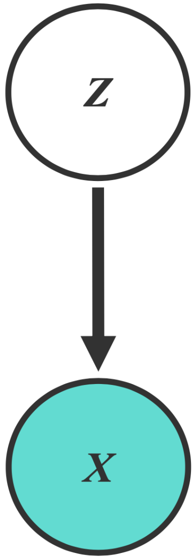
mixture proportion   mixture component

- This model can be used for unsupervised clustering.
  - This model (fit by AutoClass) has been used to discover new kinds of stars in astronomical data, etc.

# Example: Gaussian Mixture Models (GMMs)




- Consider a mixture of K Gaussian components:
  - $Z$ is a latent class indicator vector:

$$p(z_n) = \text{multi}(z_n : \pi) = \prod_k (\pi_k)^{z_n^k}$$

  - $X$ is a conditional Gaussian variable with a class-specific mean/covariance

$$p(x_n \mid z_n^k = 1, \mu, \Sigma) = N(x_n : \mu_k, \Sigma_k) \;\; = \frac{1}{(2\pi)^{m/2} |\Sigma_k|^{1/2}} \exp\left\{ -\tfrac{1}{2}(x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right\}$$

  - The likelihood of a sample:

Parameters to be learned:

mixture component

mixture proportion

$$p(x_n | \mu, \Sigma) = \sum_k p(z^k = 1 \mid \pi) p(x, \mid z^k = 1, \mu, \Sigma)$$
$$= \sum_{z_n} \prod_k \left( (\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x, \mid \mu_k, \Sigma_k)$$

# Example: Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components: $p(x_n|\mu,\Sigma) = \sum_k \pi_k N(x,|\mu_k,\Sigma_k)$
- Recall MLE for completely observed data
  - Data log-likelihood:

$$\ell(\boldsymbol{\theta};D) = \log\prod_n p(z_n,x_n) = \log\prod_n p(z_n\mid\pi)p(x_n\mid z_n,\mu,\sigma)$$

$$= \sum_n \log\prod_k \pi_k^{z_n^k} + \sum_n \log\prod_k N(x_n;\mu_k,\sigma)^{z_n^k}$$

$$= \sum_n\sum_k z_n^k \log\pi_k - \sum_n\sum_k z_n^k \tfrac{1}{2\sigma^2}(x_n - \mu_k)^2 + C$$

  - MLE:

$$\hat{\pi}_{k,MLE} = \arg\max_\pi \ell(\boldsymbol{\theta};D),$$

$$\hat{\mu}_{k,MLE} = \arg\max_\mu \ell(\boldsymbol{\theta};D) \quad\Rightarrow\quad \hat{\mu}_{k,MLE} = \frac{\sum_n z_n^k x_n}{\sum_n z_n^k}$$

$$\hat{\sigma}_{k,MLE} = \arg\max_\sigma \ell(\boldsymbol{\theta};D)$$

- What if we do not know $z_n$?

# Why is Learning Harder?

- Complete log likelihood: if both $\boldsymbol{x}$ and $\boldsymbol{z}$ can be observed, then

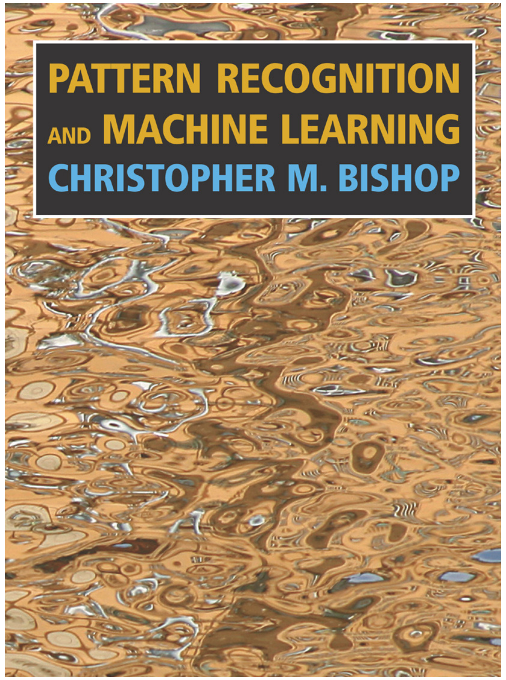
$$\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z}) = \log p(\boldsymbol{x}, \boldsymbol{z}|\theta) = \log p(\boldsymbol{z}|\theta_z) + \log p(\boldsymbol{x}|\boldsymbol{z}, \theta_x)$$

  - Decomposes into a sum of factors, the parameter for each factor can be estimated separately
- But given that $\boldsymbol{z}$ is not observed, $\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})$ is a random quantity, cannot be maximized directly
- Incomplete (or marginal) log likelihood: with $\boldsymbol{z}$ unobserved, our objective becomes the log of a marginal probability:

$$\ell(\theta; \boldsymbol{x}) = \log p(\boldsymbol{x}|\theta) = \log \sum_{z} p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

  - All parameters become coupled together
  - In other models when $\boldsymbol{z}$ is complex (continuous) variables (as we'll see later), marginalization over $\boldsymbol{z}$ is intractable.

# Expectation Maximization (EM)



# Expectation Maximization (EM)

- For any distribution $q(\boldsymbol{z}|\boldsymbol{x})$, define expected complete log likelihood:

$$\mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] = \sum_z q(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

    - A deterministic function of $\theta$
    - Inherit the factorizability of $\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})$
- Use this as the surrogate objective
- Does maximizing this surrogate yield a maximizer of the likelihood?
    - We can show that:

$$\ell(\theta; \boldsymbol{x}) \geq \mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] + H(q)$$

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- **Question**: show that $\ell(\theta;\boldsymbol{x}) \geq \mathbb{E}_q[\ell_c(\theta;\boldsymbol{x},\boldsymbol{z})] + H(q)$

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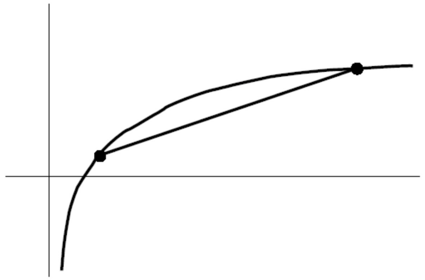
$$\begin{aligned}
\ell(\theta;x) &= \log p(x|\theta) \\
&= \log \sum_z p(x,z|\theta) \\
&= \log \sum_z q(z|x) \frac{p(x,z|\theta)}{q(z|x)} \\
&\geq \sum_z q(z|x) \log \frac{p(x,z|\theta)}{q(z|x)} \quad \text{Evidence Lower Bound (ELBO)} \\
&= \sum_z q(z|x) \log p(x,z|\theta) - \sum_z q(z|x) \log q(z|x) \\
&= \mathbb{E}_q[\ell_c(\theta;\boldsymbol{x},\boldsymbol{z})] + H(q)
\end{aligned}$$

Jensen's inequality



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$$\mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] = \sum_z q(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

- Conclusion-1:

$$\ell(\theta; \boldsymbol{x}) \geq \mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] + H(q) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] \quad \text{(ELBO)}$$

- **Question**: show that

$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

# Expectation Maximization (EM)

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  - Since KL divergence is non-negative, this is another way to prove Conclusion-1

# Lower Bound and Free Energy

- For fixed data $\boldsymbol{x}$, define a functional called the (variational) free energy:

$$F(q,\theta) = -\mathbb{E}_q[\ell_c(\theta;\boldsymbol{x},\boldsymbol{z})] - H(q) \geq -\ell(\theta;\boldsymbol{x})$$

- The EM algorithm is coordinate-decent on $F$
  - At each step $t$:
    - E-step: $q^{t+1} = \arg\min_q F\left(q, \theta^t\right)$
    - M-step: $\theta^{t+1} = \arg\min_\theta F\left(q^{t+1}, \theta^t\right)$

# E-step: minimization of $F(q, \theta)$ w.r.t $q$

- Claim:

$$q^{t+1} = \text{argmin}_q \, F(q, \theta^t) = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$$

  - This is the posterior distribution over the latent variables given the data and the current parameters.

- Proof (easy): recall

$$\ell(\theta^t; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta^t)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \text{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)\big)$$

Independent of $q$ ; $-F(q, \theta^t)$ ; $\geq 0$

  - $F(q, \theta^t)$ is minimized when $\text{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)\big) = 0$, which is achieved only when $q(\boldsymbol{z}|\boldsymbol{x}) = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$

# M-step: minimization of $F(q, \theta)$ w.r.t $\boldsymbol{\theta}$

- Note that the free energy breaks into two terms:

$$F(q,\theta) = -\mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] - H(q) \geq -\ell(\theta; \boldsymbol{x})$$

  - The first term is the expected complete log likelihood and the second term, which does not depend on q, is the entropy.
- Thus, in the M-step, maximizing with respect to $\theta$ for fixed $q$ we only need to consider the first term:

$$\theta^{t+1} = \text{argmax}_\theta \, \mathbb{E}_q[\ell_c(\theta; \boldsymbol{x}, \boldsymbol{z})] = \text{argmax}_\theta \sum_z q^{t+1}(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

  - Under optimal $q^{t+1}$, this is equivalent to solving a standard MLE of fully observed model $p(\boldsymbol{x}, \boldsymbol{z}|\theta)$, with z replaced by its expectation w.r.t $p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$

# EM Algorithm: Quick Summary

- Observed variables $\boldsymbol{x}$, latent variables $\boldsymbol{z}$
- To learn a model $p(\boldsymbol{x}, \boldsymbol{z}|\theta)$, we want to maximize the marginal log-likelihood

$$\ell(\theta; \boldsymbol{x}) = \log p(\boldsymbol{x}|\theta) = \log \sum_{z} p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

  - But it's too difficult
- EM algorithm:
  - maximize a lower bound of $\ell(\theta; \boldsymbol{x})$
  - Or equivalently, minimize an upper bound of $-\ell(\theta; \boldsymbol{x})$
- Key equation:

Evidence Lower Bound (ELBO)

$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

$$= -F(q, \theta) + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

Variational free energy

# EM Algorithm: Quick Summary

- The EM algorithm is coordinate-decent on $F(q, \theta)$
  - E-step: $q^{t+1} = \arg\min_q F\left(q, \theta^t\right) = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$
    - the posterior distribution over the latent variables given the data and the current parameters
  - M-step: $\theta^{t+1} = \arg\min_\theta F\left(q^{t+1}, \theta^t\right) = \text{argmax}_\theta \sum_z q^{t+1}(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$

$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

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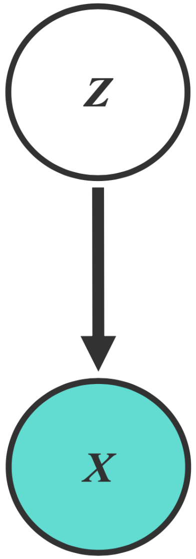


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  - $Z$ is a latent class indicator vector:

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  - The likelihood of a sample:

mixture component

mixture proportion

$$\begin{aligned} p(x_n | \mu, \Sigma) &= \sum_k p(z^k = 1 \mid \pi) p(x, \mid z^k = 1, \mu, \Sigma) \\ &= \sum_{z_n} \prod_k \left( (\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x, \mid \mu_k, \Sigma_k) \end{aligned}$$

# Example: Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components
- The expected complete log likelihood

$$\mathbb{E}_q\left[\ell_c(\boldsymbol{\theta}; x, z)\right] = \sum_n \mathbb{E}_q\left[\log p\left(z_n \mid \pi\right)\right] + \sum_n \mathbb{E}_q\left[\log p\left(x_n \mid z_n, \mu, \Sigma\right)\right]$$

$$= \sum_n \sum_k \mathbb{E}_q\left[z_n^k\right] \log \pi_k - \frac{1}{2} \sum_n \sum_k \mathbb{E}_q\left[z_n^k\right] \left(\left(x_n - \mu_k\right)^T \Sigma_k^{-1} \left(x_n - \mu_k\right) + \log\left|\Sigma_k\right| + C\right)$$

- E-step: computing the posterior of $z_n$ given the current estimate of the parameters (i.e., $\pi$ , $\mu, \Sigma$)

$$p(z_n^k = 1 \mid x, \mu^{(t)}, \Sigma^{(t)}) = \frac{\pi_k^{(t)} N(x_n, \mid \mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_i \pi_i^{(t)} N(x_n, \mid \mu_i^{(t)}, \Sigma_i^{(t)})}$$

Numerator → $p(z_n^k = 1, x, \mu^{(t)}, \Sigma^{(t)})$

Denominator → $p(x, \mu^{(t)}, \Sigma^{(t)})$

# Example: Gaussian Mixture Models (GMMs)

- E-step: computing the posterior of $z_n$ given the current estimate of the parameters (i.e., $\pi$ , $\mu, \Sigma$)

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

# Example: Gaussian Mixture Models (GMMs)

- M-step: computing the parameters given the current estimate of $z_n$
  - Once we have $q^{t+1}(z^k|x) = p(z^k|x, \theta^t) = \gamma^k$, we can compute the expected likelihood:

$$\theta^{t+1} = \text{argmax}_\theta \sum_k q^{t+1}(z^k = 1|x) \log p(x, z^k = 1|\theta)$$

$$\mathbb{E}_{q^{t+1}} [\log (p (\boldsymbol{x}, z \mid \boldsymbol{\theta}))]$$

$$= \sum_k \gamma_k \left(\log p \left(z^k = 1|\boldsymbol{\theta}\right) + \log P \left(\boldsymbol{x} \mid z^k = 1, \boldsymbol{\theta}\right)\right)$$

$$= \sum_k \gamma_k \log \pi_k + \sum_k \gamma_k \log \mathcal{N} (\boldsymbol{x}; \mu_k, \Sigma_k)$$

  - We need to fit $K$ Gaussians, just need to weight examples by $\gamma_k$

# Example: Gaussian Mixture Models (GMMs)

- M-step: computing the parameters given the current estimate of $z_n$

$$\pi_k^* = \arg\max \langle l_c(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \frac{\partial}{\partial \pi_k} \langle l_c(\boldsymbol{\theta}) \rangle = 0, \forall k, \quad \text{s.t.} \sum_k \pi_k = 1$$

$$\Rightarrow \pi_k^* = \sum_n \langle z_n^k \rangle_{q^{(t)}} \Big/ N = \sum_n \tau_n^{k(t)} \Big/ N = \langle n_k \rangle \Big/ N$$

$$\mu_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \mu_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} x_n}{\sum_n \tau_n^{k(t)}}$$

$$\Sigma_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \Sigma_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} (x_n - \mu_k^{(t+1)})(x_n - \mu_k^{(t+1)})^T}{\sum_n \tau_n^{k(t)}}$$

Fact:

$$\frac{\partial \log |\mathrm{A}^{-1}|}{\partial \mathrm{A}^{-1}} = \mathrm{A}^T$$

$$\frac{\partial \mathbf{x}^T \mathrm{A} \mathbf{x}}{\partial \mathrm{A}} = \mathbf{x}\mathbf{x}^T$$

# EM Algorithm for GMM: Quick Summary

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

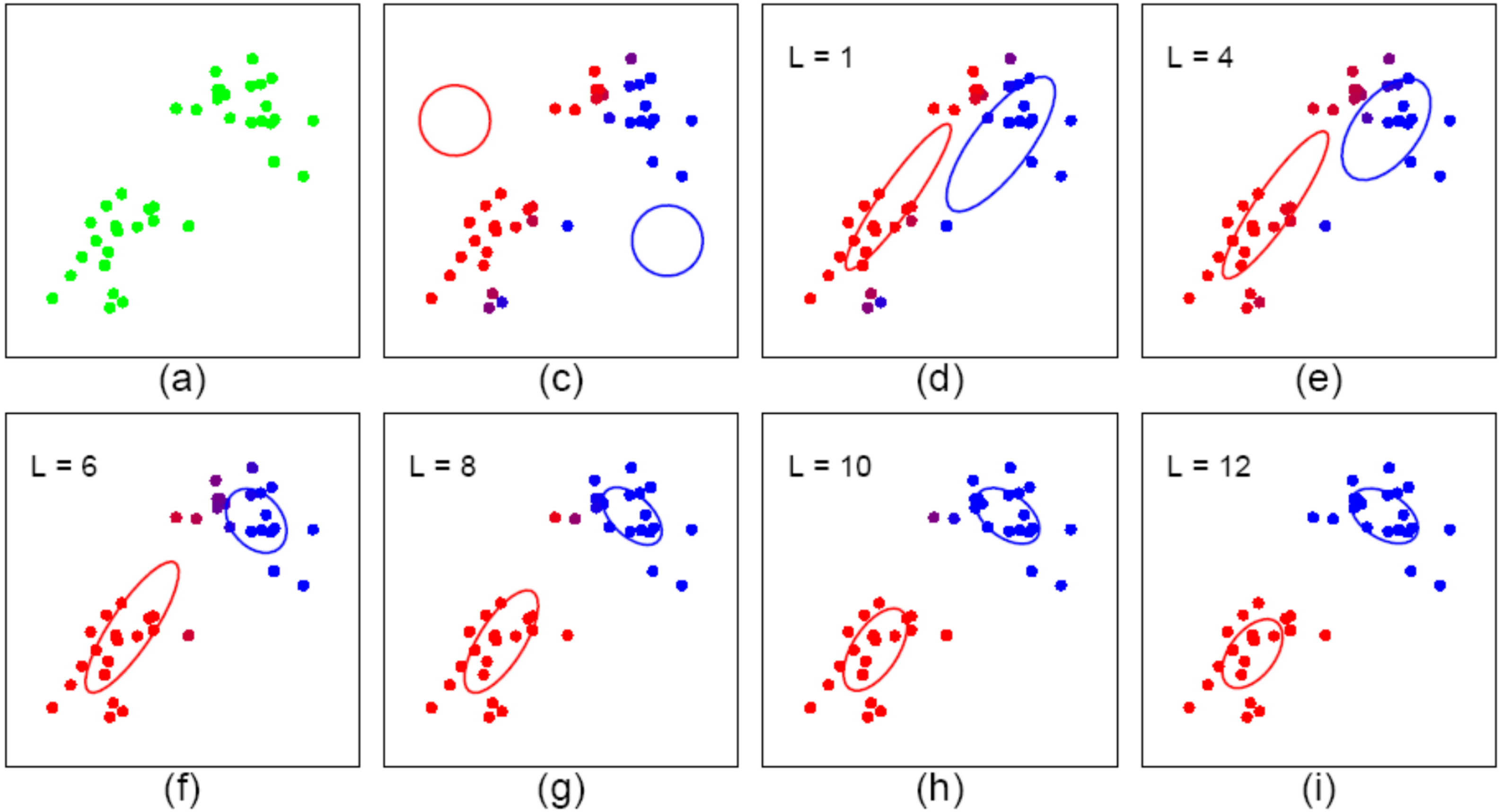
$$p(z^k = 1 \mid \boldsymbol{x}) = \frac{\pi_k \mathcal{N}(\boldsymbol{x} \mid \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x} \mid \mu_j, \Sigma_j)} := \gamma_k$$

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


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

# Example: Gaussian Mixture Models (GMMs)

- Start: "guess" the centroid $\mu_k$ and covariance $\Sigma_k$ of each of the K clusters
- Loop:



# Summary: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces
  - Estimate some “missing” or “unobserved” data from observed data and current parameters.
  - Using this “complete” data, find the maximum likelihood parameter estimates.

# Summary: EM Algorithm

- The EM algorithm is coordinate-decent on $F(q, \theta)$
  - E-step: $q^{t+1} = \arg\min_q F\left(q, \theta^t\right) = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$
  - M-step: $\theta^{t+1} = \arg\min_\theta F\left(q^{t+1}, \theta^t\right) = \text{argmax}_\theta \sum_z q^{t+1}(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$

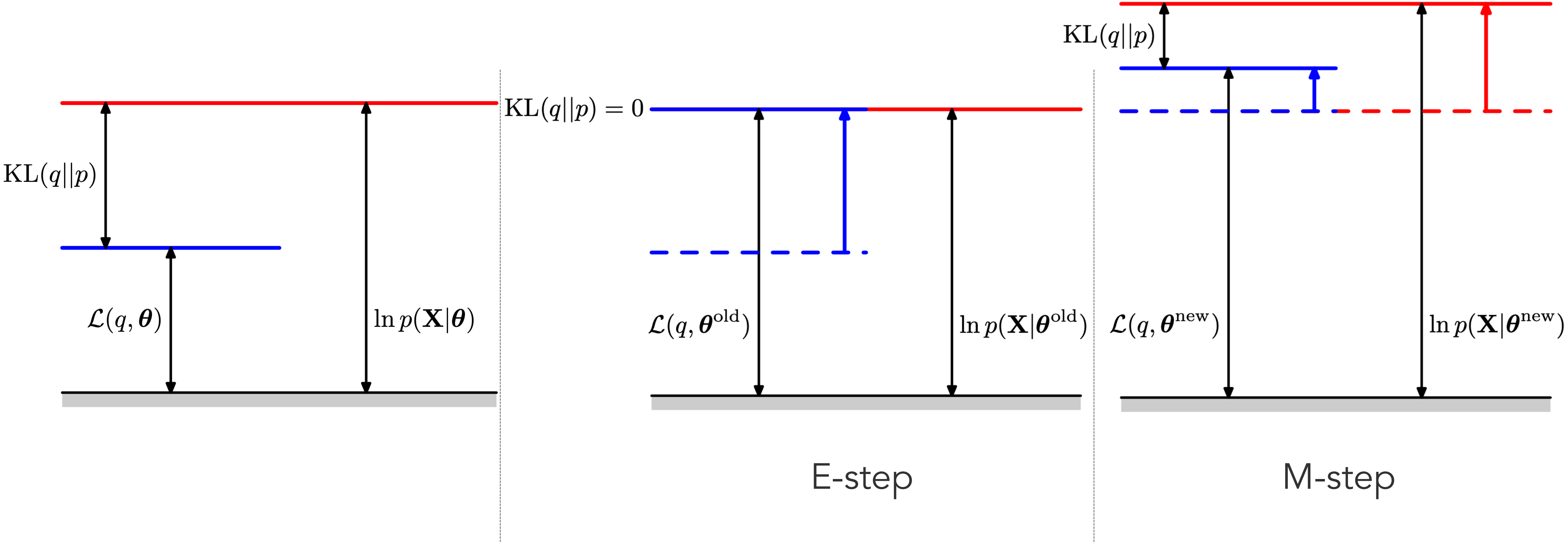
$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \text{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

$$= -F(q, \theta) + \text{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

- Limitation: need to be able to compute $p(\boldsymbol{z}|\boldsymbol{x}, \theta)$, not possible for more complicated models --- solution: Variational inference

# Each EM iteration guarantees to improve the likelihood

$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$




[PRML, Chap 9.4]

# EM Variants

- Sparse EM
  - Do not re-compute exactly the posterior probability on each data point under all models, because it is almost zero.
  - Instead keep an “active list” which you update every once in a while.

- Generalized (Incomplete) EM:
  - It might be hard to find the ML parameters in the M-step, even given the completed data. We can still make progress by doing an M-step that improves the likelihood a bit (e.g. gradient step).

# Questions?