15. Clustering

STA3142 Statistical Machine Learning

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Applied Statistics / Statistics and Data Science

Apr 30, 2024

Announcement

- No class @ week 10 (May 7, 9)

- No class & no final exam @ week 16
  - Assignment 5 is the replacement
  - You should submit A5 for your attendance @ week 16

Midterm Grading

- Ongoing; we are trying to release it this week

- If you don’t agree with the Honor code – your midterm score is 0.
  - If you didn’t write the pledge and your name on the first page properly, you receive 0 point.
  - If you did so, your submission will be graded after you complete it.
  - Your academic career is built on academic honesty.

Post-Midterm

- Let’s solve some questions that you felt difficult.
- A survey will be out together with midterm results.
  - To determine questions we are going to solve together

- If you feel you didn’t do well,
  - You are not alone; other students would too.
  - Problem-solving skills can be improved by practice.
    - E.g., Derive ML algorithms we have learned from scratch
    - Don’t just memorize them

Assignment 3

- Due **Friday 5/3, 11:59pm**
- Topics
  - (Programming) K-Nearest Neighbors
  - (Math) MLE vs. MAP
  - (Math) Kernel Methods
  - (Math/Programming) SVM Primal
- Please read the instruction carefully!
  - Submit one pdf and one zip file separately
  - Write your code only in the designated spaces
  - Do not import additional libraries
  - …
- If you feel difficult, consider to take **option 2**.

Recap: Machine Learning Tasks

- Supervised Learning
  - Classification
  - Regression
- Unsupervised Learning
  - Clustering
  - Density estimation
  - Embedding / Dimensionality reduction
- Reinforcement Learning
  - Learning to act
    (e.g., robot control, decision making, etc.)

Recap: Supervised Learning

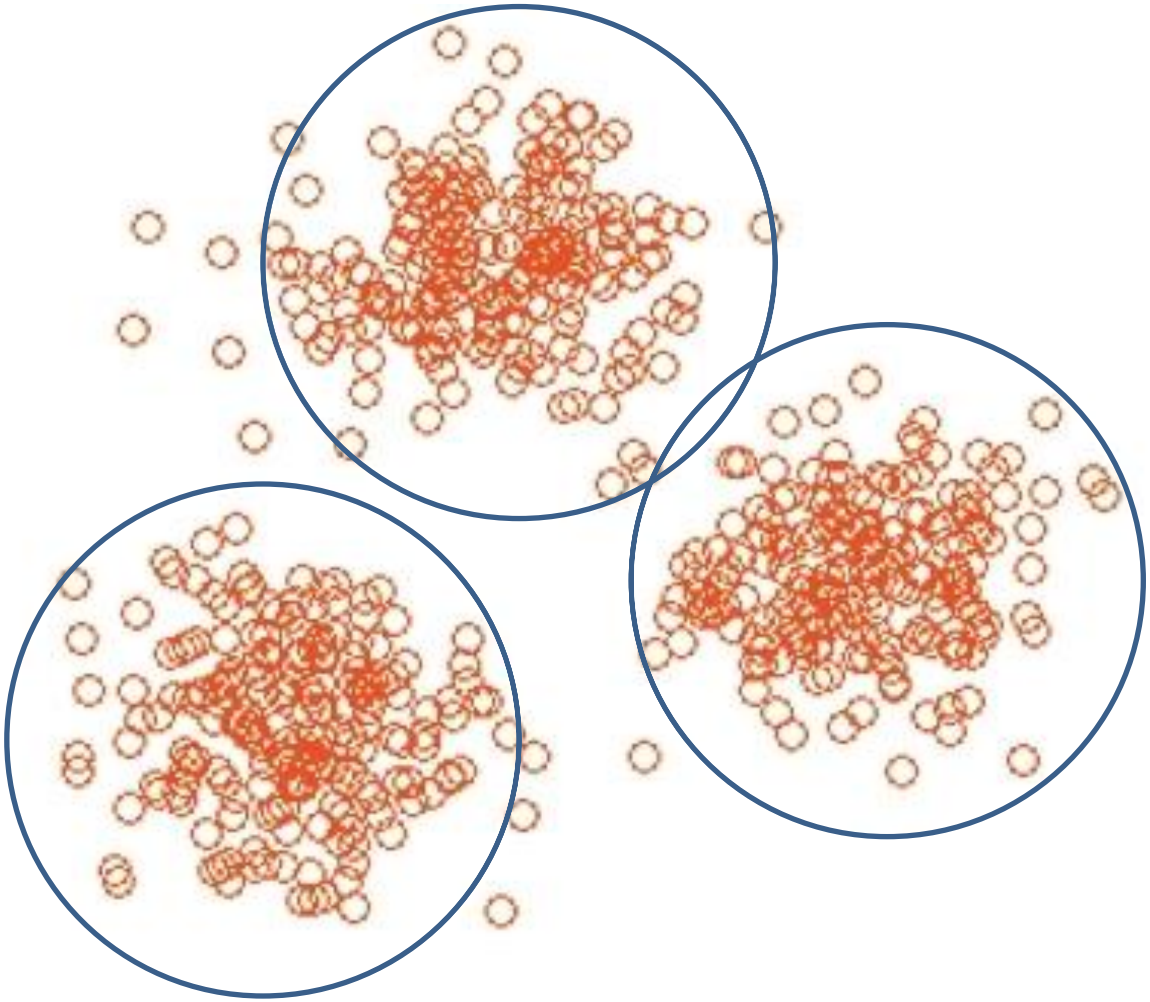
- Given a dataset $D = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, where
  - $x_i \in \mathcal{X}$: input (feature)
  - $y_i \in \mathcal{Y}$: output (label)
- A black box ML algorithm produces a prediction function $h: \mathcal{X} \to \mathcal{Y}$, such that $h(x)$ can predict the y values for all x
  - Not only for all training data $x_i \in D$,
    but also for unseen test data $x^* \in \mathcal{X}$.
- Labels could be discrete or continuous
  - Discrete labels: **classification**
  - Continuous labels: **regression**

Unsupervised Learning

- Given a dataset $D = \{x_1, \ldots, x_n\}$ without any labels, learning the underlying **structure** or **distribution** of the data
  - Clustering
  - Probability distribution (density)
  - Generating data
  - Embedding & neighborhood relations
- "Learning without teacher (supervision)"

Unsupervised Learning: Clustering

- Grouping into similar examples



Unsupervised Learning: Clustering

- Grouping into similar examples

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Slide Credit: Justin Johnson

Outline

- Expectation Maximization (EM)
  - K-Means
  - Gaussian Mixture Models (GMM)
- General View of EM

Expectation Maximization (EM)

- Iteratively learning parameters when data is not fully observed
- Suppose we have observed variables X and latent (hidden) variables Z
  - e.g., clustering: X: data, Z: cluster labels
- Iterate **E-steps** and **M-steps** until converged:
  - **E-step**: Inference about Z given X: $Q = P(Z|X)$
  - **M-step**: Update parameters with Q found at E-step
- EM algorithms for clustering:
  - K-Means (a special case of GMM)
  - Gaussian Mixture Models (GMM)

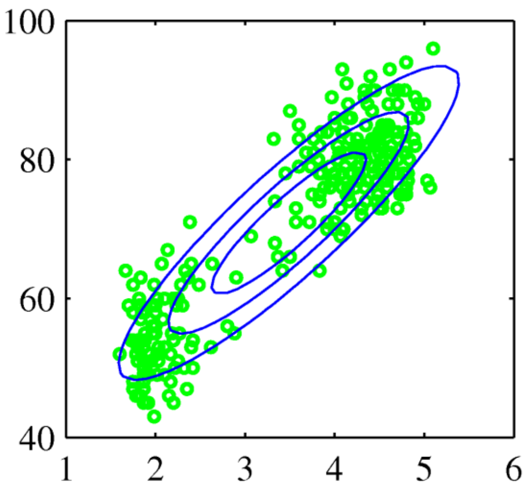
K-Means

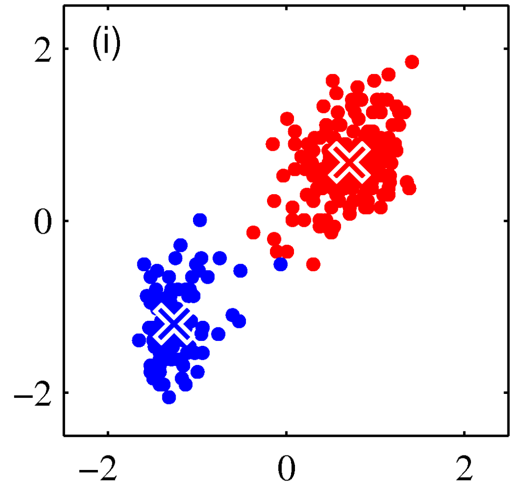
K-Means

- Given unlabeled data $x^{(n)}$ for $n = 1, \ldots, N$,

- Assume that each data belongs to one of the K clusters,

- How do we find the cluster labels?





K-Means: Formulation

- Cluster centers: $\boldsymbol{\mu}_k, k = 1, \dots, K$
- Indicator variables: $r_{nk} \in \{0,1\}, n = 1, \dots, N$
  - $r_{nk} = 1$ if $\mathbf{x}^{(n)}$ is in cluster k.
  - $r_{nj} = 0$ for all $j \neq k$.

- Minimize $J(r, \boldsymbol{\mu})$: sum of squared distances of points from the center of its assigned cluster.

$$J(r, \boldsymbol{\mu}) = \sum_{k=1}^{K} \sum_{n=1}^{N} r_{nk} \left\| \mathbf{x}^{(n)} - \boldsymbol{\mu}_k \right\|^2$$

K-Means Algorithm

- Initialize the cluster centers arbitrarily.
- Repeat the following updates until convergence:
  1. **E-Step**:
  $$r := \operatorname*{argmin}_{r} J(r, \boldsymbol{\mu})$$
  2. **M-Step**:
  $$\boldsymbol{\mu} := \operatorname*{argmin}_{\boldsymbol{\mu}} J(r, \boldsymbol{\mu})$$

K-Means Algorithm

- Initialize the cluster centers arbitrarily.
- Repeat the following updates until convergence:
  1. **E-Step**: Cluster assignment
     - Assign each point to the closest center.

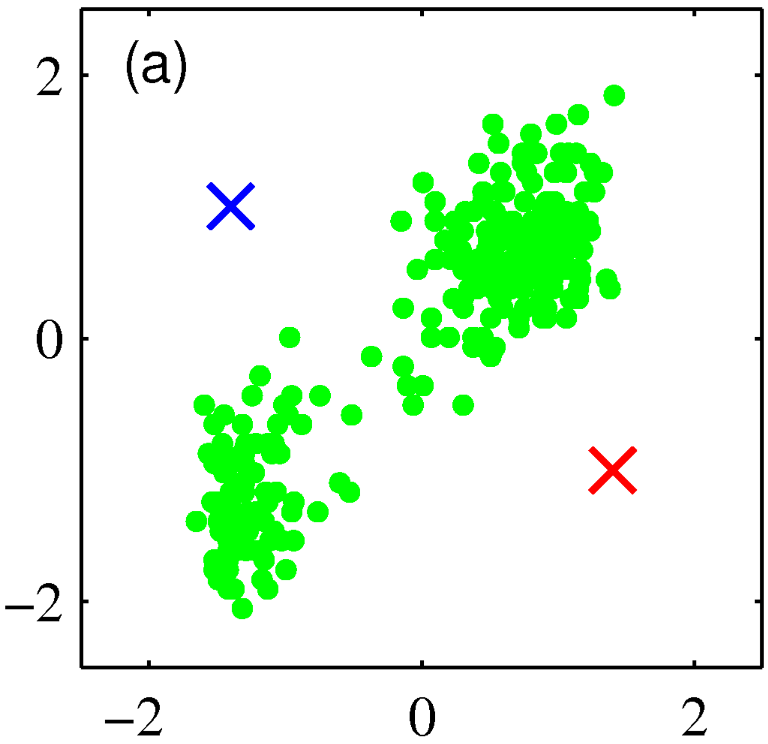
$$r_{nk} := \begin{cases} 1 & \text{if } k = \operatorname*{argmin}_j \left\| \mathbf{x}^{(n)} - \boldsymbol{\mu}_k \right\|^2 \\ 0 & \text{otherwise} \end{cases}$$

  2. **M-Step**: Parameter update
     - Update cluster centers

$$\boldsymbol{\mu} := \frac{\sum_{n=1}^{N} r_{nk} \mathbf{x}^{(n)}}{\sum_{n=1}^{N} r_{nk}}$$

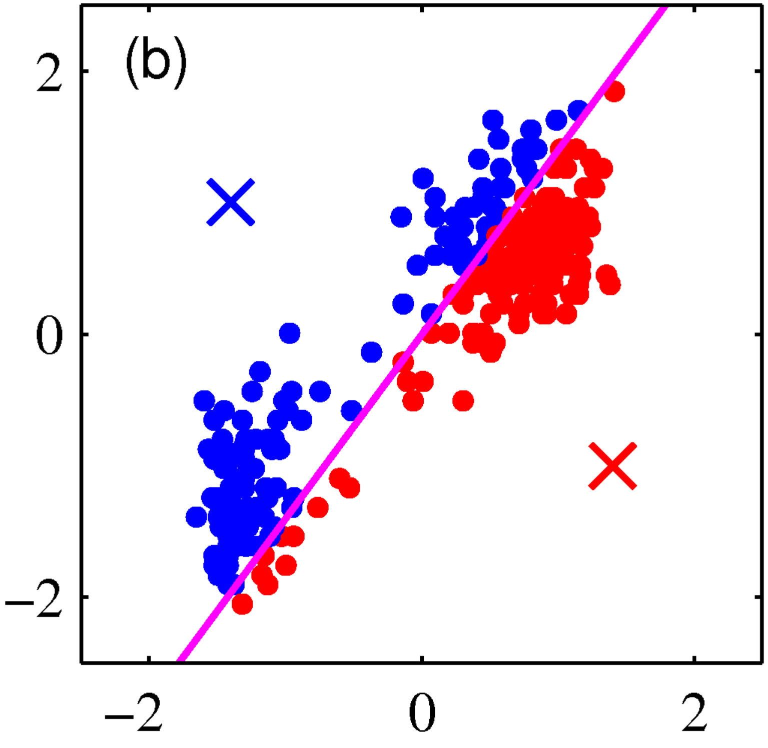
K-Means Example: Initialization

- Choose K and pick random means.
- In this example, $K = 2$.



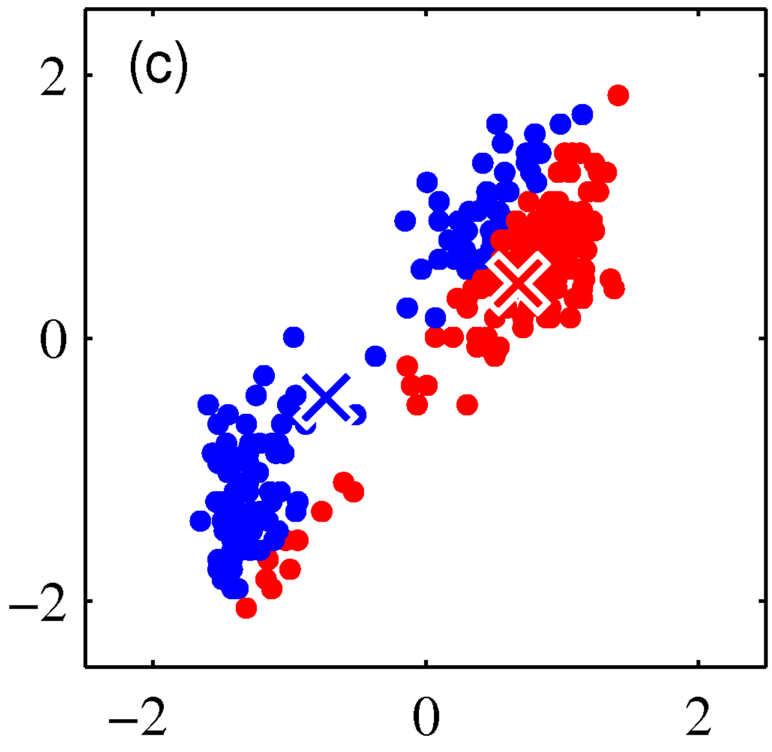
K-Means Example: 1st E-Step

- Assign each data to the nearest center.



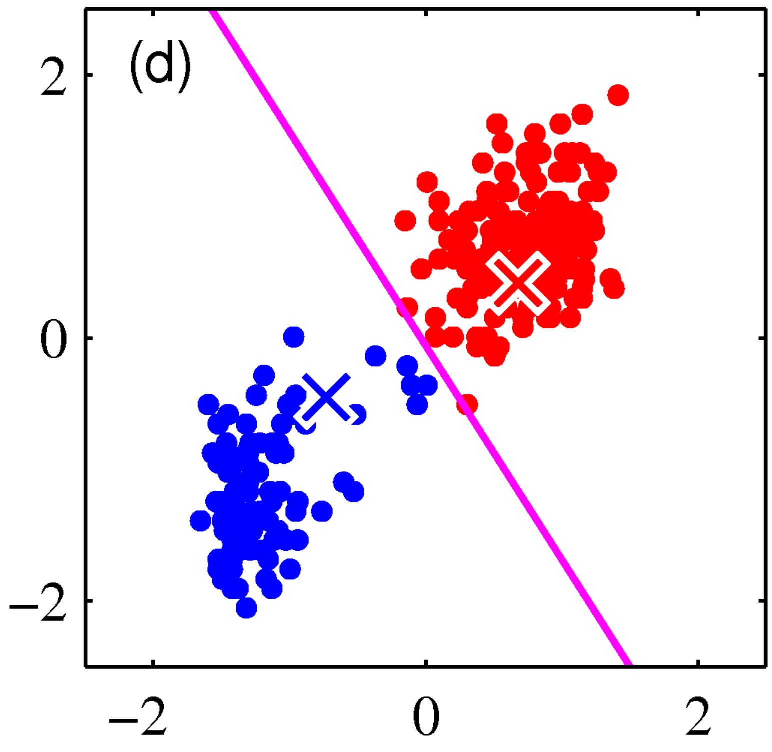
K-Means Example: 1st M-Step

- Compute new centers for each cluster.



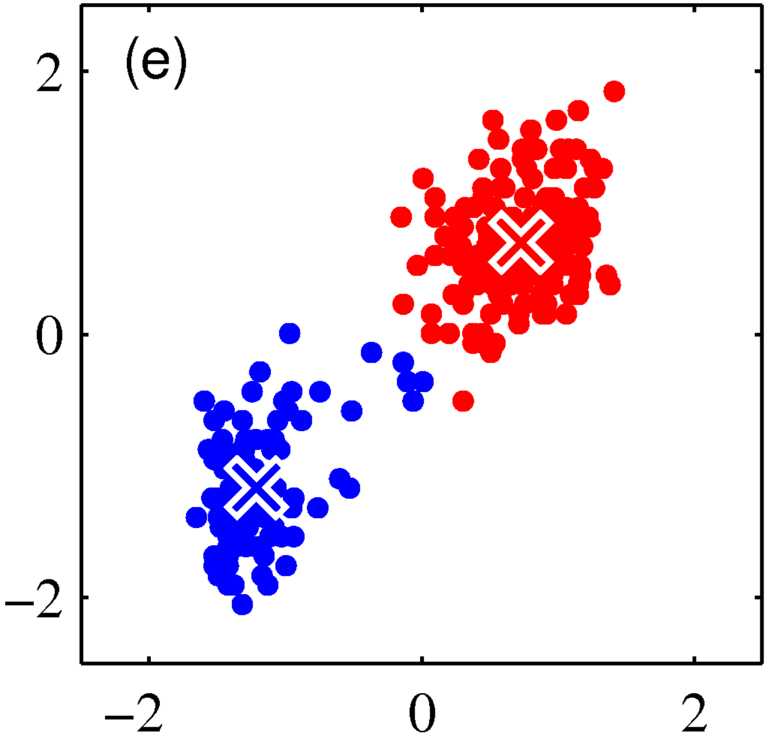
K-Means Example: 2nd E-Step

- Reassign data to the nearest center.



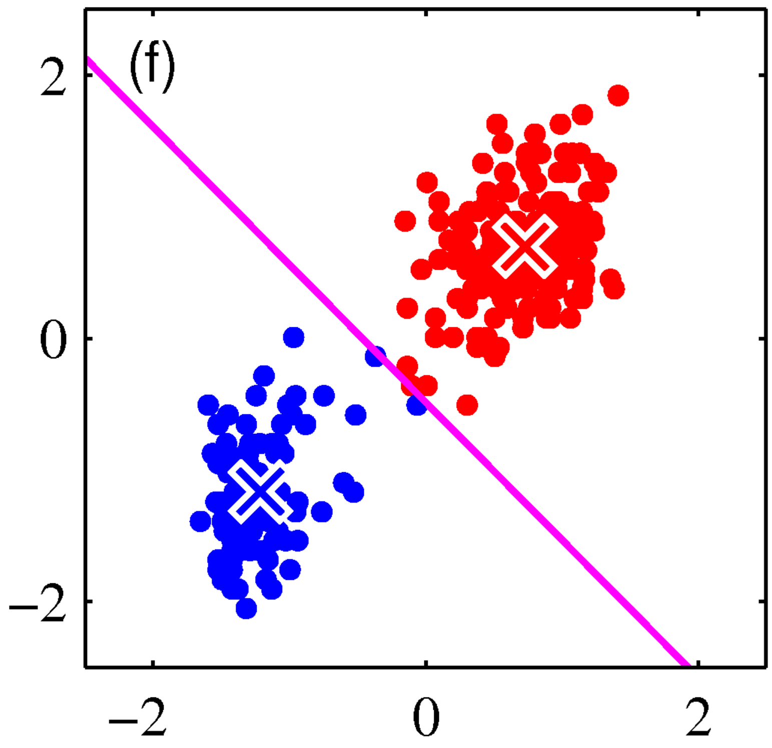
K-Means Example: 2nd M-Step

- Compute new centers for each cluster.



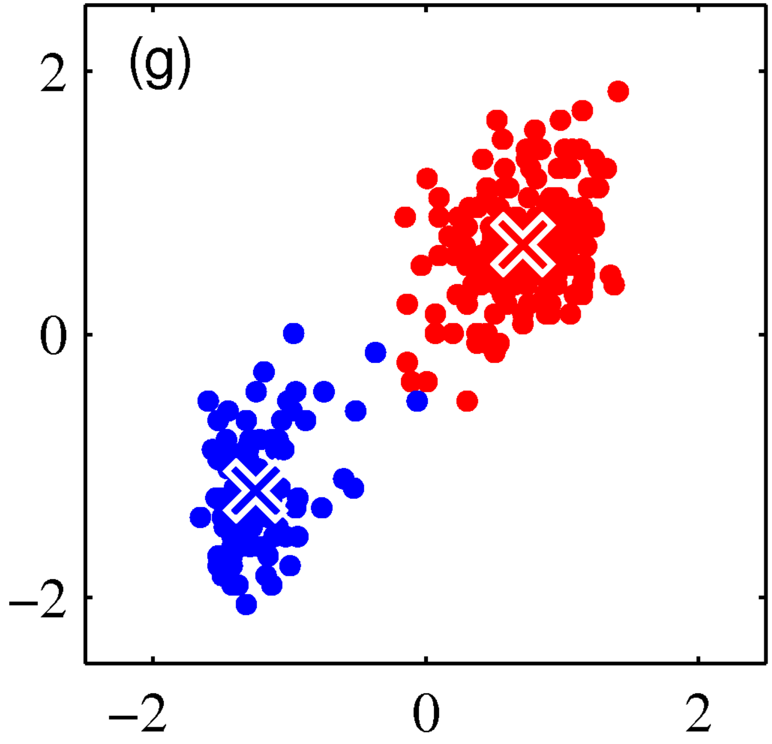
K-Means Example: 3rd E-Step

- Reassign data to the nearest center.



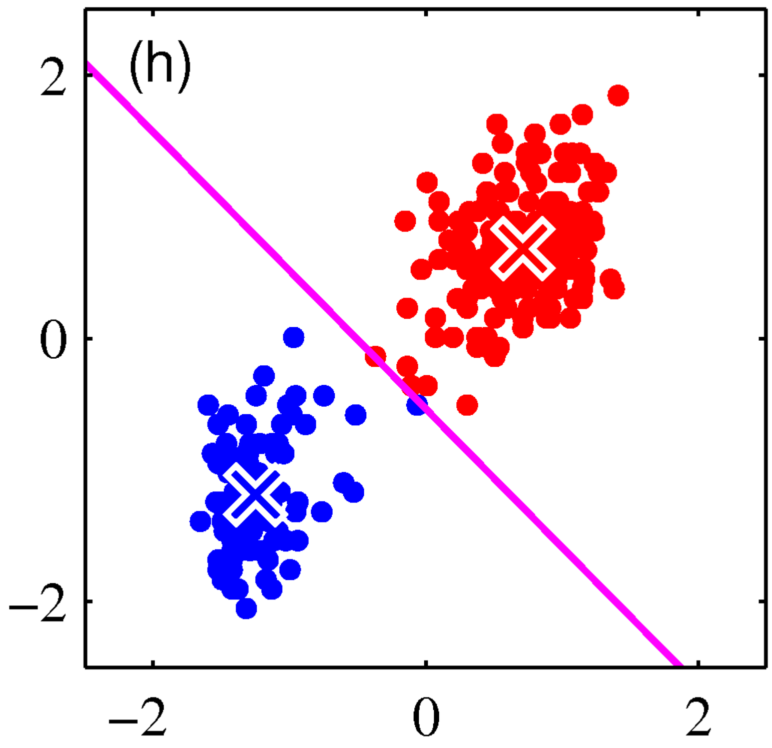
K-Means Example: 3rd M-Step

- Compute new centers for each cluster.



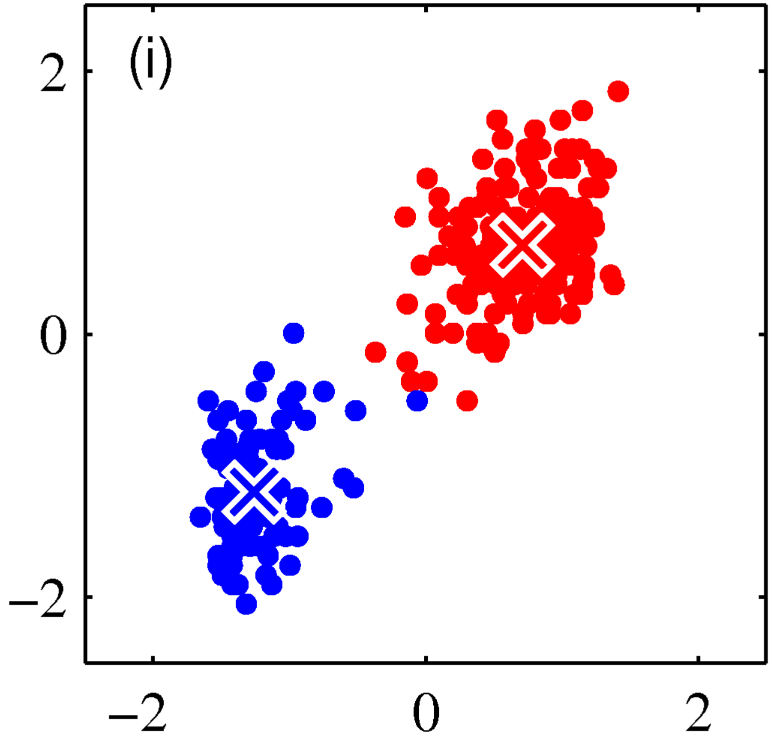
K-Means Example: 4th E-Step

- Reassign data to the nearest center.



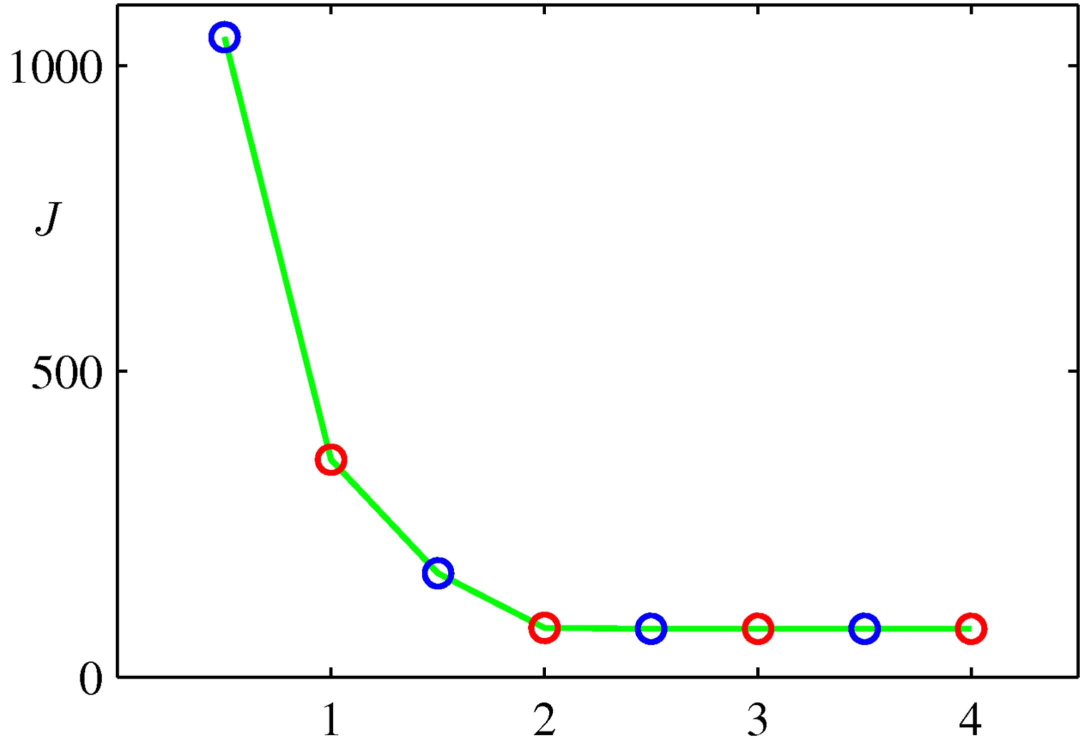
K-Means Example: 4th M-Step

- Compute new centers for each cluster.
- Stop here; cluster centers have stopped changing.



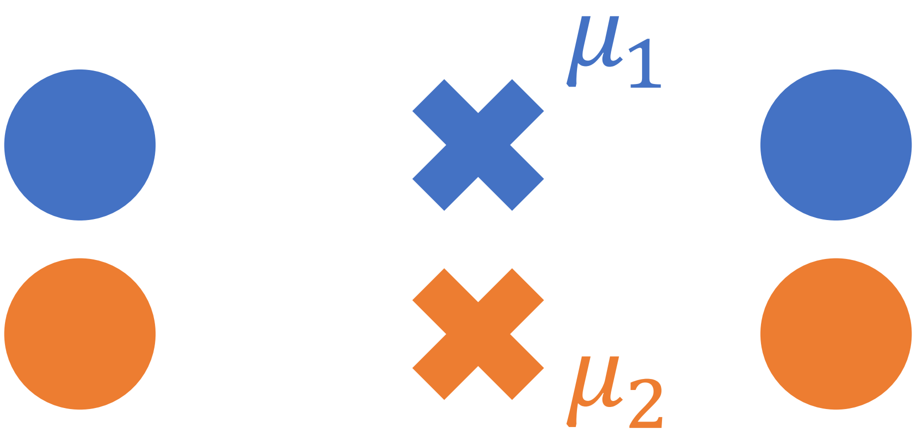
K-Means: Convergence

- Convergence is relatively quick, in # of steps.
  - Blue circles after **E-step**: Assign each point to a cluster
  - Red circles after **M-step**: Recompute the cluster centers
  - However, all those distance computations are expensive.



K-Means: Properties

- The objective function $J(r, \boldsymbol{\mu})$ monotonically decreases over time.
  - It is a general property of the EM algorithm.
- No guarantee to find the **global optimum**.
  - Guaranteed to converge to **local optimum**.
  - Clustering result depends on the initial values.
  - e.g., the following clustering is a stable local optimum



Gaussian Mixture Models

Hard vs. Soft Clusters

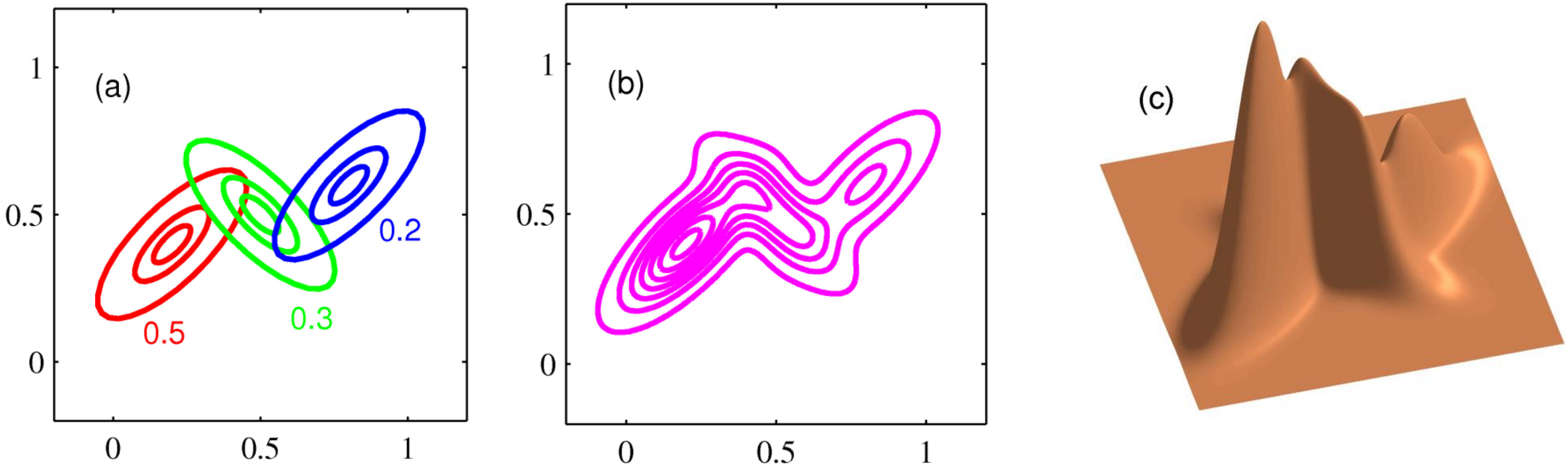
- K-means uses **hard** clustering assignment.
  - Each data belongs to exactly one cluster.

- Gaussian mixture model (GMM) for **soft** clustering
  - Each data is assigned to more than one cluster.
  - Different clusters take different levels of responsibility (posterior probability) for each point.
    - Each data was generated by only one cluster, but we don’t know which one.
  - Note that GMM itself is a probabilistic model, not a clustering method; **EM for GMM** is a clustering method on top of the probabilistic model.

Gaussian Mixture Models

- GMMs make it possible to describe much richer distributions.

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)$$



GMM: Formulation

- Mixing coefficients: π_k, where $\sum_{k=1}^{K} \pi_k = 1$
- Cluster assignments: $\mathbf{z} \in \{0,1\}^K$ (1-of-K)
- Marginal distribution of $\mathbf{z}$:

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

- Conditional distribution of $\mathbf{x}$:

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)$$

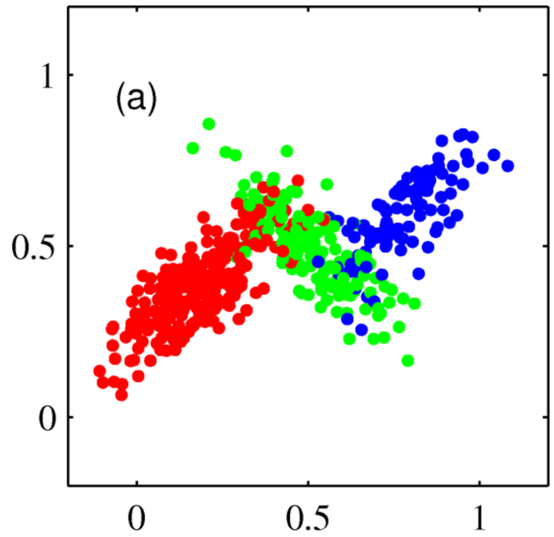
- Marginal distribution of $\mathbf{x}$:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)$$

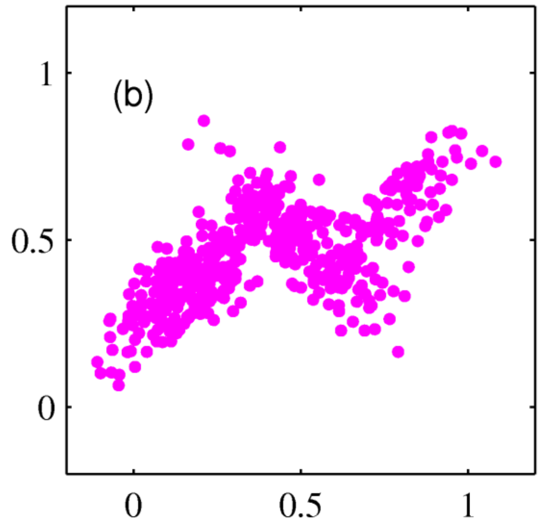
GMM: Formulation

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

$p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$



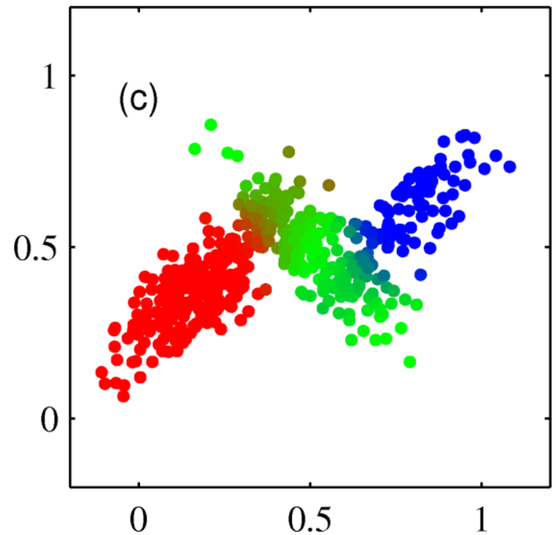
$p(\mathbf{x})$



EM for GMM: E-Step

- Responsibility $\gamma(z_k)$: The degree (posterior prob.) to which each Gaussian explains an observation $\mathbf{x}$.

$$\gamma(z_k) = p(z_k = 1|\mathbf{x})$$
$$= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}_j, \Sigma_j\right)}$$



EM for GMM: M-Step Formulation

- Log-likelihood of observing the data $\mathbf{x}$

$$
\begin{aligned}
\log p(\mathbf{x}) &= \sum_{k=1}^{K} \gamma(z_k) \log p(\mathbf{x}) \\
&= \sum_{k=1}^{K} \gamma(z_k) \log \frac{p(\mathbf{x}, z_k = 1)}{p(z_k = 1 | \mathbf{x})} \\
&= \sum_{k=1}^{K} \gamma(z_k) \log p(\mathbf{x}, z_k = 1) - \sum_{k=1}^{K} \gamma(z_k) \log \gamma(z_k)
\end{aligned}
$$

- Assume $\gamma(z_k)$ is a constant

$$
\log p(\mathbf{x}) = \sum_{k=1}^{K} \gamma(z_k) \log\big(\pi_k \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_k, \Sigma_k)\big) + C
$$

EM for GMM: M-Step Formulation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \sum_{k=1}^{K} \gamma(z_k) \log\left(\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)\right) + C \\
&= \sum_{k=1}^{K} \gamma(z_k) \log \pi_k + \sum_{k=1}^{K} \gamma(z_k) \log \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) + C \\
&= \sum_{k=1}^{K} \gamma(z_k) \log \pi_k + \frac{1}{2} \sum_{k=1}^{K} \gamma(z_k) \log\left|\Sigma_k^{-1}\right| \\
&\quad - \frac{1}{2} \sum_{k=1}^{K} \gamma(z_k) (\mathbf{x} - \boldsymbol{\mu}_k)^T \Sigma_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) + C
\end{aligned}
$$

EM for GMM: M-Step Formulation

- Log-likelihood:

$$L = \log p\left(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\right) = \sum_{n=1}^{N} \log p\left(\mathbf{x}^{(n)}\right)$$

$$= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log \pi_k + \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log\left|\Sigma_k^{-1}\right|$$

$$- \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k\right)^T \Sigma_k^{-1} \left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k\right) + C$$

EM for GMM: M-Step Formulation

- Learning objective: maximum log-likelihood

$$\max_{\{\boldsymbol{\mu}_k, \Sigma_k, \pi_k\}_{k=1}^{K}} L$$

$$\text{subject to} \sum_{k=1}^{K} \pi_k = 1$$

  - where

$$L = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log \pi_k + \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log\left|\Sigma_k^{-1}\right|$$
$$- \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k\right)^T \Sigma_k^{-1} \left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k\right)$$

EM for GMM: M-Step Derivation

- MLE with respect to $\boldsymbol{\mu}_k$:

$$L = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\log\pi_k + \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\log\left|\Sigma_k^{-1}\right|$$
$$-\frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)^T\Sigma_k^{-1}\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)$$

$$\frac{\partial L}{\partial\boldsymbol{\mu}_k} = \frac{1}{2}\sum_{n=1}^{N}\gamma(z_{nk})\Sigma_k^{-1}\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right) = 0$$
$$\therefore\ \boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}^{(n)}}{\sum_{n=1}^{N}\gamma(z_{nk})}$$

EM for GMM: M-Step Derivation

- MLE with respect to $M = \Sigma_k^{-1}$:

$$L = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\log\pi_k + \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\log|M|$$

$$-\frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)^T M\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)$$

$$\frac{\partial\log|X|}{\partial X} = (X^{-1})^T \qquad \frac{\partial\mathbf{a}^T X\mathbf{b}}{\partial X} = \mathbf{a}\mathbf{b}^T$$

$$\frac{\partial L}{\partial M} = \frac{1}{2}\sum_{n=1}^{N}\gamma(z_{nk})M^{-1} - \frac{1}{2}\sum_{n=1}^{N}\gamma(z_{nk})\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)^T = 0$$

$$\therefore M^{-1} = \Sigma_k = \frac{\sum_{n=1}^{N}\gamma(z_{nk})\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)\left(\mathbf{x}^{(n)}-\boldsymbol{\mu}_k\right)^T}{\sum_{n=1}^{N}\gamma(z_{nk})}$$

EM for GMM: M-Step Derivation

- MLE with respect to π_k:

$$\max_{\{\pi_k\}_{k=1}^K} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log \pi_k$$

$$\text{subject to } \sum_{k=1}^{K} \pi_k = 1$$

- Lagrangian function:

$$\mathcal{L}(\pi_1, \dots, \pi_K) = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log \pi_k - \alpha \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

EM for GMM: M-Step Derivation

- Lagrangian function:

$$\mathcal{L}(\pi_1, \ldots, \pi_K) = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log \pi_k - \alpha \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = \sum_{n=1}^{N} \frac{\gamma(z_{nk})}{\pi_k} - \alpha = 0$$

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

- From the constraint:

$$\sum_{k=1}^{K} \pi_k = \frac{1}{\alpha} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) = \frac{N}{\alpha} = 1$$

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

EM for GMM: M-Step

- The mean of a cluster is the weighted mean, weighted by the responsibilities $\gamma(z_{nk})$.

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}^{(n)}$$

  - where $N_k = \sum_{n=1}^{N} \gamma(z_{nk})$ is the effective number of data in cluster k

- Likewise for covariance:

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k\right)\left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k\right)^T$$

- Mixing coefficients: $\pi_k = \frac{N_k}{N}$

EM for GMM: Summary

- Initialize means $\boldsymbol{\mu}_k$, covariances Σ_k, and mixing coefficients π_k for K Gaussians.
- **E-Step**: Given the parameters $\{\boldsymbol{\mu}_k, \Sigma_k, \pi_k\}$, evaluate the responsibilities $\gamma(z_{nk})$.

$$\gamma(z_{nk}) = p\left(z_k = 1 | \mathbf{x}^{(n)}\right) = \frac{\pi_k \mathcal{N}\left(\mathbf{x}^{(n)} \middle| \boldsymbol{\mu}_k, \Sigma_k\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\mathbf{x}^{(n)} \middle| \boldsymbol{\mu}_j, \Sigma_j\right)}$$

- **M-Step**: Given the responsibilities $\gamma(z_{nk})$, estimate the parameters $\{\boldsymbol{\mu}_k, \Sigma_k, \pi_k\}$.

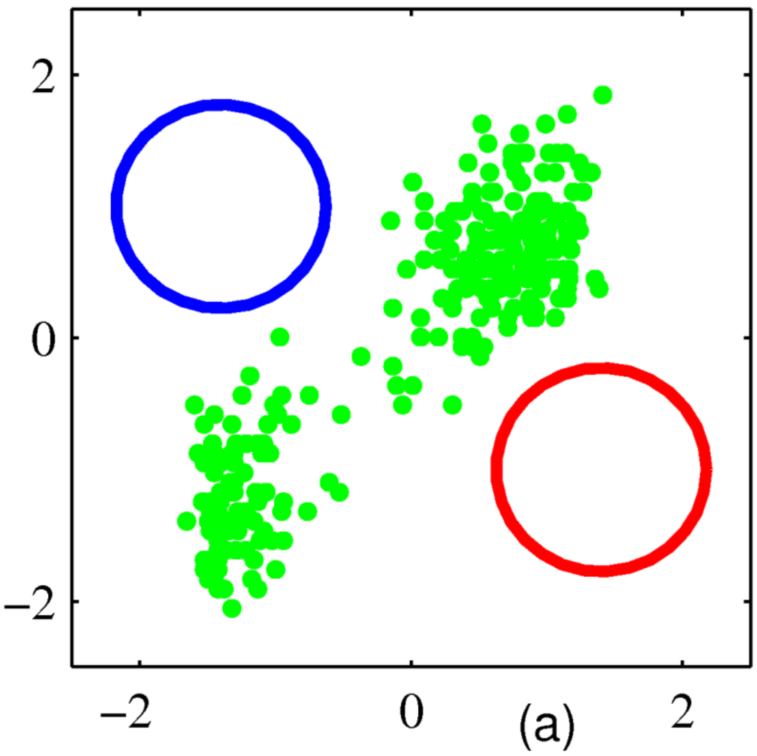
$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}^{(n)}, \pi_k^{\text{new}} = \frac{N_k}{N}, \text{where } N_k = \sum_{n=1}^{N} \gamma(z_{nk})$$

$$\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k^{\text{new}}\right) \left(\mathbf{x}^{(n)} - \boldsymbol{\mu}_k^{\text{new}}\right)^T$$

- Stop when the parameters or likelihood converges.

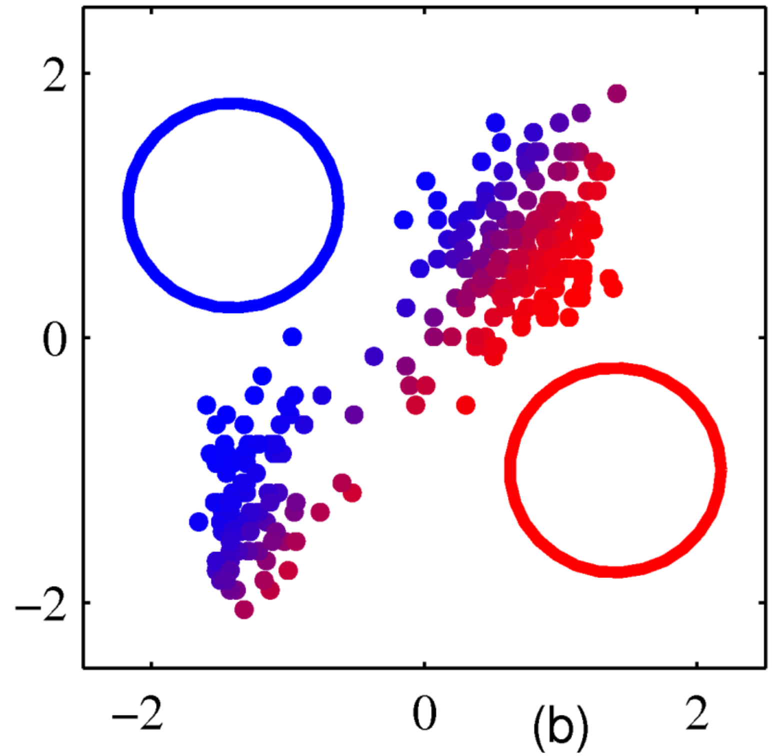
EM for GMM Example

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



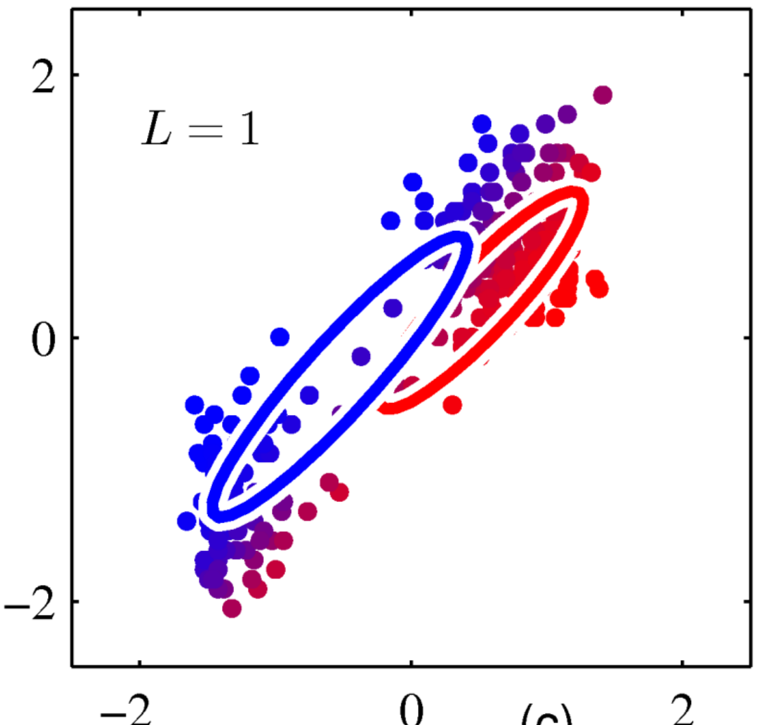
EM for GMM Example: 1st E-Step

- Evaluate the responsibilities.



EM for GMM Example: 1st M-Step

- Estimate the parameters.



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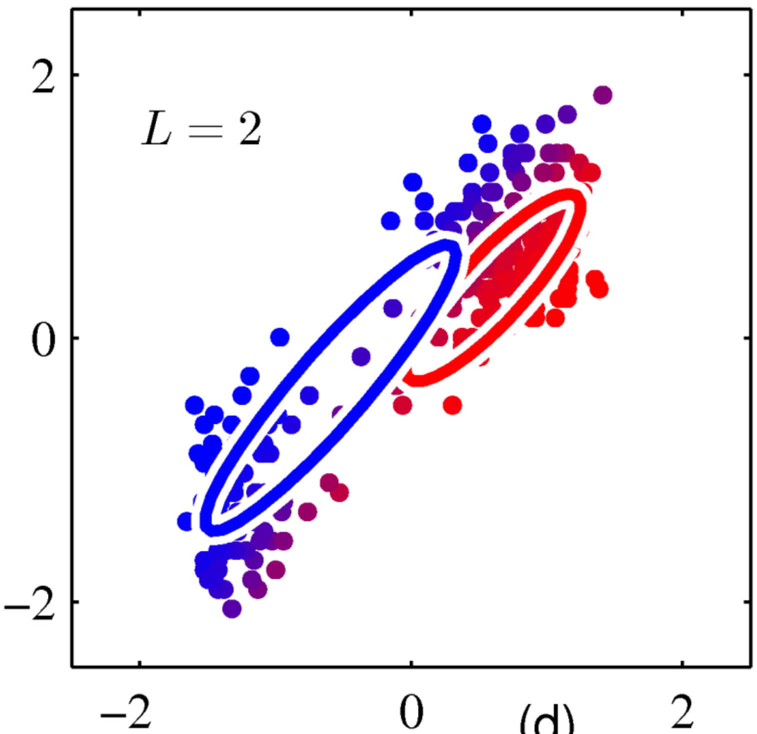
EM for GMM Example: 2nd Steps

- Evaluate the responsibilities first, then estimate the parameters.



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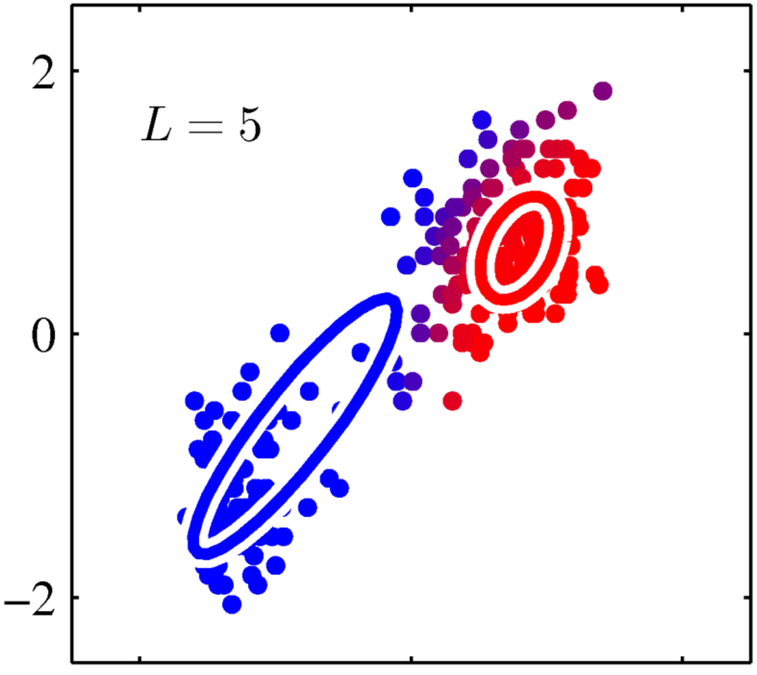
EM for GMM Example: 5^{th} Steps

- Evaluate the responsibilities first, then estimate the parameters.



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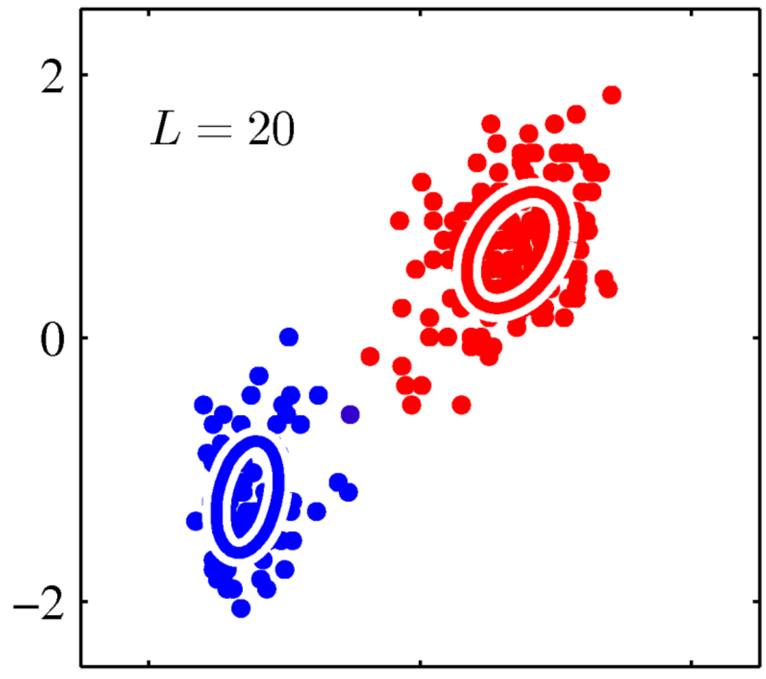
EM for GMM Example: 20^{th} Steps

- Evaluate the responsibilities first, then estimate the parameters.



(f)

EM for GMM vs. K-Means

- Fix the covariance matrix for each cluster as a diagonal matrix:

$$\Sigma_k = \sigma^2 I$$

- If we take $\sigma^2 \rightarrow 0$, then the update rules converge to K-means clustering.

General View of EM

EM: Motivation

- Suppose a system with observed variables X.
- It may be easier to understand with additional latent variables Z, which are not observed.

- E.g., in GMM, the latent variable Z specifies which Gaussian generated the sample X.
  - The responsibility is the posterior $p(Z|X)$.

EM: Motivation

- In ML, we usually find model parameters θ by maximizing log-likelihood of observed data.
- If we had complete data $\{X, Z\}$, we could easily maximize likelihood $p(X, Z|\theta)$.
- However, when not all variables are observed, we can marginalize over the unobserved variables:

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

  - If Z is continuous, replace the sum with integral
- The summation over the latent variables is inside the logarithm, resulting in complicated expressions.

EM: Formulation

- EM finds the local maximum likelihood of $\log p(X)$ by alternating:
- **E-Step**: Given current parameters θ^{old}, find the posterior distribution of Z given X: $p(Z|X, \theta^{\text{old}})$
- Then, we find the expectation of the complete-data log-likelihood using the posterior:

$$Q(\theta, \theta^{\text{old}}) = \sum_{Z} \underbrace{p(Z|X, \theta^{\text{old}})}_{\text{Constant w.r.t. } \theta} \log p(X, Z|\theta)$$

- **M-Step**: Maximize the expectation:

$$\theta^{\text{new}} = \underset{\theta}{\operatorname{argmax}}\, Q(\theta, \theta^{\text{old}})$$

EM: Derivation

- Goal: Maximize $p(X|\theta) = \sum_Z p(X, Z|\theta)$
- For any distribution $q(Z)$, $(q(Z) \geq 0, \sum_Z q(Z) = 1)$

$$\log p(X|\theta) = \sum_Z q(Z) \log p(X|\theta)$$

  - $\log p(X|\theta)$ is independent to Z

EM: Derivation

- Goal: Maximize $p(X|\theta) = \sum_Z p(X, Z|\theta)$
- For any distribution $q(Z)$, $(q(Z) \geq 0, \sum_Z q(Z) = 1)$

$$\log p(X|\theta) = \sum_Z q(Z) \log p(X|\theta)$$
$$= \sum_Z q(Z) \log \frac{p(X, Z|\theta)}{p(Z|X, \theta)}$$

  - Conditional probability: $p(X, Z|\theta) = p(X|\theta)p(Z|X, \theta)$

EM: Derivation

- Goal: Maximize $p(X|\theta) = \sum_Z p(X, Z|\theta)$
- For any distribution $q(Z)$, ($q(Z) \geq 0, \sum_Z q(Z) = 1$)

$$\log p(X|\theta) = \sum_Z q(Z) \log p(X|\theta)$$
$$= \sum_Z q(Z) \log \frac{p(X, Z|\theta)}{p(Z|X, \theta)}$$
$$= \sum_Z q(Z) \log \frac{p(X, Z|\theta)}{q(Z)} \frac{q(Z)}{p(Z|X, \theta)}$$

  - Introduce auxiliary $q(Z)$

EM: Derivation

- Goal: Maximize $p(X|\theta) = \sum_Z p(X,Z|\theta)$
- For any distribution $q(Z)$, $(q(Z) \geq 0, \sum_Z q(Z) = 1)$

$$
\begin{aligned}
\log p(X|\theta) &= \sum_Z q(Z) \log p(X|\theta) \\
&= \sum_Z q(Z) \log \frac{p(X,Z|\theta)}{p(Z|X,\theta)} \\
&= \sum_Z q(Z) \log \frac{p(X,Z|\theta)}{q(Z)} \frac{q(Z)}{p(Z|X,\theta)} \\
&= \sum_Z q(Z) \log \frac{p(X,Z|\theta)}{q(Z)} + \sum_Z q(Z) \log \frac{q(Z)}{p(Z|X,\theta)} \\
&= \mathcal{L}(q,\theta) + KL\big(q(Z)||p(Z|X)\big)
\end{aligned}
$$

- $\mathcal{L}(q,\theta)$: The lower bound we maximize
- $KL\big(q(Z)||p(Z|X)\big)$: Gap between $q(Z)$ and $p(Z|X)$

EM: Derivation

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&= \sum_Z q(Z) \log \frac{p(X, Z|\theta)}{q(Z)} + \sum_Z q(Z) \log \frac{q(Z)}{p(Z|X, \theta)} \\
&= \mathcal{L}(q, \theta) + KL\big(q(Z) || p(Z|X)\big) \\
&\geq \mathcal{L}(q, \theta)
\end{aligned}
$$

- KL divergence is nonnegative: $KL\big(q(Z) || p(Z|X)\big) \geq 0$

EM: Another Derivation

- Given the observed variables X, latent variables Z, and parameters θ:

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

  - Introduce Z

EM: Another Derivation

- Given the observed variables X, latent variables Z, and parameters θ:

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

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

  - Introduce auxiliary $q(Z)$ where $q(Z) \geq 0, \sum_Z q(Z) = 1$

EM: Another Derivation

- Given the observed variables X, latent variables Z, and parameters θ:

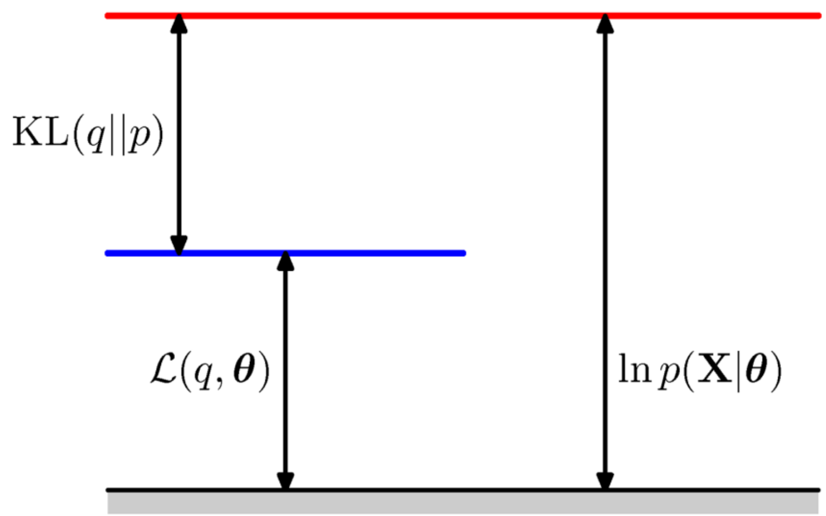
$$\log p(X|\theta) = \log \sum_{Z} p(X,Z|\theta)$$
$$= \log \sum_{Z} q(Z) \frac{p(X,Z|\theta)}{q(Z)}$$
$$\geq \sum_{Z} q(Z) \log \frac{p(X,Z|\theta)}{q(Z)} = \mathcal{L}(q,\theta)$$

  - Jensen's inequality
  - Equality holds when $p(X,Z|\theta)/q(Z)$ is constant.

EM: Visualizing Decompositions

$$\log p(X|\theta) = \mathcal{L}(q, \theta) + KL\big(q(Z)||p(Z|X)\big)$$

- $KL(q||p) \geq 0$; equality holds only when $q = p$.
- Thus, $\mathcal{L}(q, \theta)$ is the lower bound of $\log p(X|\theta)$, which EM maximizes.

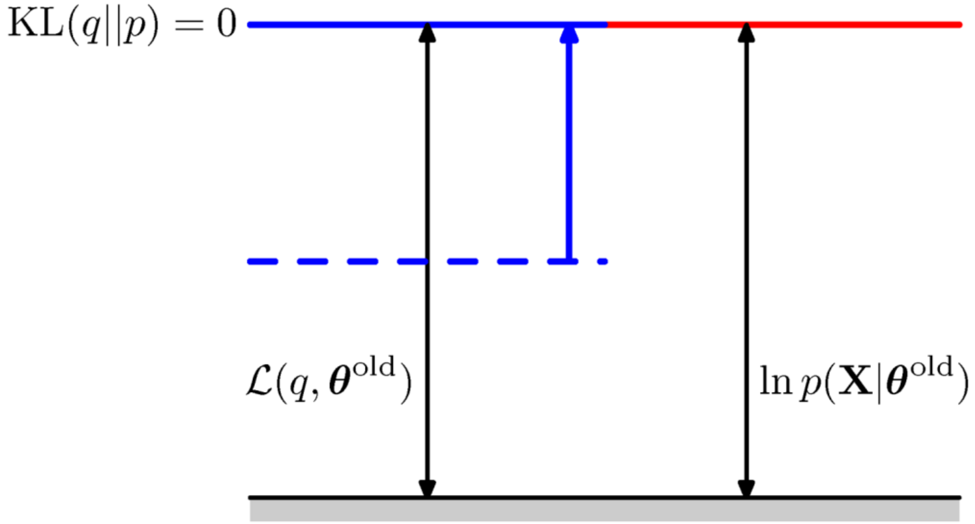


EM: Visualizing Decompositions

$$\log p(X|\theta) = \mathcal{L}(q,\theta) + KL\big(q(Z)||p(Z|X)\big)$$

- **E-Step** updates $q(Z)$ to maximize $\mathcal{L}(q,\theta)$.
- $q(Z)$ is maximized when $KL\big(q(Z)||p(Z|X)\big) = 0$

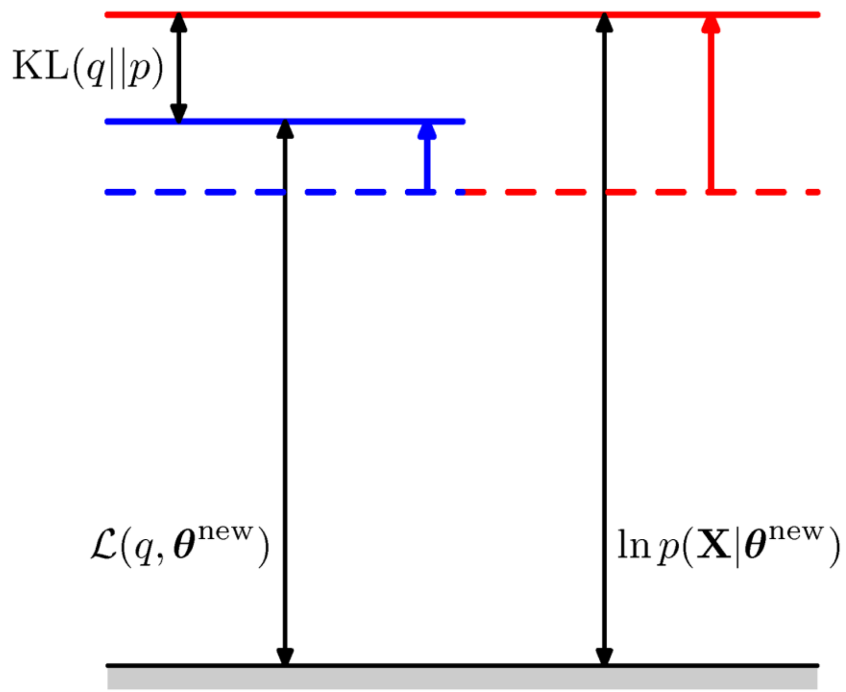
$$q(Z) = p(Z|X,\theta)$$



EM: Visualizing Decompositions

$$\log p(X|\theta) = \mathcal{L}(q,\theta) + KL\big(q(Z)||p(Z|X)\big)$$

- **M-Step**: Increase $\mathcal{L}(q,\theta)$ with $q(Z)$ as constant
  - This increases $\log p(X|\theta)$, but then $q(Z) \neq p(Z|X,\theta)$
- Iterate EM until converged



Next: Dimensionality Reduction