# EECS 545: Machine Learning

# Lecture 17. Learning in Graphical Models

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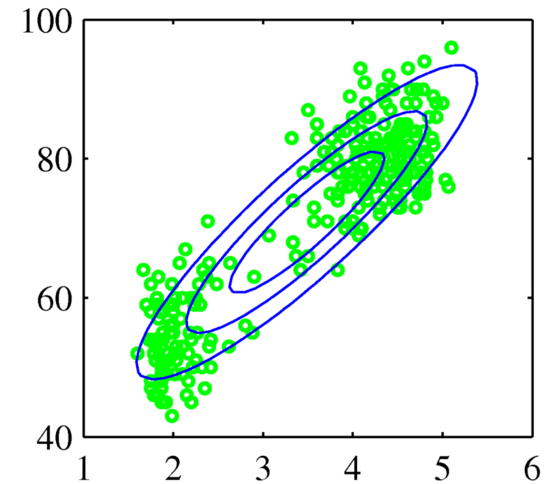
# Expectation Maximization

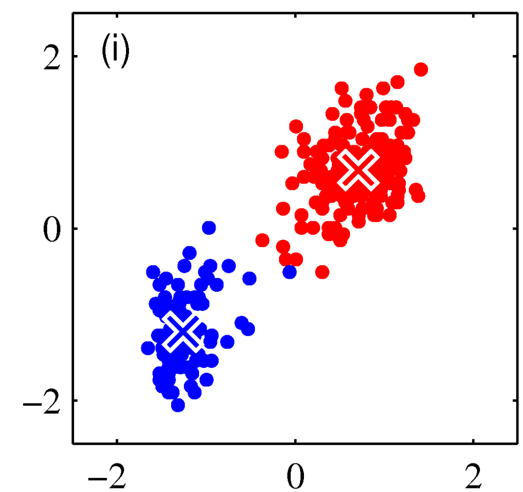
# Expectation Maximization

- Parameter learning when the data is not fully observed.
  - Suppose that we have observed varaibles X, and hidden variables Z
- Main idea:
  - Run inference about Z given X: $Q=P(Z|X)$
  - Update parameters by treating Q as observation!
- Example:
  - Gaussian mixtures
  - (We will start with Kmeans which is a special case of Gaussian mixtures)

# The K-Means Algorithm

- Given unlabeled data $x_n$, ($n=1,\ldots,N$),
- And believing it belongs in $K$ clusters,
- How do we find the clusters?



# The K-Means Algorithm

- We need indicator variables $r_{nk}$ in {0,1}.
  - $\boldsymbol{r_{nk}} = 1$ if $\mathbf{x}_n$ is in cluster $k$.
  - and $\boldsymbol{r_{nj}} = 0$ for all $j$ other than $k$.

- Minimize the distortion measure $J$: sum of squared distance of points from the center of its own cluster.

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} ||\underbrace{\mathbf{x}_n}_{\in \mathbb{R}^d} - \underbrace{\mu_k}_{\in \mathbb{R}^d}||^2$$

Variables =

$\{\mu_1, \dots, \mu_k\}$

$\{r_{nk}\}$

$$\min_{\mu, r} \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \| x_n - \mu_k \|^2$$

<u>Fix $\mu$.</u> for every $n$, $\sum_{k=1}^{K} r_{nk} \| x_n - \mu_k \|^2$

$$\begin{cases} r_{n1} = 1 & \Rightarrow \| x_n - \mu_1 \|^2 \\ r_{n2} = 1 & \Rightarrow \| x_n - \mu_2 \|^2 \\ \vdots & \vdots \\ r_{nK} = 1 & \Rightarrow \| x_n - \mu_K \|^2 \end{cases}$$

$$\mu_k = \frac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$$

For every $n$, $k^* = \arg\min_{k \in \{1, \dots, K\}} \| x_n - \mu_k \|^2$, set $r_{nk^*} = 1$

---

Fix $r$,

$$\nabla_{\mu_k} J = \sum_{n=1}^{N} r_{nk} \underbrace{\nabla_k \| x_n - \mu_k \|^2}_{2(\mu_k - x_n)} = 2\left[\sum_n r_{nk} \mu_k - \sum_n r_{nk} x_n\right] = 0$$

# The K-Means Algorithm

- Set the cluster centers arbitrarily.
- Repeat until quiescence:
  - **E Step: assign each point to closest center.**

Fix $\mu$
optimize $r$

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j ||\mathbf{x}_n - \mu_j||^2 \\ 0 & \text{otherwise} \end{cases}$$

  - **M Step: update the centers**

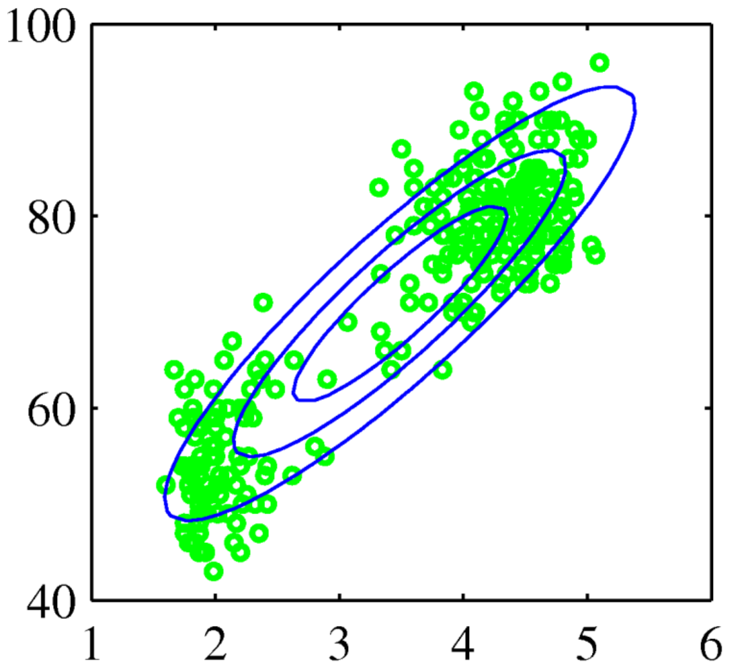
Fix $r$
optimize $\mu$

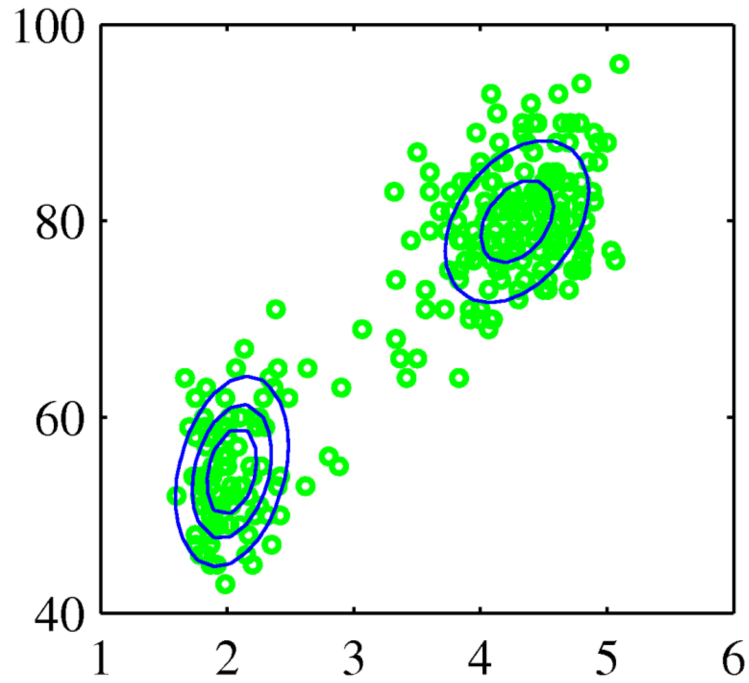
$$\mu_k = \frac{\sum_n r_{nk}\mathbf{x}_n}{\sum_n r_{nk}}$$

Q. Verify this

# Clustering Pixels

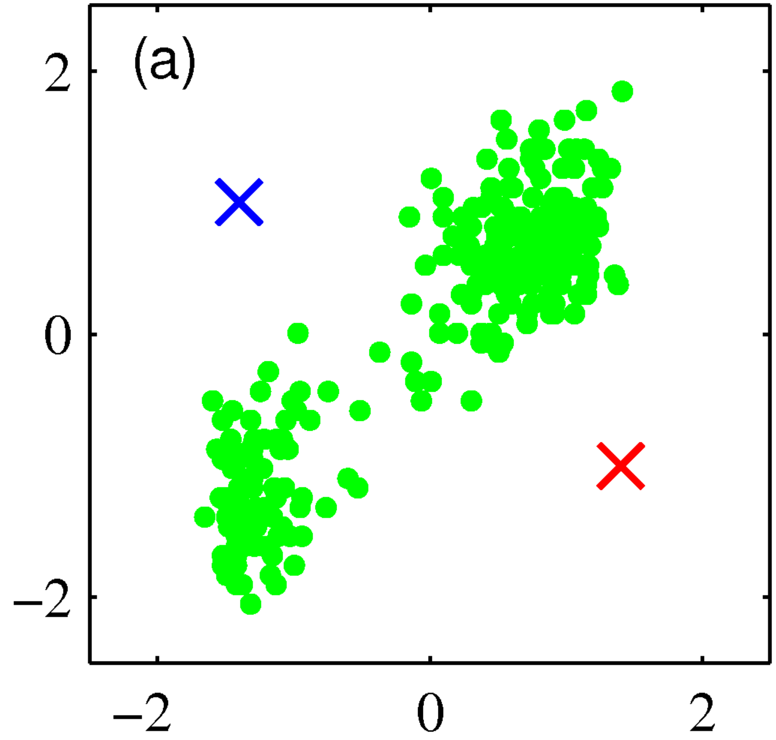
- How do we find clusters of pixels?



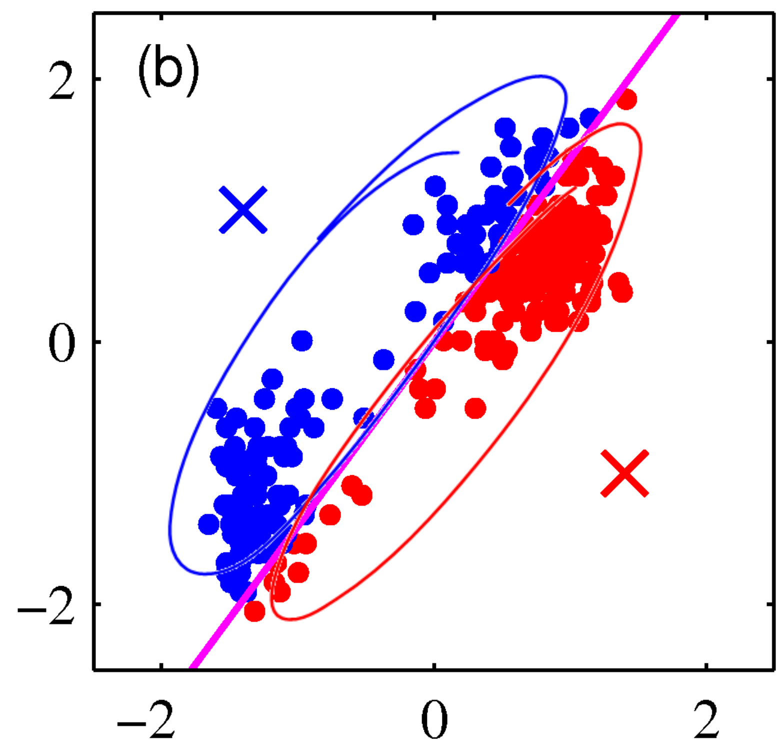
# K-Means Clustering

- Select K. Pick random means.
  - Here K=2.



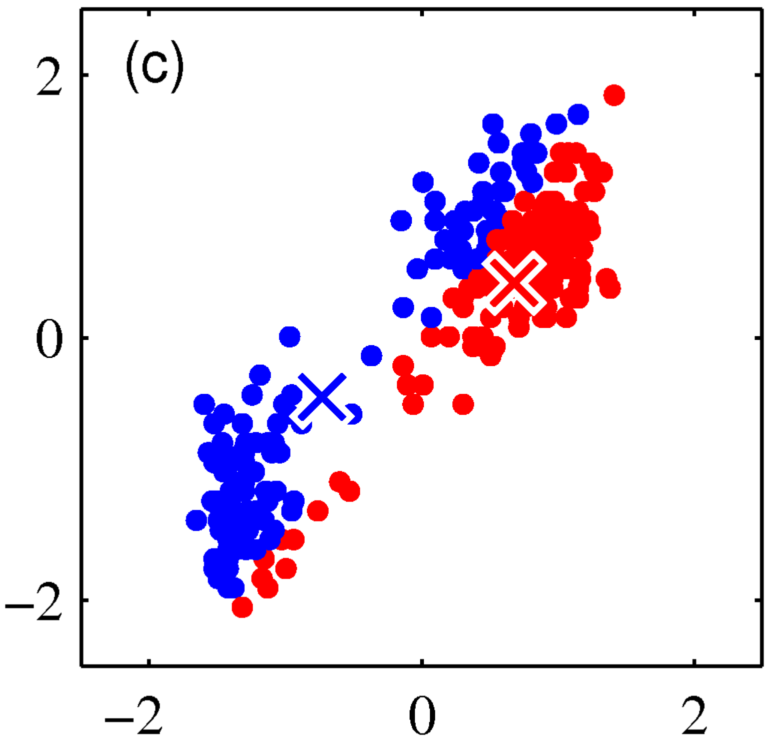
# The E Step

- Assign each point to the nearest center.



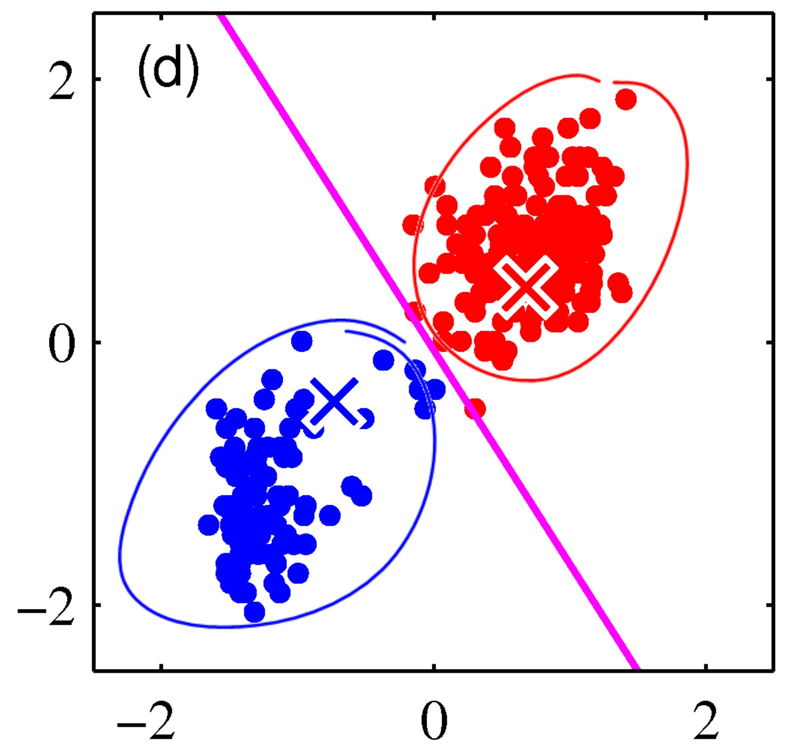
# The M-Step

- Compute new centers for each cluster.



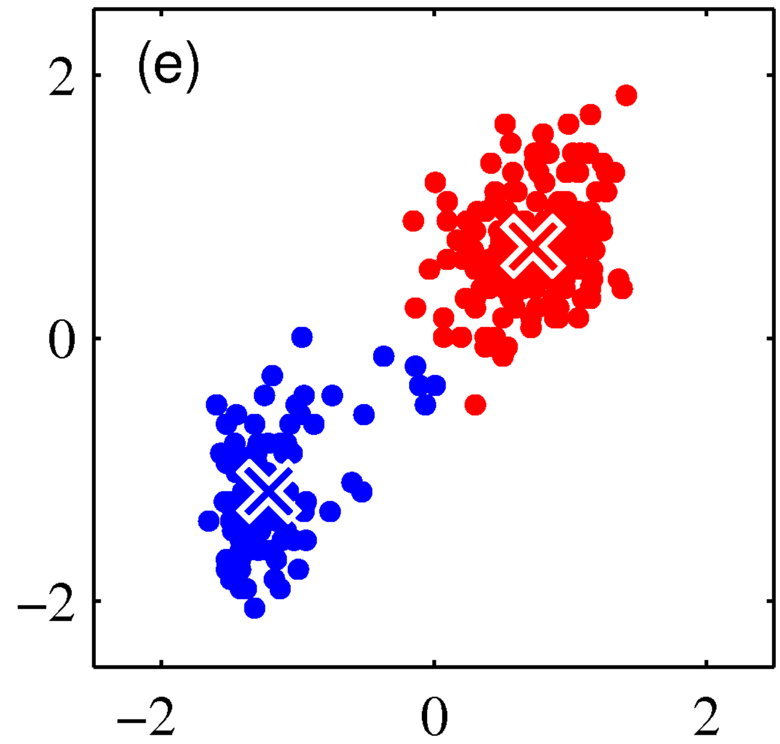
# The E-Step Again

- Re-assign points to the now-nearest center.



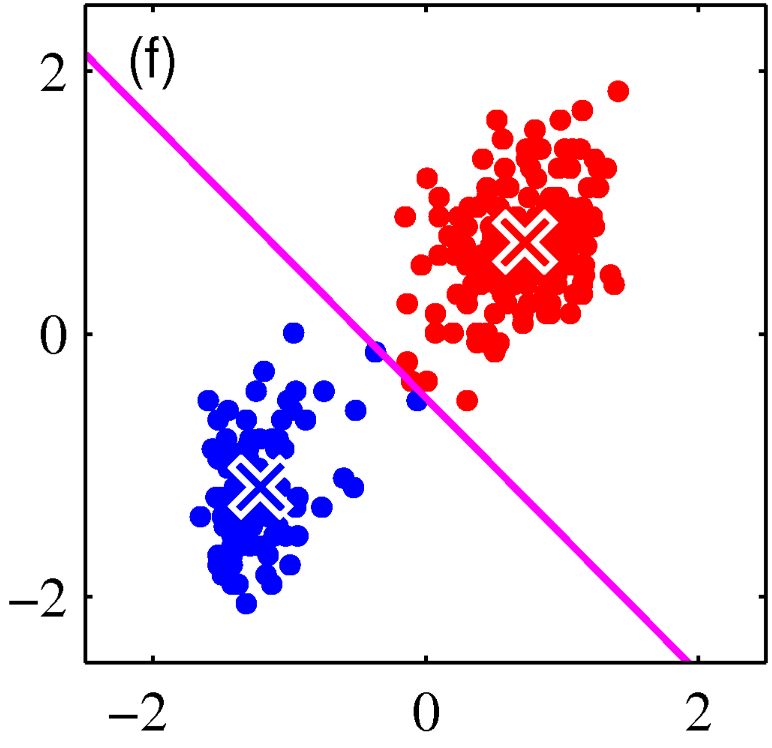
# The M-Step Again

- Compute centers for the new clusters.



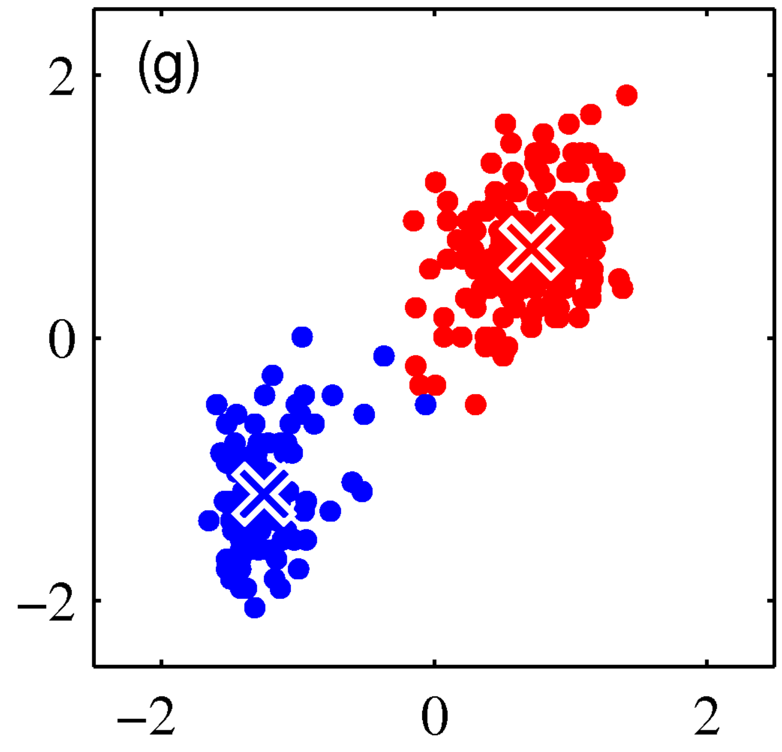
# Another E-Step

- Reassign the pixels to centers.



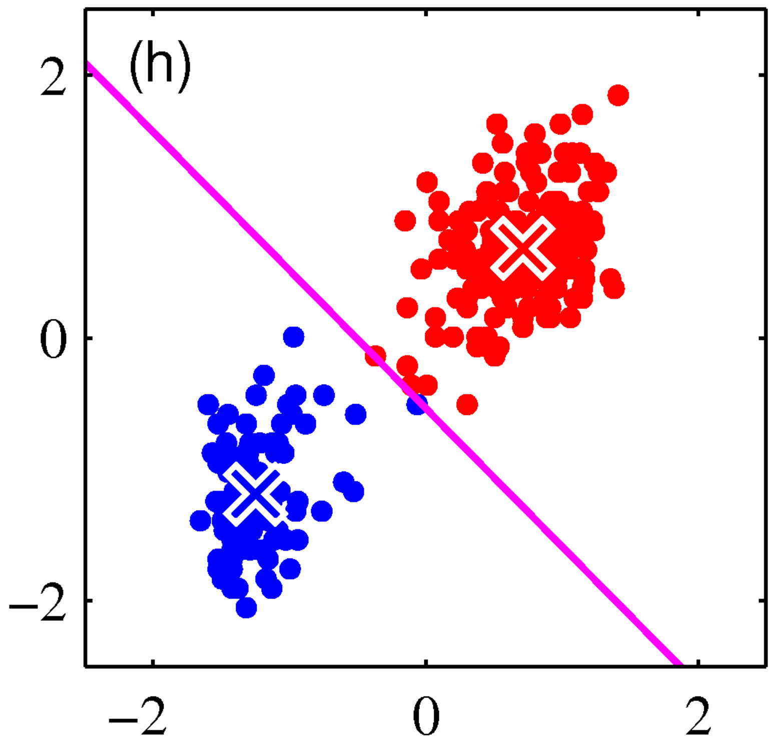
# Another M-Step

- New centers.



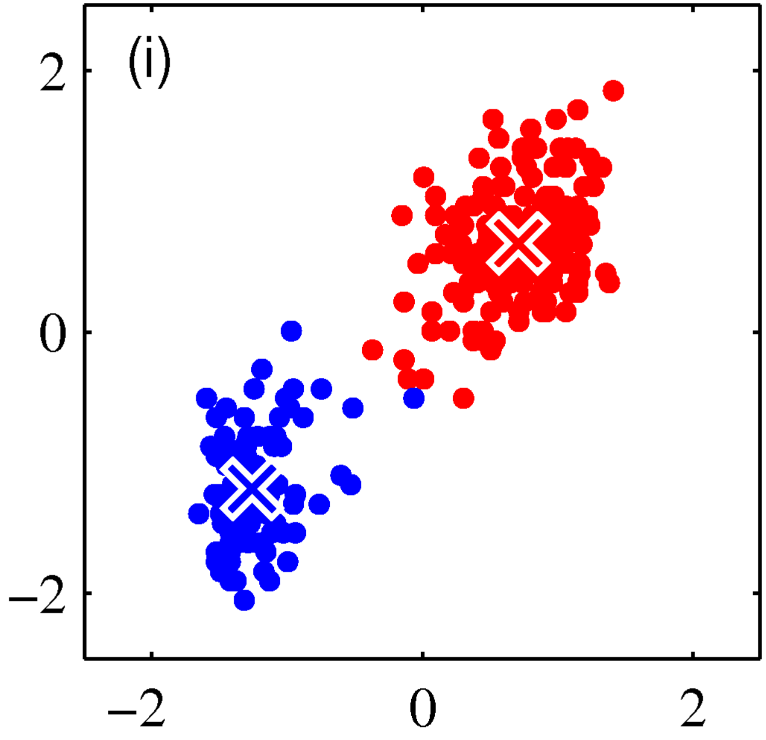
# Another E-Step.

- New cluster assignments.



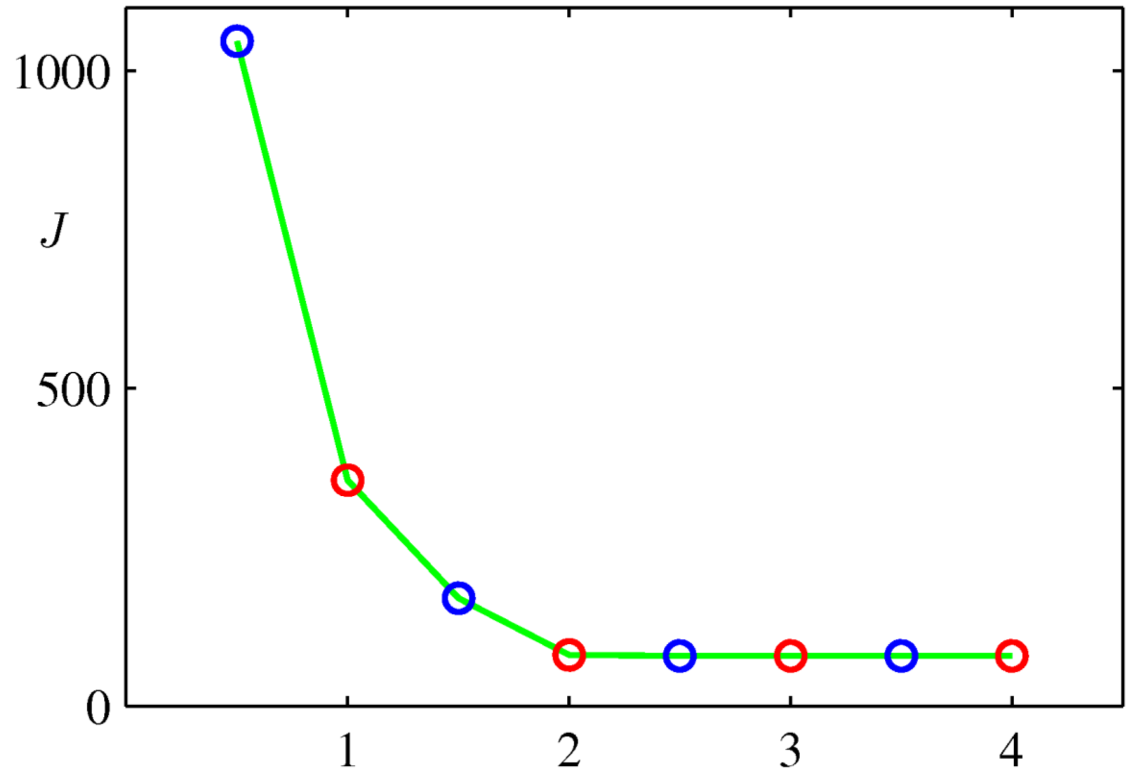
# M-Step again.

- The cluster centers have stopped changing.



# Convergence

- Convergence is relatively quick, in steps.
  - But: all those distance computations are expensive.



# Hard and Soft Clusters

- K-Means uses hard clustering.
  - A point belongs to exactly one cluster.

- Mixture of Gaussians uses soft clustering.
  - A point could be explained by any cluster.
  - Different clusters take different levels of responsibility for that point.
  - (It was actually generated by only one cluster, but we don't know which one.)

# Expectation Maximization

- Parameter learning when the data is not fully observed.
  - Suppose that we have observed varaibles X, and hidden variables Z
- Main idea:
  - E-step: Run inference about Z given X: Q=P(Z|X)
  - M-step: Update parameters by treating Q as observation!
- Example:
  - Gaussian mixtures
  - (We will start with Kmeans which is a special case of Gaussian mixtures)

# One page-derivation of EM

- Given the observed input data x, latent variable z, and parameter $\theta$:

$$\sum_z Q(z)\, g(z) = \mathbb{E}_Q\, g(z)$$

prob. over z.

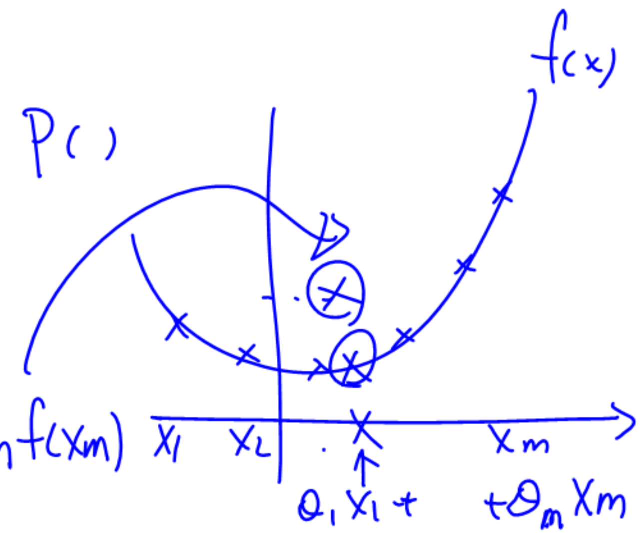
$$\begin{aligned}
\log P_\theta(x) &= \log \sum_z P_\theta(x,z) \\
&= \log \underbrace{\sum_z Q(z)}_{\mathbb{E}_Q} \overbrace{\frac{P_\theta(x,z)}{Q(z)}}^{g(z)} \quad (Set\, Q(z) \geq 0, \sum_z Q(z) = 1) \\
&\geq \underbrace{\sum_z Q(z)}_{\mathbb{E}_Q} \log \frac{P_\theta(x,z)}{Q(z)} \quad (Jensen's\, inequality)
\end{aligned}$$

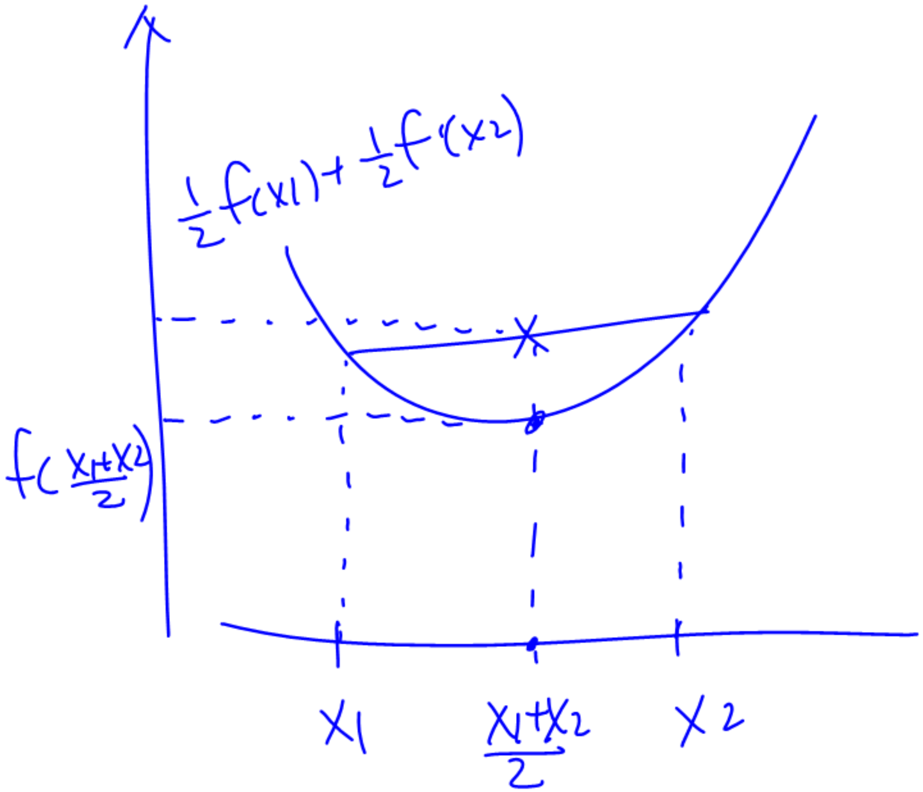
- For convex function $f(x)$ and prob. $P(\,)$

$$\mathbb{E}_P[f(x)] \geq f(\mathbb{E}_P[X])$$

- $\theta_1 + \dots + \theta_m = 1.$ $\theta_i \geq 0$

$$\theta_1 f(x_1) + \theta_2 f(x_2) + \dots \theta_m f(x_m)$$

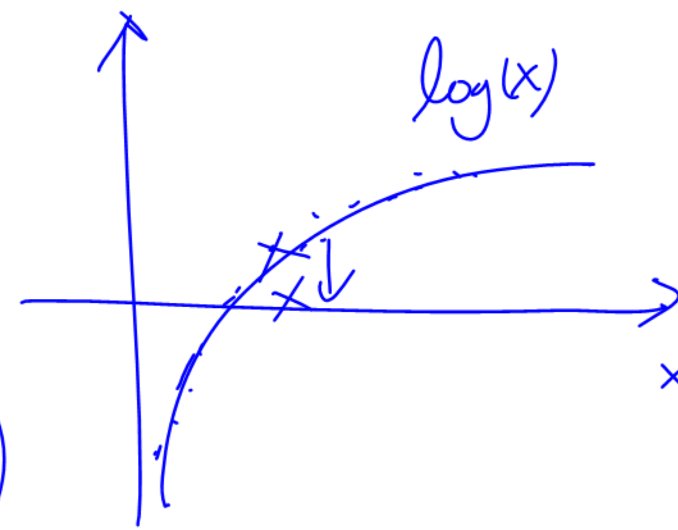





$\theta_1 = \frac{1}{2}$

$\theta_2 = \frac{1}{2}$

if $x_1 = x_2$ equality holds.




$\log(x)$ is concave function

$$\mathbb{E}_Q[\log(x)] \leq \log(\mathbb{E}_Q[x])$$

# One page-derivation of EM

- Given the observed input data x, latent variable z, and parameter $\theta$:

$$
\begin{aligned}
\log P_\theta(x) &= \log \sum_z P_\theta(x, z) \\
&= \log \sum_z Q(z) \frac{P_\theta(x, z)}{Q(z)} \quad (Set\, Q(z) \geq 0, \sum_z Q(z) = 1) \\
&\geq \sum_z Q(z) \log \frac{P_\theta(x, z)}{Q(z)} \quad (Jensen's\, inequality)
\end{aligned}
$$

- Equality holds when $\mathrm{Q(z)} \propto P_\theta(x,z) = P_\theta(z|x)$
  - (E-step) Compute the posterior of z given x
- Fix Q, update $\theta$ that maximize the "data completion" log-likelihood (M-step)

maximize $\Theta$

$$\sum_i \sum_{z^{(i)}} Q\left(z^{(i)}\right) \log P_\theta\left(x^{(i)}, z^{(i)}\right)$$

Q. Verify this!

$z$ : assignment

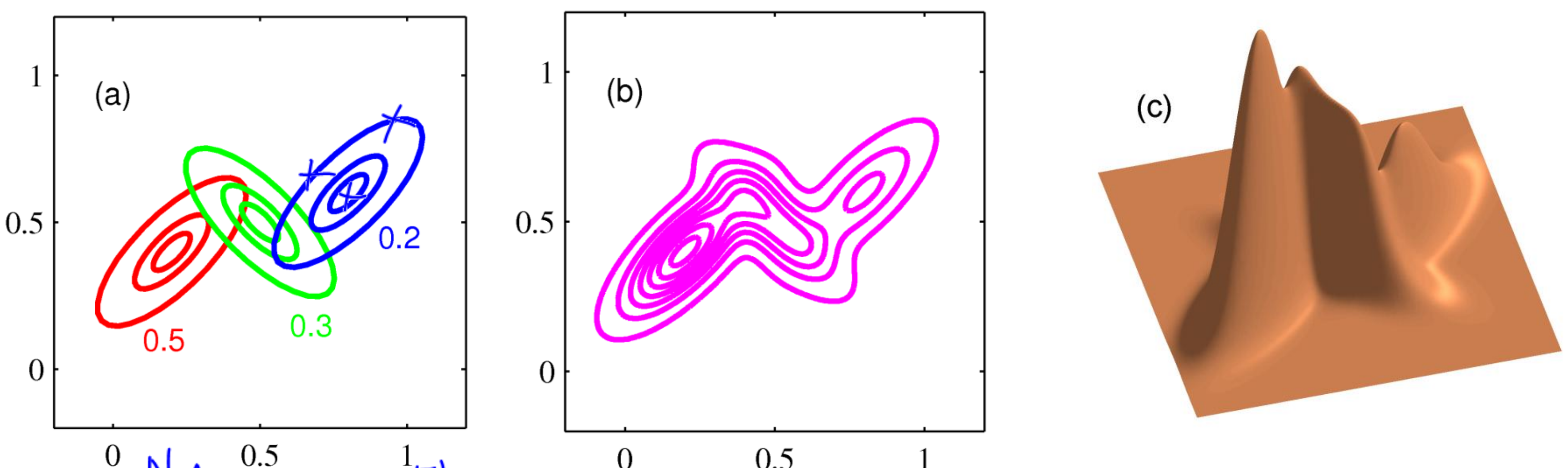
# Mixtures of Gaussians

$z_{nk} = 1$
if example $n$ is assigned to cluster $k$

$$\boxed{P(x, z) = \prod_{k=1}^{N} \left[ \pi_k \mathcal{N}(x \mid \mu_k, \Sigma_k) \right]^{z_{nk}}}$$

- Mixtures of Gaussians make it possible to describe much richer distributions.

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x} \mid \mu_k, \mathbf{\Sigma}_k) \quad \sum_{z} P(x, z)$$




$$\max_{\pi_k, \mu_k, \Sigma_k} \sum_{i=1}^{N} \log P(x^{[i]})$$

# Mixtures of Gaussians

- Note the mixing coefficients in

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

- Let z in $\{0,1\}^K$ be a 1-of-*K* random variable;

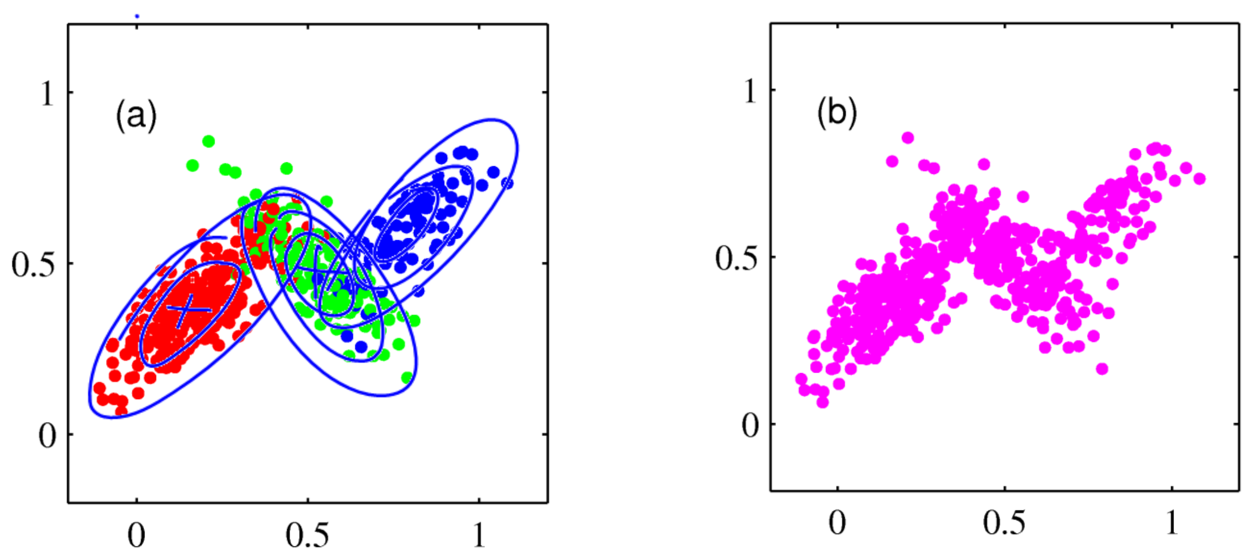
$$p(z_k = 1) = \pi_k \qquad p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}$$

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\mu_k, \mathbf{\Sigma}_k)$$

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

# Mixtures of Gaussians

- To generate samples from a Gaussian mixture distribution $p(\mathrm{x})$, use $p(\mathrm{x},\mathrm{z})$:
  - Select a value $\mathbf{z}$ from the marginal $p(\mathbf{z})$;
  - Then select a value $\mathbf{x}$ from $p(\mathbf{x} \mid \mathbf{z})$ for that $\mathbf{z}$.



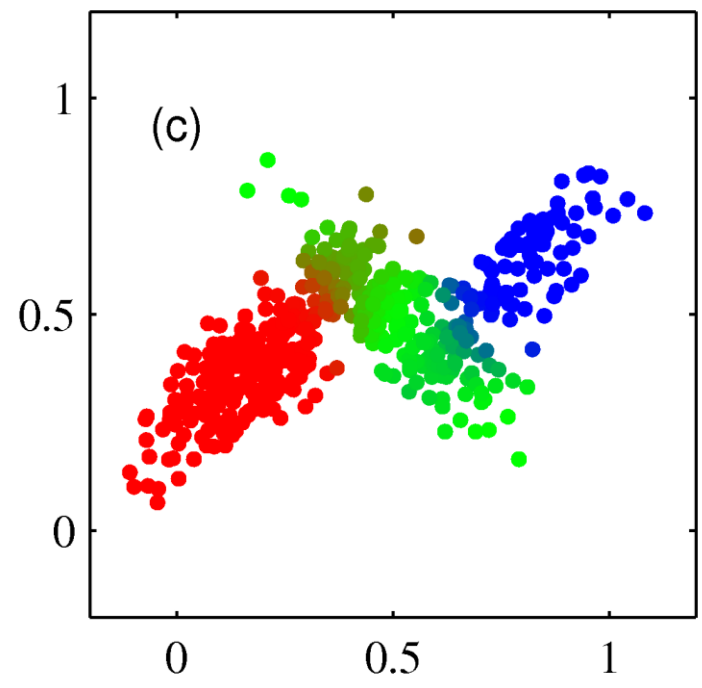
# Mixtures of Gaussians

- Responsibility is the degree to which each Gaussian explains an observation x.

$$\gamma(z_k) \equiv p(z_k = 1|\mathbf{x})$$

$$= \frac{P(z_k=1, x)}{\sum_k P(z_k=1, x)}$$

$$\gamma(z_k) = \frac{\pi_k \mathcal{N}(\mathbf{x}|\mu_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\mu_j, \boldsymbol{\Sigma}_j)}$$




Q. Verify this!

# Mixtures of Gaussians

- The mean of a cluster is the weighted mean, weighted by the responsibilities.

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

weighted average of $x_n$ with weights $\gamma(z_{nk})$

  - $N_k$ is the effective number of points in cluster $k$

$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}) \qquad \pi_k = \frac{N_k}{N}$$

- Likewise for covariance:

$$\mathbf{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \mu_k)(\mathbf{x}_n - \mu_k)^T$$

# EM for Gaussian Mixtures

- Initialize means, covariances, and mixing coefficients for the K Gaussians.

- E Step: Given the coefficients, evaluate the responsibilities.

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \mathbf{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_j, \mathbf{\Sigma}_j)}$$

# EM for Gaussian Mixtures

- M Step: Given the responsibilities, re-evaluate the coefficients.

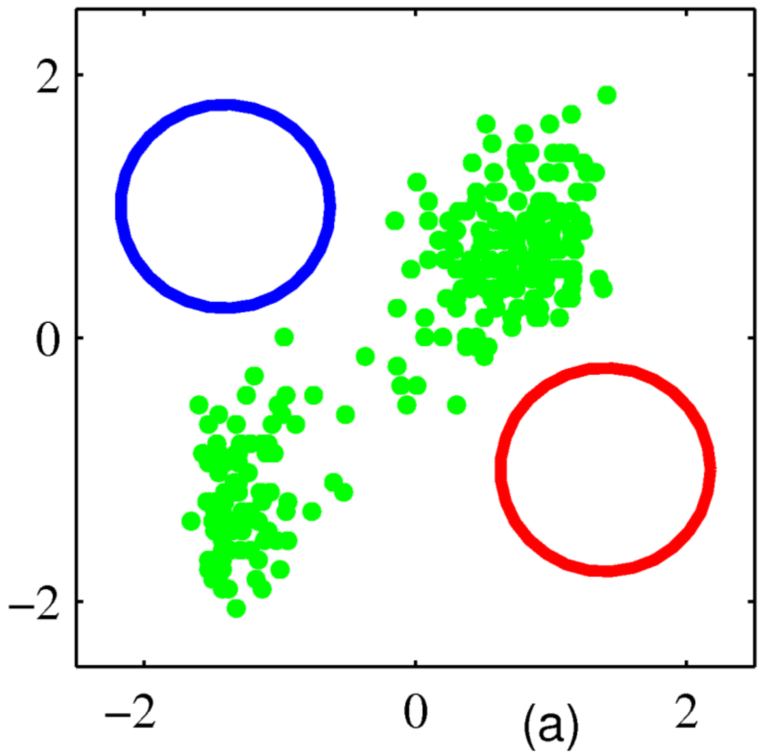
$$\mu_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n \qquad \pi_k^{\text{new}} = \frac{N_k}{N}$$

$$\mathbf{\Sigma}_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})(\mathbf{x}_n - \mu_k^{\text{new}})(\mathbf{x}_n - \mu_k^{\text{new}})^T$$

- Stop when either coefficients or log likelihood converges.

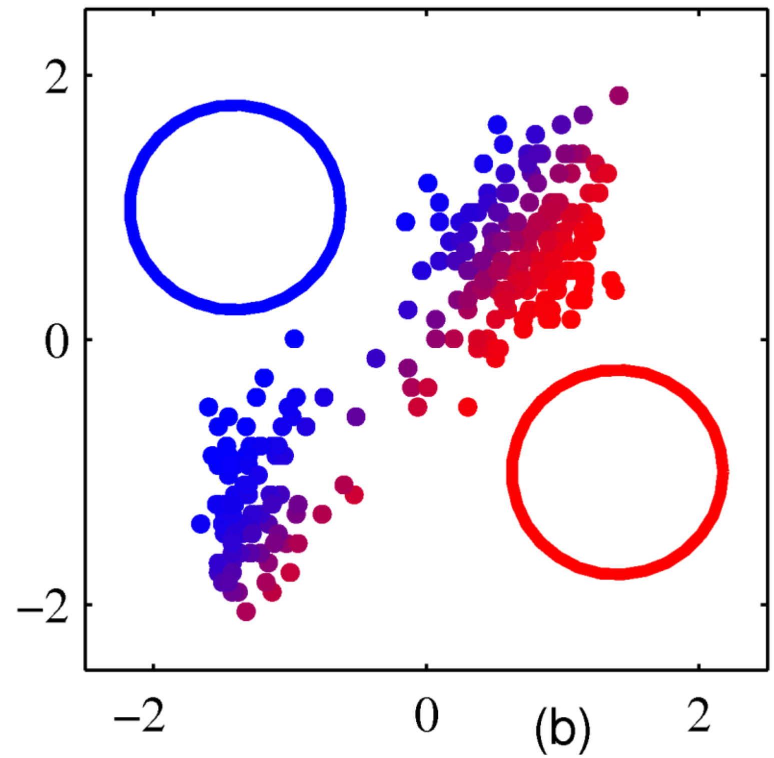
# EM Example

- Initialize parameters: means, covariances, and mixing coefficients.



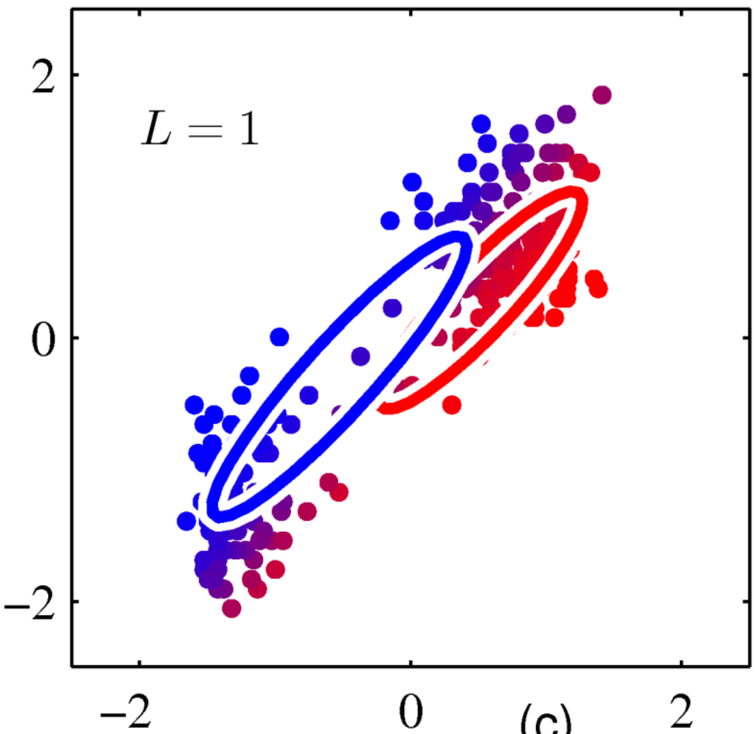
# EM Example

- First E Step



# EM Example

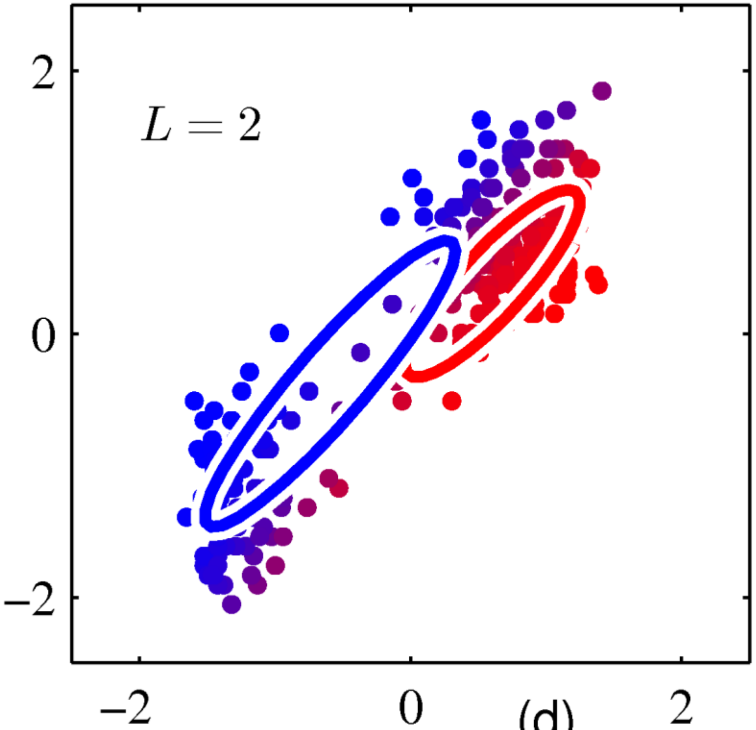
- First M Step



(c)

# EM Example

- Second E and M Steps



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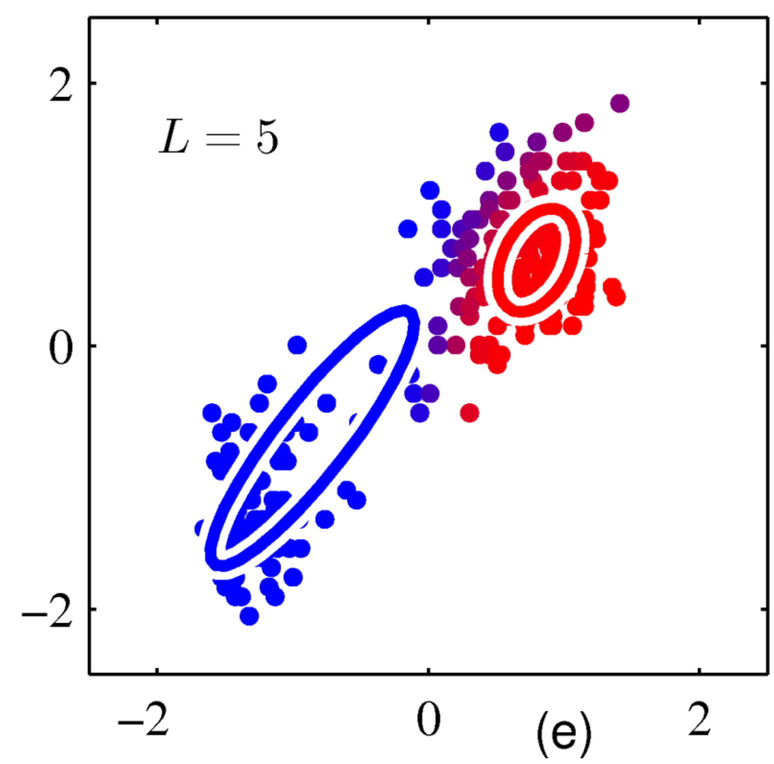
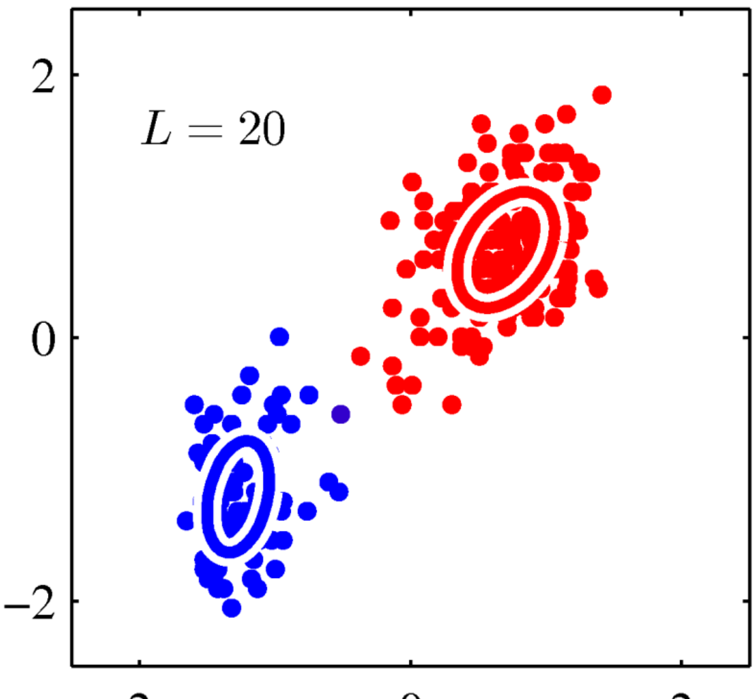
# EM Example

- Three more E-M cycles



# EM Example

- Fifteen E-M cycles later



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# Abstract view of EM

# Latent Variables

- A system with observed variables X,
  - may be far easier to understand in terms of additional variables **Z**,
  - but they are not observed (latent).

- For example, in a mixture of Gaussians,
  - The latent variable **z** specifies which Gaussian generated the sample **x**.
  - The *responsibility* is essentially p(**z** | **x**).

# Latent Variables

- We find model parameters by maximizing log likelihood of observed data.
- If we had complete data {X,Z}, we could easily maximize likelihood $p(\mathbf{X},\mathbf{Z}|\theta)$
- Unfortunately, with incomplete data (X only), we must marginalize over Z, so

$$\ln p(\mathbf{X}|\theta) = \ln\left\{\sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\theta)\right\}$$

- (The sum inside the log makes it hard.)

# Expectation, then Maximization

- E-Step:
  - Given current parameter values, find the *distribution* $p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}})$
  - This lets us define the *expectation*

$$\mathcal{Q}(\theta, \theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\theta)$$

- M-Step:
  - Maximize the expectation of log likelihood, over the distribution $p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}})$

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

# The E-M Algorithm

- Choose initial values for the parameters.

- Repeat:
  - **E-Step:**
  - **M-Step** $p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}})$

$$\theta^{\text{new}} = \arg\max_{\theta} \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\theta)$$

- Until convergence
  - of parameters or log likelihood

# K-Means and E-M

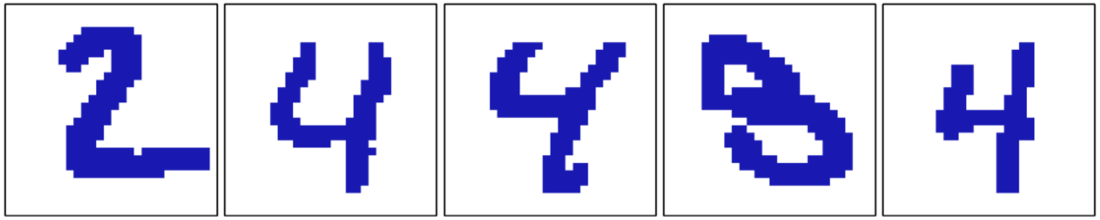
- Consider E-M over Gaussian models with fixed covariance matrix $\epsilon\mathbf{I}$

- In the limit as $\epsilon \to 0$ the responsibility goes to 1 for the closest Gaussian, and 0 elsewhere.

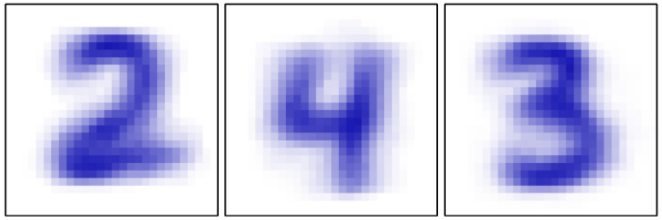
- This gives hard assignment to clusters, and the K-Means algorithm.

# More Clustering

- These images are points in $\{0,1\}^D$.



- We find three clusters:



- The clusters are (very large) mixtures of Bernoulli distributions. These images show the latent responsibilities.

# The EM Algorithm in General

- Our goal is to maximize $p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$
- For any distribution *q*(Z) over latent variables

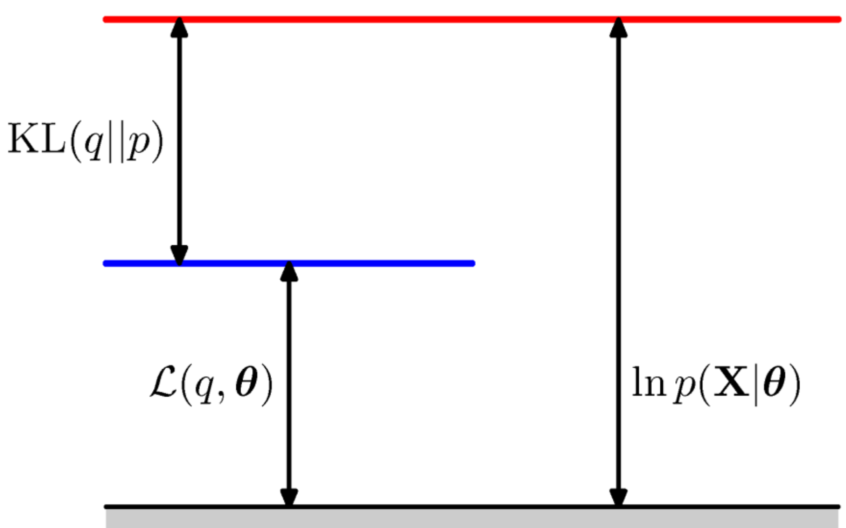
$$\ln p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + KL(q||p)$$

- where

$$\mathcal{L}(q, \theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right\}$$

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

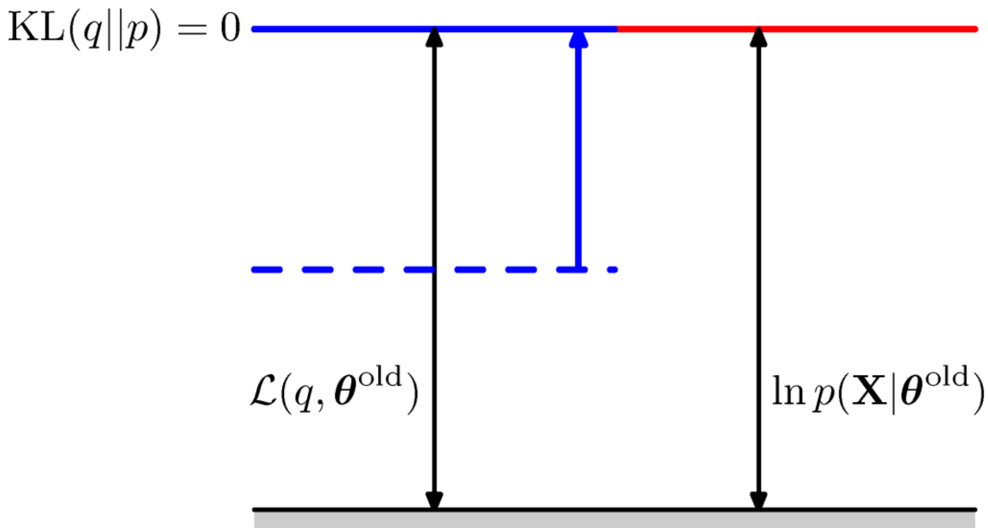
# Visualize the Decomposition




$$\ln p(\mathbf{X}|\theta) = \mathcal{L}(q,\theta) + KL(q||p)$$

- Recall: $KL(q||p) \geq 0$
  - with equality only when *q*=*p*.
- Thus, $\mathcal{L}(q,\theta)$
  - is a lower bound on $\ln p(\mathbf{X}|\theta)$
- which EM tries to maximize.

# Visualize the E-Step

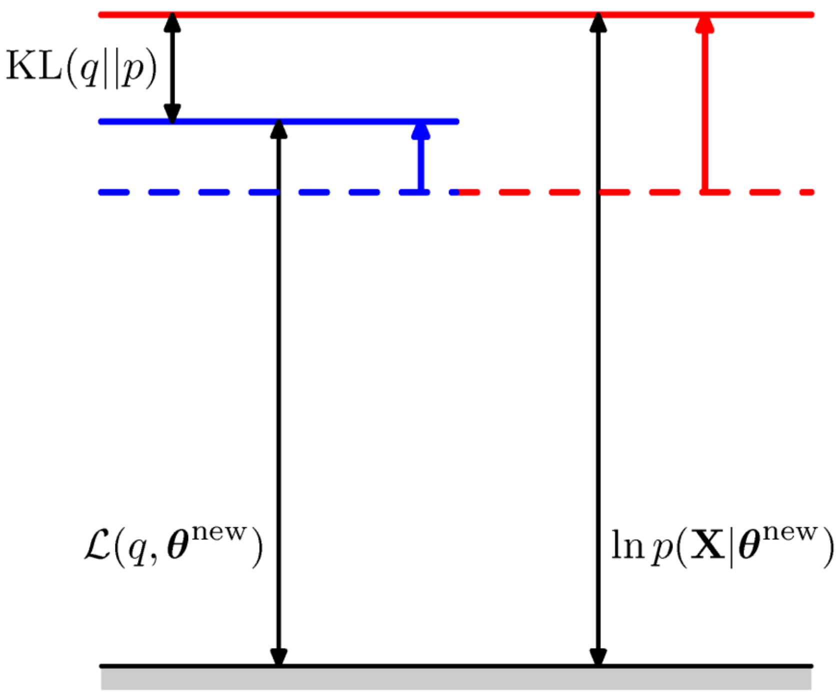



$$\ln p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + KL(q||p)$$

- E-Step changes *q*(Z) to maximize $\mathcal{L}(q, \theta)$
- *q* has no effect on $\ln p(\mathbf{X}|\theta)$
- So maximizes when $KL(q||p) = 0$

$$q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta)$$

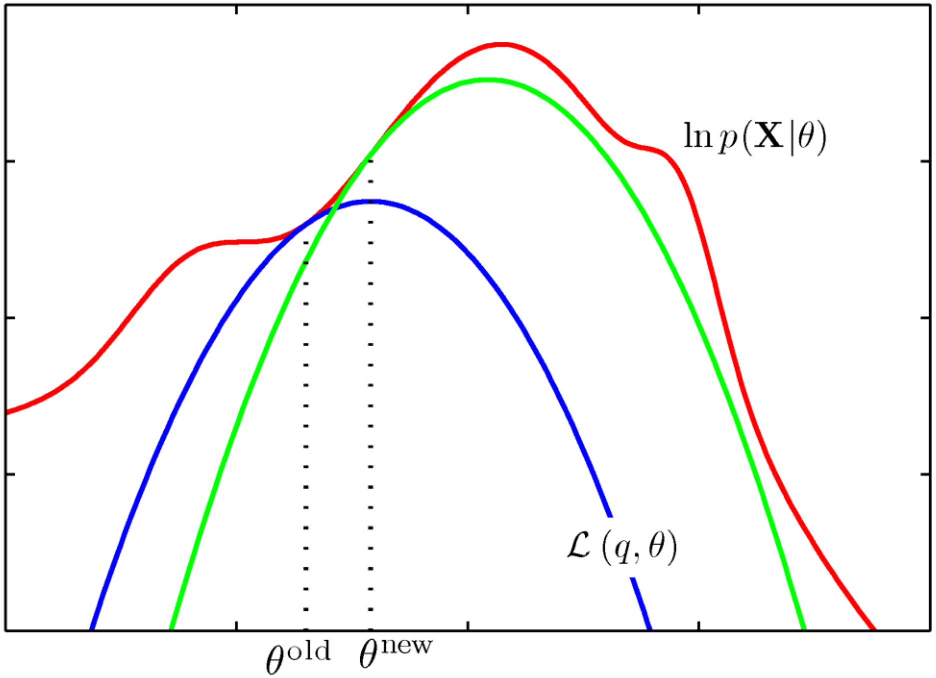
# Visualize the M-Step




$$\ln p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + KL(q||p)$$

- Holding *q*(Z) constant increase $\mathcal{L}(q, \theta)$
- This increases $\ln p(\mathbf{X}|\theta)$
- But now $p \neq q$
- so $KL(q||p) > 0$

# Another view of E-M




- Given old params, find *q* so that
- $\mathcal{L}(q, \theta)$ is tangent to $\ln p(\mathbf{X}|\theta)$
- Find new params to maximize $\mathcal{L}(q, \theta)$
- Then find new *q* to be tangent at a higher point.

# Next

- Unsupervised Learing