

DSC291: Machine Learning with Few Labels

Unsupervised Learning

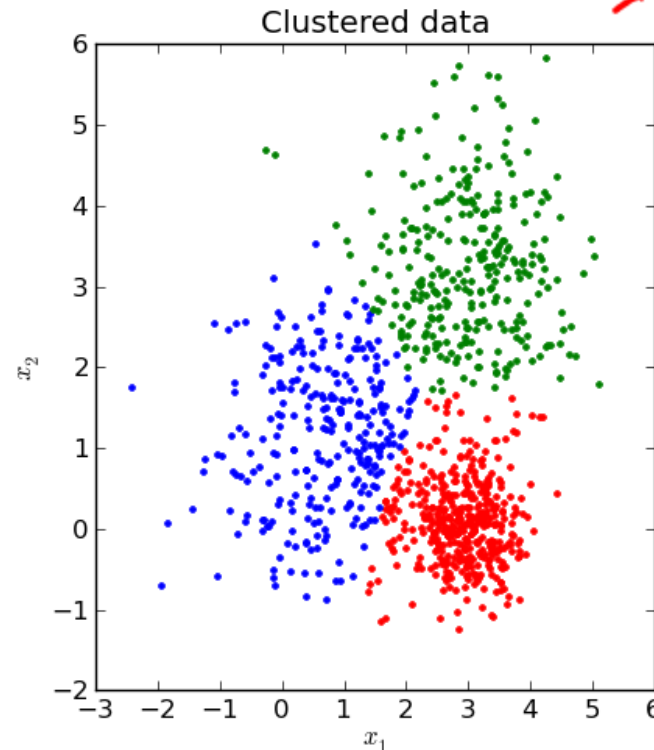
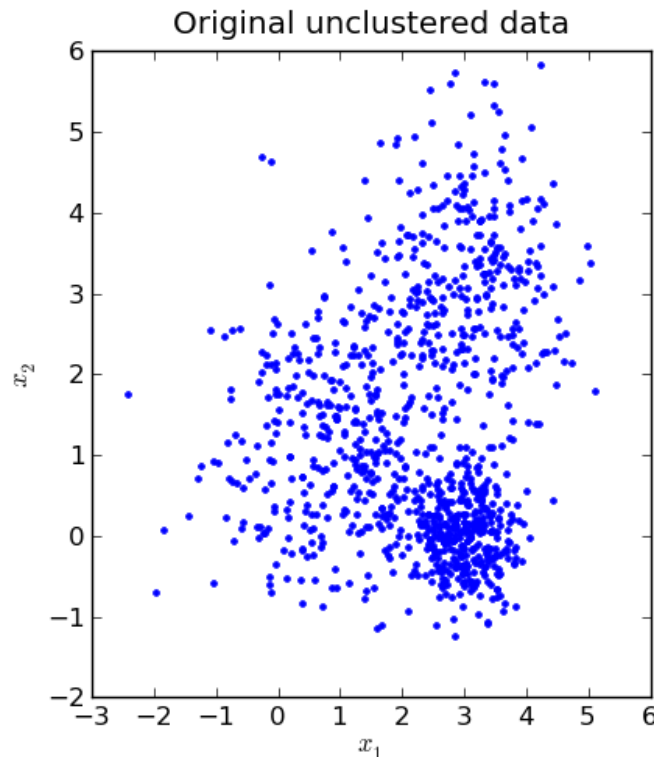
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Lecture 4, April 10, 2025

Unsupervised Learning

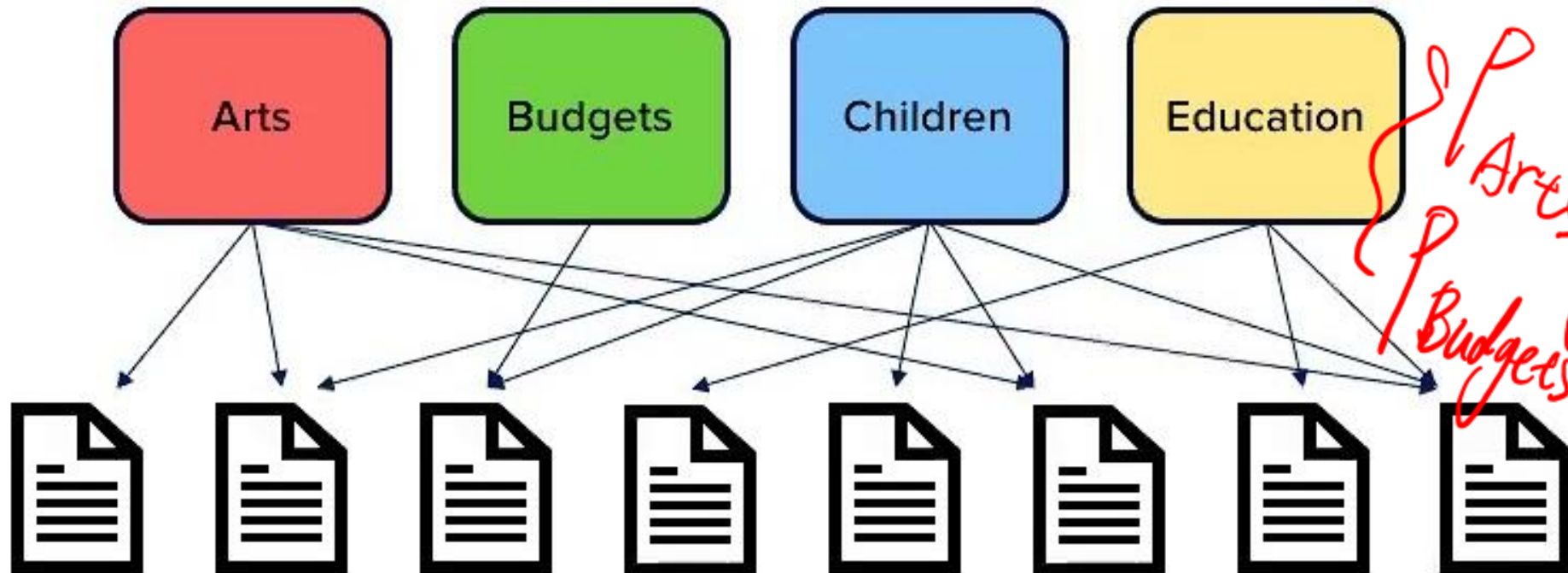
- Each data instance is partitioned into two parts:
 - observed variables x
 - latent (unobserved) variables z
- Want to learn a model $p_{\theta}(x, z)$

$$x = (x_1, x_2)$$
$$z \in \{1, 2, 3\}$$



Unsupervised Learning

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Unsupervised Learning

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

Input Space



Unsupervised Learning

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

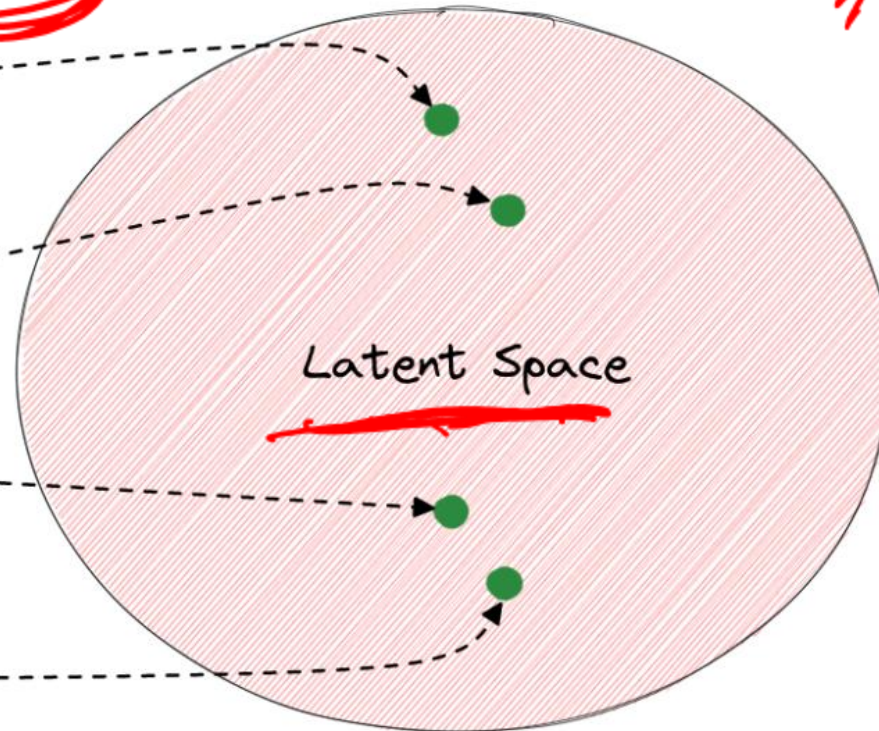
~~VAE~~ ~~GAN~~
Diffusion

$p_\theta(x/z) p(z)$
 ~~$p_\theta(x/z) p(z)$~~
prior
 $x = \text{image}$
 $z \in \mathbb{R}^{100}$

Latent-space
model

deep generative
models

Input Space



$p_\theta(x^*, z)$

$$p(x, z | \theta) = p(x | z, \theta) \cdot p(z | \theta)$$

Why is Unsupervised Learning Harder?

- **Complete log likelihood:** if both x and z can be observed, then

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

- Decomposes into a sum of factors, the parameter for each factor can be estimated separately

Now z is not observed:

- **Incomplete (or marginal) log likelihood:** with z unobserved, our objective becomes the log of a marginal probability:

$$\ell(\theta; x) = \log p(x | \theta)$$

Supervised, Complete data (x, z)

$$\nabla_{\theta} \ell_c(\theta; x, z) = \nabla_{\theta} \log p(x, z | \theta)$$

$$p(x, z | \theta)$$

$$p(x | \theta) = \sum_z p(x, z | \theta)$$

Why is Unsupervised Learning Harder?

- **Complete log likelihood:** if both x and z can be observed, then

$$\textcircled{\text{d}} \quad \ell_c(\theta; x, z) = \log p(x, z | \theta) = \log p(z | \theta_z) + \log p(x | z, \theta_x)$$

- Decomposes into a sum of factors, the parameter for each factor can be estimated separately

Now z is not observed:

- **Incomplete (or marginal) log likelihood:** with z unobserved, our objective becomes the log of a marginal probability:

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

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

$$z \in \mathbb{R}^{100} \\ \nabla_{\theta_z} \int_z p(x, z | \theta_z, \theta_x) \\ \int_z p(x, z | \theta_z, \theta_x)$$

$$\nabla_{\theta_z} \ell(\theta; x) = \nabla_{\theta_z} \log \sum_z p(x, z | \theta_z, \theta_x)$$

$$= \frac{\nabla_{\theta_z} \sum_z p(x, z | \theta_z, \theta_x)}{\sum_z p(x, z | \theta_z, \theta_x)}$$

Expectation Maximization (EM)

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This class

EM → VAEs → diffusion 8

Expectation Maximization (EM): Intuition

Expectation Maximization (EM): Intuition

- Supervised MLE is easy:

$$\max_{\theta} \ell_c(\theta; \mathbf{x}, \mathbf{z}) = \log p(\mathbf{x}, \mathbf{z} | \theta)$$

- Observe both $\mathbf{x}$ and $\mathbf{z}$

- Unsupervised MLE is hard:

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

- Observe only $\mathbf{x}$

- EM, intuitively:

E-step: $q(\mathbf{z} | \mathbf{x}) = p(\mathbf{z} | \mathbf{x}, \theta)$

We don't actually observe q , let's estimate it

M-step: $\max_{\theta} \mathbb{E}_{q(\mathbf{z} | \mathbf{x})} [\log p(\mathbf{x}, \mathbf{z} | \theta)]$

Let's "pretend" we also observe $\mathbf{z}$ (its distribution)

Expectation Maximization (EM): Intuition

- Supervised MLE is easy:

- Observe both x and z

$$\max_{\theta} \ell_c(\theta; x, z) = \log p(x, z | \theta)$$

posterior

- Unsupervised MLE is hard:

- Observe only x

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

- EM, intuitively:

E-step:

$$q^{t+1}(z|x) = p(z|x, \theta^t)$$

M-step:

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

This is an iterative process

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E-step: $q^{t+1}(\mathbf{z} | \mathbf{x}) = p(\mathbf{z} | \mathbf{x}, \theta^t)$

We don't actually observe q , let's estimate it

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Expectation Maximization (EM): Intuition

- Supervised MLE is easy:

- Observe both x and z

$$\max_{\theta} \ell_c(\theta; x, z) = \log p(x, z | \theta)$$

- Unsupervised MLE is hard:

- Observe only x

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

- EM, intuitively

$$\ell(\theta; x) \geq \mathbb{E}_{q(z|x)} [\log p(x, z | \theta)] + H(q)$$

M-step: $\max_{\theta} \mathbb{E}_{q(z|x)} [\log p(x, z | \theta)]$

This is an iterative process

Lower bound

Let's "pretend" we also observe z (its distribution)

only observe q , let's

Expectation Maximization (EM): Intuition

- **Question:** show that $\ell(\theta; \mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}, \mathbf{z}|\theta)] + H(q)$

Expectation Maximization (EM): Intuition

- **Question:** show that

$$\begin{aligned}\ell(\theta; \mathbf{x}) &\geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}, \mathbf{z}|\theta)] + H(q) \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \right]\end{aligned}$$

$$- \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} [\log q(\mathbf{z}|\mathbf{x})]$$

Expectation Maximization (EM): Intuition

- **Question:** show that

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

- **Hint:** first show that

$$\ell(\theta; \mathbf{x}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \right] + \text{KL}(q(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}|\mathbf{x}, \theta)) \geq 0$$

- Since KL divergence is non-negative, we arrive at the conclusion

Expectation Maximization (EM): Intuition

- **Question:** show that $\ell(\theta; \mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}, \mathbf{z}|\theta)] + H(q)$

$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \right]$$

- **Hint:** first show that

$$\ell(\theta; \mathbf{x}) = \underbrace{\mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \right]}_{\text{Evidence Lower Bound (ELBO)}} + \text{KL}(q(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}|\mathbf{x}, \theta))$$
$$= \underbrace{-F(q, \theta)}_{\text{Variational free energy}} + \text{KL}(q(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}|\mathbf{x}, \theta))$$

$$F(q, \theta) = - \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}, \mathbf{z}|\theta)] - H(q)$$

Lower Bound and Free Energy

- Variational free energy:

$$\min_{q, \theta} \quad \underline{F(q, \theta)} = -\mathbb{E}_{q(z|x)}[\log p(x, z|\theta)] - H(q)$$

- The EM algorithm is coordinate-decent on F

- At each step t :

- E-step: $q^{t+1} = \arg \min_q F(q, \theta^t) \Rightarrow q^{t+1}(z|x) = p(z|x, \theta^t)$

- M-step: $\theta^{t+1} = \arg \min_{\theta} F(q^{t+1}, \theta) \Rightarrow \max_{\theta} \mathbb{E}_{q^{t+1}(z|x)}[\log p(x, z|\theta)]$

Lower Bound and Free Energy

- Variational free energy:

$$F(q, \theta) = - \mathbb{E}_{q(z|x)} [\log p(x, z|\theta)] - H(q)$$

- The EM algorithm is coordinate-decent on F

- At each step t :

- E-step: $q^{t+1} = \arg \min_q F(q, \theta^t)$  $q^{t+1}(z|x) = p(z|x, \theta^t)$
- M-step: $\theta^{t+1} = \arg \min_{\theta} F(q^{t+1}, \theta)$ $\Rightarrow \max_{\theta} \mathbb{E}_{q^{t+1}(z|x)} [\log p(x, z|\theta)]$

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

- **Question:** show that that optimal solution of E-step is

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

- I.e., the posterior distribution over the latent variables given the data and the current parameters.

- **Hint:** use the fact

$$F = -\ell + \text{KL}$$

$$\underbrace{\ell(\theta^t; \mathbf{x})}_{\substack{\downarrow \\ \text{Independent of } q}} = \underbrace{-F(q, \theta^t)}_{\substack{\downarrow \\ \geq 0}} + \text{KL}(q(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}|\mathbf{x}, \theta^t))$$

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

Lower Bound and Free Energy

- Variational free energy:

$$\underline{F(q, \theta) = - \mathbb{E}_{q(z|x)} [\log p(x, z|\theta)] - H(q)}$$

- The EM algorithm is coordinate-decent on F

- At each step t :

- E-step: $q^{t+1} = \arg \min_q F(q, \theta^t)$

✓ $\Rightarrow q^{t+1}(z|x) = p(z|x, \theta^t)$

- M-step: $\theta^{t+1} = \arg \min_{\theta} F(q^{t+1}, \theta)$

? $\Rightarrow \max_{\theta} \mathbb{E}_{q^{t+1}(z|x)} [\log p(x, z|\theta)]$

EM Algorithm: Quick Summary

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

○ But it's too difficult $\ell(\theta; \mathbf{x}) = \log p(\mathbf{x}|\theta) = \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta)$

- EM algorithm:
 - maximize a lower bound of $\ell(\theta; \mathbf{x})$
 - Or equivalently, minimize an upper bound of $-\ell(\theta; \mathbf{x})$
- Key equation:

$$\ell(\theta; \mathbf{x}) = \underbrace{\mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \right]}_{\text{Evidence Lower Bound (ELBO)}} + \text{KL}(q(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}|\mathbf{x}, \theta))$$
$$= \underbrace{-F(q, \theta)}_{\text{Variational free energy}} + \text{KL}(q(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}|\mathbf{x}, \theta))$$

Variational free energy

EM Algorithm: Quick Summary

- The EM algorithm is coordinate-decent on $F(q, \theta)$

- E-step: $q^{t+1} = \arg \min_q F(q, \theta^t) = \underline{p(\mathbf{z}|\mathbf{x}, \theta^t)}$

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

- M-step: $\theta^{t+1} = \arg \min_{\theta} F(q^{t+1}, \theta) = \arg \max_{\theta} \sum_{\mathbf{z}} q^{t+1}(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta)$

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

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

Surrogate objective

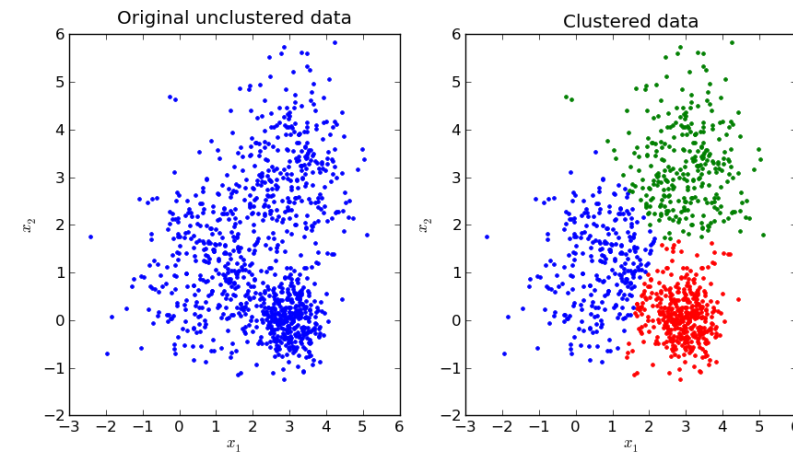
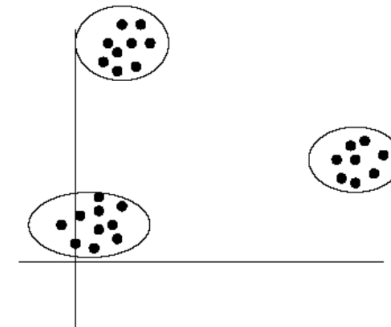
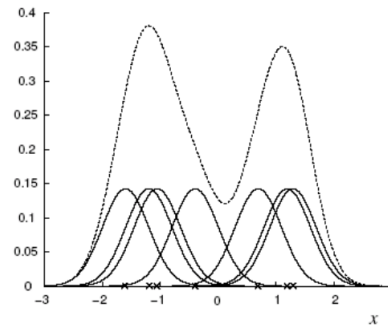
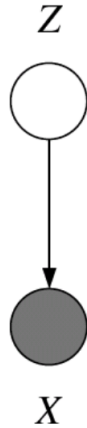
Example: Gaussian Mixture Models

- Consider a mixture of K Gaussian components:

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

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

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

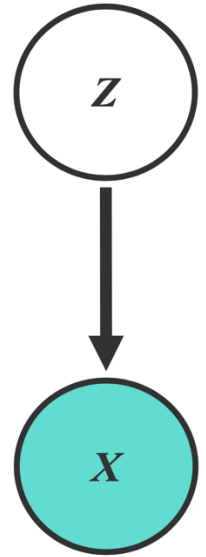
- The likelihood of a sample:

Parameters to be learned:

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

mixture proportion

mixture component



Example: Gaussian Mixture Models (GMMs)

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

$$\begin{aligned}\mathbb{E}_q [\ell_c(\boldsymbol{\theta}; x, z)] &= \sum_n \mathbb{E}_q [\log p(z_n | \pi)] + \sum_n \mathbb{E}_q [\log p(x_n | z_n, \mu, \Sigma)] \\ &= \sum_n \sum_k \mathbb{E}_q [z_n^k] \log \pi_k - \frac{1}{2} \sum_n \sum_k \mathbb{E}_q [z_n^k] \left((x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) + \log |\Sigma_k| + C \right)\end{aligned}$$

- E-step: computing the posterior of z_n given the current estimate of the parameters (i.e., π, μ, Σ)

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

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

Example: Gaussian Mixture Models (GMMs)

- M-step: computing the parameters given the current estimate of Z_n

$$\pi_k^* = \arg \max \langle l_c(\boldsymbol{\theta}) \rangle, \quad \Rightarrow \quad \frac{\partial}{\partial \pi_k} \langle l_c(\boldsymbol{\theta}) \rangle = 0, \forall k, \quad \text{s.t.} \sum_k \pi_k = 1$$
$$\Rightarrow \pi_k^* = \frac{\sum_n \langle Z_n^k \rangle_{q^{(t)}}}{N} = \frac{\sum_n \tau_n^{k(t)}}{N} = \frac{\langle n_k \rangle}{N}$$

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

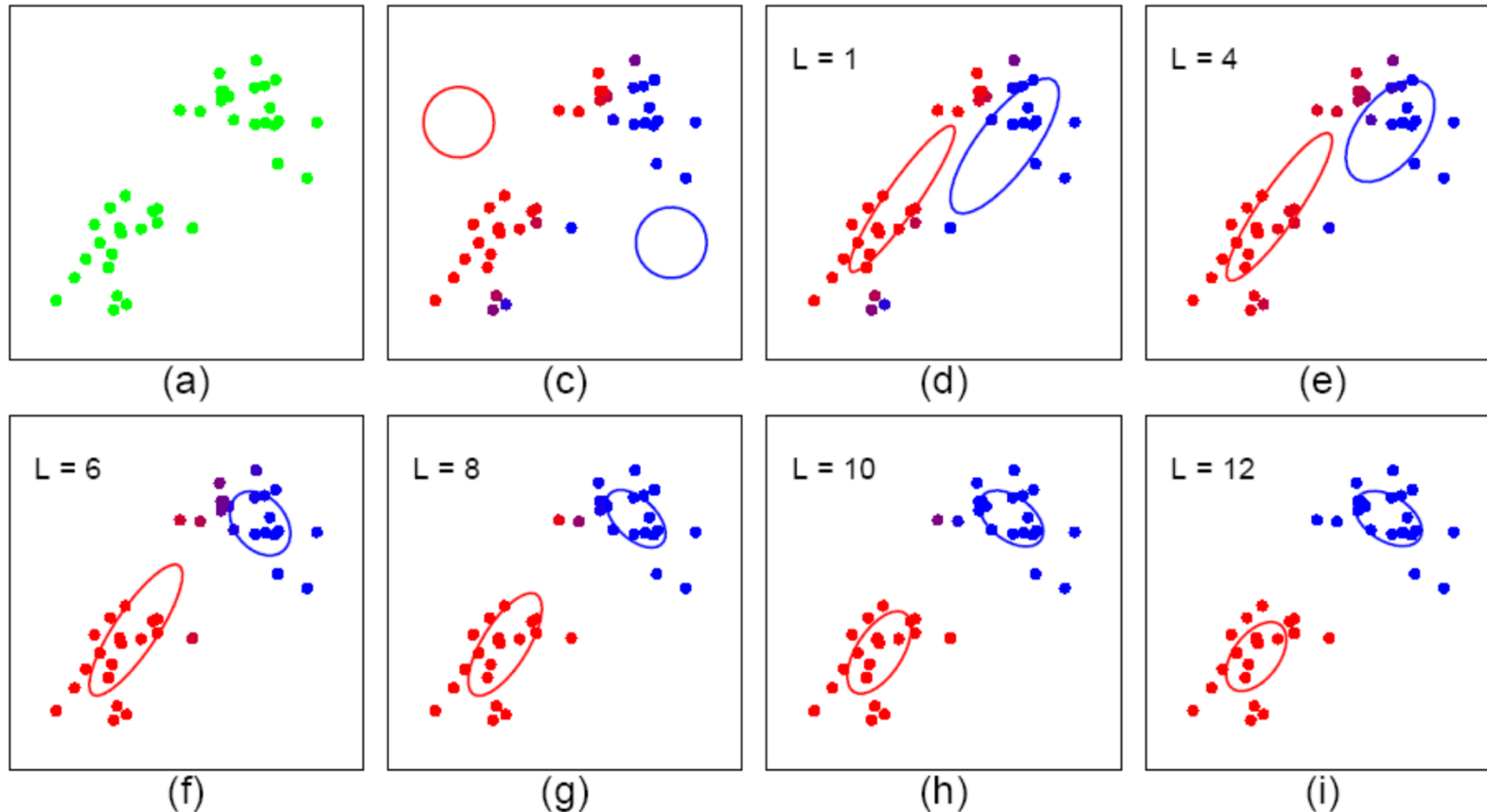
$$\Sigma_k^* = \arg \max \langle l(\boldsymbol{\theta}) \rangle, \quad \Rightarrow \quad \Sigma_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} (x_n - \mu_k^{(t+1)})(x_n - \mu_k^{(t+1)})^T}{\sum_n \tau_n^{k(t)}}$$

Fact :

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

Example: Gaussian Mixture Models (GMMs)

- Start: “guess” the centroid μ_k and covariance Σ_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.
- Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:
 - E-step:
 - M-step: $q^{t+1} = \arg \min_q F(q, \theta^t)$
 $\theta^{t+1} = \arg \min_{\theta} F(q^{t+1}, \theta)$

Questions?