

k -Means Clustering

He He

Slides based on Lecture 13a from David Rosenberg's course materials
(<https://github.com/davidrosenberg/mlcourse>)

CDS, NYU

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Final exam

- Period: 6:00pm EST, May 12 – 8:00pm EST, May 12
- Format: on Gradescope, same as midterm
- Coverage: mainly about material from week 6 onwards but can overlap with basic concepts before midterm
- Submission: **Make sure you leave enough time for submission!**

K-means Clustering

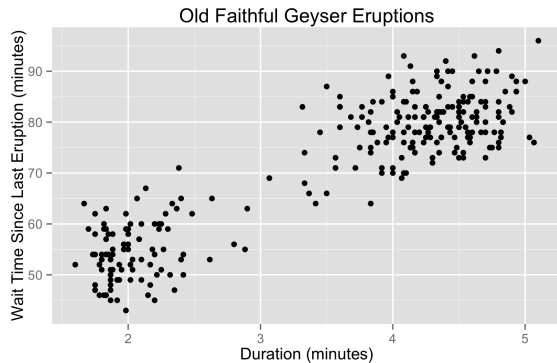
Unsupervised learning

Goal Discover interesting *structure* in the data.

Formulation Density estimation: $p(x; \theta)$ (often with *latent* variables).

- Examples**
- Discover *clusters*: cluster data into groups.
 - Discover *factors*: project high-dimensional data to a small number of “meaningful” dimensions, i.e. dimensionality reduction.
 - Discover *graph structures*: learn joint distribution of correlated variables, i.e. graphical models.

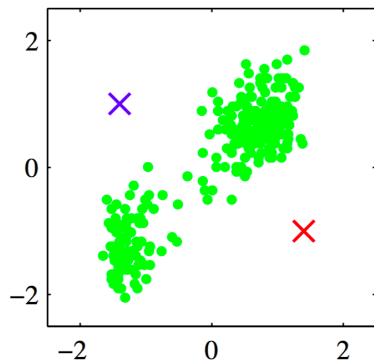
Example: Old Faithful Geyser



- Looks like two clusters.
- How to find these clusters algorithmically?

k -Means: By Example

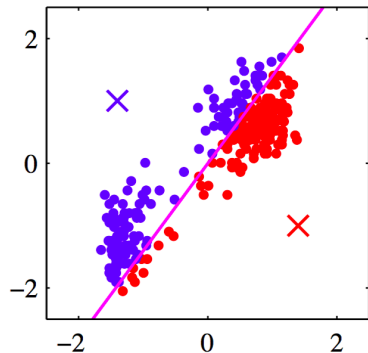
- Standardize the data.
- Choose two cluster centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(a).

k-means: by example

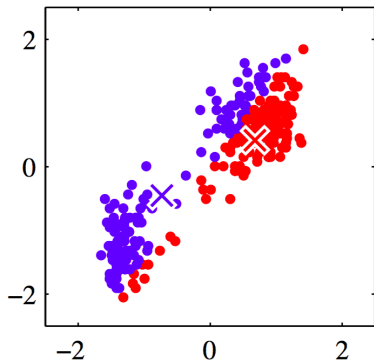
- Assign each point to closest center.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(b).

k -means: by example

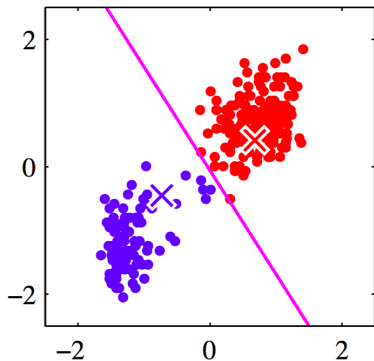
- Compute new cluster centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(c).

k -means: by example

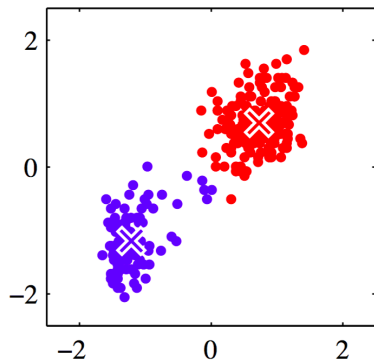
- Assign points to closest center.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(d).

k -means: by example

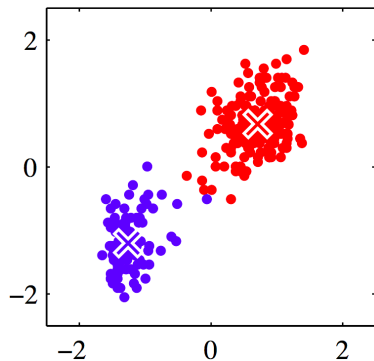
- Compute cluster centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(e).

k -means: by example

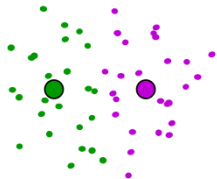
- Iterate until convergence.



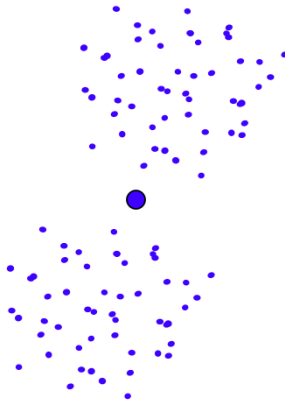
From Bishop's *Pattern recognition and machine learning*, Figure 9.1(i).

Suboptimal Local Minimum

- The clustering for $k = 3$ below is a local minimum, but suboptimal:



Would be better to have
one cluster here



... and two clusters here

Formalize k -Means

- Dataset $\mathcal{D} = \{x_1, \dots, x_n\} \subset \mathcal{X}$ where $\mathcal{X} = \mathbb{R}^d$.
- Goal: Partition data \mathcal{D} into k disjoint sets C_1, \dots, C_k .
- Let $c_i \in \{1, \dots, k\}$ be the cluster assignment of x_i .
- The **centroid** of C_i is defined to be

$$\mu_i = \arg \min_{\mu \in \mathcal{X}} \sum_{x \in C_i} \|x - \mu\|^2. \quad \text{mean of } C_i \quad (1)$$

- The k -means objective is to minimize the distance between each example and its cluster centroid:

$$J(c, \mu) = \sum_{i=1}^n \|x_i - \mu_{c_i}\|^2. \quad (2)$$

k-Means: Algorithm

- 1 Initialize: Randomly choose initial centroids $\mu_1, \dots, \mu_k \in \mathbb{R}^d$.
- 2 Repeat until convergence (i.e. c_i doesn't change anymore):

- 1 For all i , set

$$c_i \leftarrow \arg \min_j \|x_i - \mu_j\|^2. \quad \text{Minimize } J \text{ w.r.t. } c \text{ while fixing } \mu \quad (3)$$

- 2 For all j , set

$$\mu_j \leftarrow \frac{1}{|C_j|} \sum_{x \in C_j} x. \quad \text{Minimize } J \text{ w.r.t. } \mu \text{ while fixing } c. \quad (4)$$

- Recall the objective: $J(c, \mu) = \sum_{i=1}^n \|x_i - \mu_{c_i}\|^2$.

Avoid bad local minima

k -means converges to a local minimum.

- J is non-convex, thus no guarantee to converging to the global minimum.

Avoid getting stuck with bad local minima:

- Re-run with random initial centroids.
- **k -means++**: choose initial centroids that spread over all data points.
 - Randomly choose the first centroid from the data points \mathcal{D} .
 - Sequentially choose subsequent centroids from points that are farther away from current centroids:
 - Compute distance between each x_i and the closest already chosen centroids.
 - Randomly choose next centroid with probability proportional to the computed distance squared.

Summary

We've seen

- Clustering—an unsupervised learning problem that aims to discover group assignments.
- k -means:
 - Algorithm: alternating between assigning points to clusters and computing cluster centroids.
 - Objective: minimizing some loss function by coordinate descent.
 - Converge to a local minimum.

Next, probabilistic model of clustering.

- A generative model of x .
- Maximum likelihood estimation.

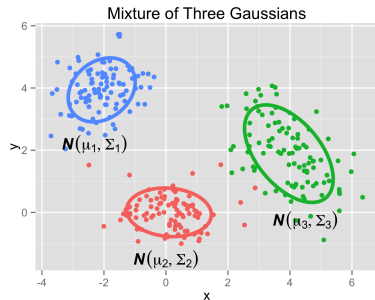
Gaussian Mixture Models

Probabilistic Model for Clustering

- Problem setup:
 - There are k clusters (or **mixture components**).
 - We have a probability distribution for each cluster.
- Generative story of a **mixture distribution**:
 - 1 Choose a random cluster $z \in \{1, 2, \dots, k\}$.
 - 2 Choose a point from the distribution for cluster z .

Example:

- 1 Choose $z \in \{1, 2, 3\}$ with $p(1) = p(2) = p(3) = \frac{1}{3}$.
- 2 Choose $x \mid z \sim \mathcal{N}(X \mid \mu_z, \Sigma_z)$.



Gaussian mixture model (GMM)

Generative story of GMM with k mixture components:

- 1 Choose cluster $z \sim \text{Categorical}(\pi_1, \dots, \pi_k)$.
- 2 Choose $x \mid z \sim \mathcal{N}(\mu_z, \Sigma_z)$.

Probability density of x :

- Sum over (marginalize) the **latent variable** z .

$$p(x) = \sum_z p(x, z) \tag{5}$$

$$= \sum_z p(x \mid z) p(z) \tag{6}$$

$$= \sum_k \pi_k \mathcal{N}(\mu_k, \Sigma_k) \tag{7}$$

Identifiability Issues for GMM

- Suppose we have found parameters

Cluster probabilities: $\pi = (\pi_1, \dots, \pi_k)$

Cluster means: $\mu = (\mu_1, \dots, \mu_k)$

Cluster covariance matrices: $\Sigma = (\Sigma_1, \dots, \Sigma_k)$

that are at a local minimum.

- What happens if we shuffle the clusters? e.g. Switch the labels for clusters 1 and 2.
- We'll get the same likelihood. How many such equivalent settings are there?
- Assuming all clusters are distinct, there are $k!$ equivalent solutions.
- Not a problem *per se*, but something to be aware of.

we should be careful when interpret the meaning of a cluster. It is tempting to say that cluster 1 is politics, 2 is sports etc. But we will always need to look at the examples in that cluster instead of just relying on the cluster id, which are interchangeable.

Learning GMMs

How to learn the parameters π_k, μ_k, Σ_k ?

- MLE (also called maximize marginal likelihood).
- Log likelihood of data:

$$L(\theta) = \sum_{i=1}^n \log p(x_i; \theta) \quad (8)$$

$$= \sum_{i=1}^n \log \sum_z p(x, z; \theta) \quad (9)$$

- Cannot push log into the sum... z and x are coupled.
- No closed-form solution for GMM—try to compute the gradient yourself!

Gradient Descent / SGD for GMM

- What about running gradient descent or SGD on

$$J(\pi, \mu, \Sigma) = - \sum_{i=1}^n \log \left\{ \sum_{z=1}^k \pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z) \right\}?$$

- Can be done, in principle – but need to be clever about it.
- For example, each covariance matrix $\Sigma_1, \dots, \Sigma_k$ has to be positive semidefinite.
- How to maintain that constraint?
 - Rewrite $\Sigma_i = M_i M_i^T$, where M_i is an unconstrained matrix.
 - Then Σ_i is positive semidefinite.
- Even then, pure gradient-based methods have trouble.¹

¹See Hosseini and Sra's [Manifold Optimization for Gaussian Mixture Models](#) for discussion and further references.

Learning GMMs: observable case

Suppose we observe cluster assignments z . Then MLE is easy:

$$n_z = \sum_{i=1}^n 1(z_i = z) \quad \# \text{ examples in each cluster} \quad (10)$$

$$\hat{\pi}(z) = \frac{n_z}{n} \quad \text{fraction of examples in each cluster} \quad (11)$$

$$\hat{\mu}_z = \frac{1}{n_z} \sum_{i: z_i = z} x_i \quad \text{empirical cluster mean} \quad (12)$$

$$\hat{\Sigma}_z = \frac{1}{n_z} \sum_{i: z_i = z} (x_i - \hat{\mu}_z)(x_i - \hat{\mu}_z)^T. \quad \text{empirical cluster covariance} \quad (13)$$

The inference problem: observe x , want to know z .

$$p(z = j | x_i) = p(x, z = j) / p(x) \quad (14)$$

$$= \frac{p(x | z = j) p(z = j)}{\sum_k p(x | z = k) p(z = k)} \quad (15)$$

$$= \frac{\pi_j \mathcal{N}(x_i | \mu_j, \Sigma_j)}{\sum_k \pi_k \mathcal{N}(x_i | \mu_k, \Sigma_k)} \quad (16)$$

- $p(z | x)$ is a *soft assignment*.
- If we know the parameters μ, Σ, π , this would be easy to compute.

Let's compute the cluster assignments and the parameters iteratively.

The expectation-minimization (EM) algorithm:

- ① Initialize parameters μ, Σ, π randomly.
- ② Run until convergence:
 - ① E-step: fill in latent variables by inference.
 - compute soft assignments $p(z | x_i)$ for all i .
 - ② M-step: standard MLE for μ, Σ, π given “observed” variables.
 - Equivalent to MLE in the observable case on data weighted by $p(z | x_i)$.

M-step for GMM

- Let $p(z | x)$ be the soft assignments:

$$\gamma_i^j = \frac{\pi_j^{\text{old}} \mathcal{N}(x_i | \mu_j^{\text{old}}, \Sigma_j^{\text{old}})}{\sum_{c=1}^k \pi_c^{\text{old}} \mathcal{N}(x_i | \mu_c^{\text{old}}, \Sigma_c^{\text{old}})}.$$

- Exercise: show that

$$n_z = \sum_{i=1}^n \gamma_i^z$$

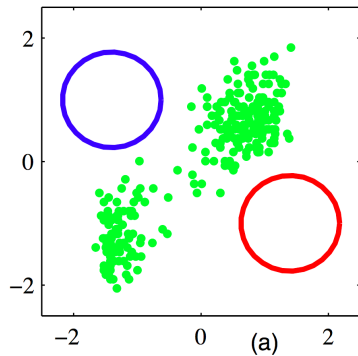
$$\mu_z^{\text{new}} = \frac{1}{n_z} \sum_{i=1}^n \gamma_i^z x_i$$

$$\Sigma_z^{\text{new}} = \frac{1}{n_z} \sum_{i=1}^n \gamma_i^z (x_i - \mu_z^{\text{new}}) (x_i - \mu_z^{\text{new}})^T$$

$$\pi_z^{\text{new}} = \frac{n_z}{n}.$$

EM for GMM

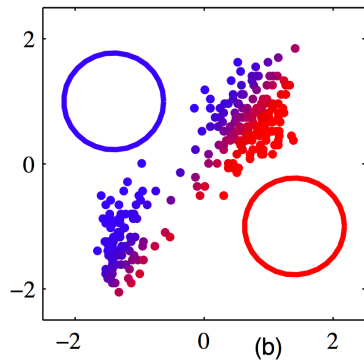
- Initialization



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

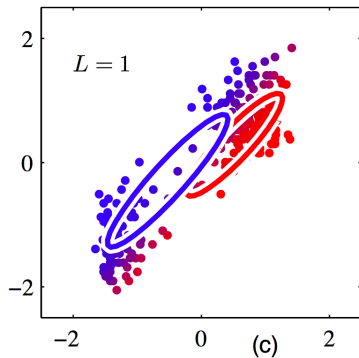
- First soft assignment:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

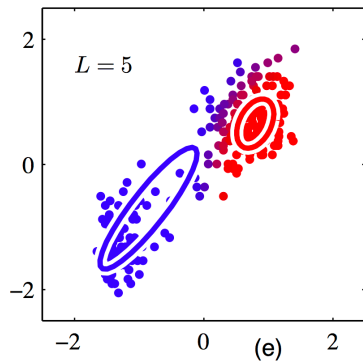
- First soft assignment:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

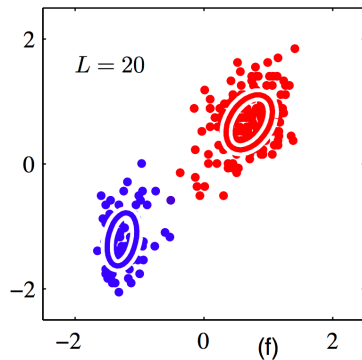
- After 5 rounds of EM:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

- After 20 rounds of EM:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM: Summary

- EM is a general algorithm for learning latent variable models.
- *Key idea*: if data was fully observed, then MLE is easy.
 - E-step: fill in latent variables by computing $p(z \mid x, \theta)$.
 - M-step: standard MLE given fully observed data.
- Simpler and more efficient than gradient methods.
- Can prove that EM monotonically improves the likelihood and converges to a local minimum.
- k -means is a special case of EM for GMM with *hard assignments*, also called hard-EM.

Latent Variable Models

General Latent Variable Model

- Two sets of random variables: z and x .
- z consists of unobserved **hidden variables**.
- x consists of **observed variables**.
- Joint probability model parameterized by $\theta \in \Theta$:

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

Definition

A **latent variable model** is a probability model for which certain variables are never observed.

e.g. The Gaussian mixture model is a latent variable model.

Complete and Incomplete Data

- Suppose we observe some data (x_1, \dots, x_n) .
- To simplify notation, take x to represent the entire dataset

$$x = (x_1, \dots, x_n),$$

and z to represent the corresponding unobserved variables

$$z = (z_1, \dots, z_n).$$

- An observation of x is called an **incomplete data set**.
- An observation (x, z) is called a **complete data set**.

Our Objectives

- **Learning problem:** Given incomplete dataset x , find MLE

$$\hat{\theta} = \arg \max_{\theta} p(x | \theta).$$

- **Inference problem:** Given x , find conditional distribution over z :

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

- For Gaussian mixture model, learning is hard, inference is easy.
- For more complicated models, inference can also be hard. (See DSGA-1005)

Log-Likelihood and Terminology

- Note that

$$\arg \max_{\theta} p(x \mid \theta) = \arg \max_{\theta} [\log p(x \mid \theta)].$$

- Often easier to work with this “**log-likelihood**”.
- We often call $p(x)$ the **marginal likelihood**,
 - because it is $p(x, z)$ with z “marginalized out”:

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

- We often call $p(x, z)$ the **joint**. (for “joint distribution”)
- Similarly, $\log p(x)$ is the **marginal log-likelihood**.

EM Algorithm

Intuition

Problem: marginal log-likelihood $\log p(x; \theta)$ is hard to optimize (observing only x)

Observation: complete data log-likelihood $\log p(x, z; \theta)$ is easy to optimize (observing both x and z)

Idea: guess a distribution of the latent variables $q(z)$ (soft assignments)

Maximize the **expected complete data log-likelihood**:

$$\max_{\theta} \sum_{z \in \mathcal{Z}} q(z) \log p(x, z; \theta)$$

EM assumption: the expected complete data log-likelihood is easy to optimize

Why should this work?

Math Prerequisites

Jensen's Inequality

Theorem (Jensen's Inequality)

If $f : \mathbb{R} \rightarrow \mathbb{R}$ is a **convex** function, and x is a random variable, then

$$\mathbb{E}f(x) \geq f(\mathbb{E}x).$$

Moreover, if f is **strictly convex**, then equality implies that $x = \mathbb{E}x$ with probability 1 (i.e. x is a constant).

- e.g. $f(x) = x^2$ is convex. So $\mathbb{E}x^2 \geq (\mathbb{E}x)^2$. Thus

$$\text{Var}(x) = \mathbb{E}x^2 - (\mathbb{E}x)^2 \geq 0.$$

Kullback-Leibler Divergence

- Let $p(x)$ and $q(x)$ be probability mass functions (PMFs) on \mathcal{X} .
- How can we measure how “different” p and q are?
- The **Kullback-Leibler** or “**KL**” **Divergence** is defined by

$$\text{KL}(p\|q) = \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)}.$$

(Assumes $q(x) = 0$ implies $p(x) = 0$.)

- Can also write this as

$$\text{KL}(p\|q) = \mathbb{E}_{x \sim p} \log \frac{p(x)}{q(x)}.$$

Gibbs Inequality ($\text{KL}(p\|q) \geq 0$ and $\text{KL}(p\|p) = 0$)

Theorem (Gibbs Inequality)

Let $p(x)$ and $q(x)$ be PMFs on \mathcal{X} . Then

$$\text{KL}(p\|q) \geq 0,$$

with equality iff $p(x) = q(x)$ for all $x \in \mathcal{X}$.

- KL divergence measures the “distance” between distributions.
- Note:
 - KL divergence **not a metric**.
 - KL divergence is **not symmetric**.

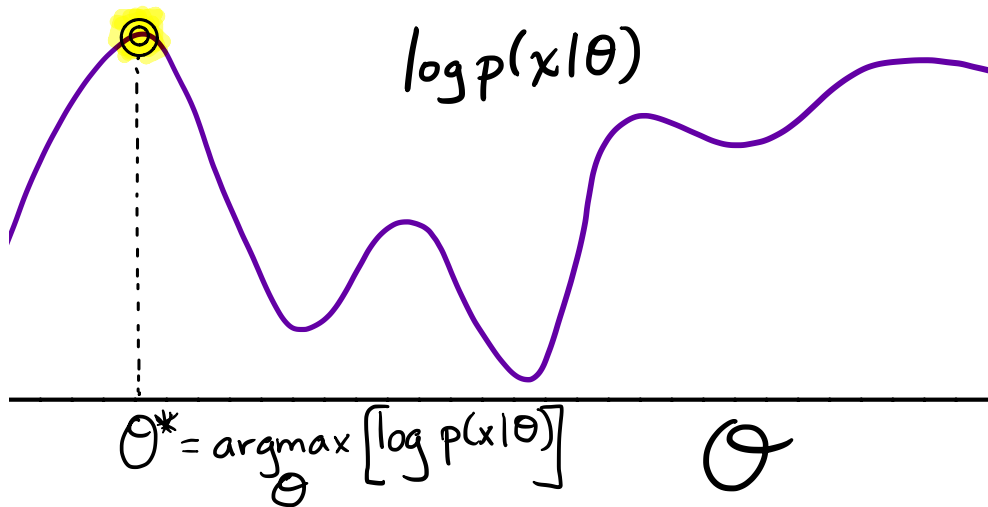
Gibbs Inequality: Proof

$$\begin{aligned}\mathrm{KL}(p\|q) &= \mathbb{E}_p \left[-\log \left(\frac{q(x)}{p(x)} \right) \right] \\ &\geq -\log \left[\mathbb{E}_p \left(\frac{q(x)}{p(x)} \right) \right] \quad (\text{Jensen's}) \\ &= -\log \left[\sum_{\{x|p(x)>0\}} p(x) \frac{q(x)}{p(x)} \right] \\ &= -\log \left[\sum_{x \in \mathcal{X}} q(x) \right] \\ &= -\log 1 = 0.\end{aligned}$$

- Since $-\log$ is strictly convex, we have strict equality iff $q(x)/p(x)$ is a constant, which implies $q = p$.

The ELBO: Family of Lower Bounds on $\log p(x | \theta)$

The Maximum Likelihood Estimator



Lower bound of the marginal log-likelihood

$$\begin{aligned}\log p(x; \theta) &= \log \sum_{z \in \mathcal{Z}} p(x, z; \theta) \\ &= \log \sum_{z \in \mathcal{Z}} q(z) \frac{p(x, z; \theta)}{q(z)} \\ &\geq \sum_{z \in \mathcal{Z}} q(z) \log \frac{p(x, z; \theta)}{q(z)} \\ &\stackrel{\text{def}}{=} \mathcal{L}(q, \theta)\end{aligned}$$

- **Evidence:** $\log p(x; \theta)$
- **Evidence lower bound (ELBO):** $\mathcal{L}(q, \theta)$
- q : chosen to be a family of tractable distributions
- Idea: *maximize the ELBO* instead of $\log p(x; \theta)$

MLE, EM, and the ELBO

- The MLE is defined as a maximum over θ :

$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta} [\log p(x | \theta)].$$

- For any PMF $q(z)$, we have a lower bound on the marginal log-likelihood

$$\log p(x | \theta) \geq \mathcal{L}(q, \theta).$$

- In EM algorithm, we maximize the lower bound (ELBO) over θ and q :

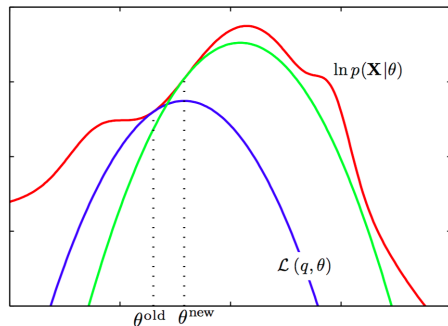
$$\hat{\theta}_{\text{EM}} \approx \arg \max_{\theta} \left[\max_q \mathcal{L}(q, \theta) \right]$$

- In EM algorithm, q ranges over all distributions on z .

EM: Coordinate Ascent on Lower Bound

- Choose sequence of q 's and θ 's by “**coordinate ascent**” on $\mathcal{L}(q, \theta)$.
- EM Algorithm (high level):
 - ① Choose initial θ^{old} .
 - ② Let $q^* = \arg \max_q \mathcal{L}(q, \theta^{\text{old}})$
 - ③ Let $\theta^{\text{new}} = \arg \max_{\theta} \mathcal{L}(q^*, \theta)$.
 - ④ Go to step 2, until converged.
- Will show: $p(x | \theta^{\text{new}}) \geq p(x | \theta^{\text{old}})$
- **Get sequence of θ 's with monotonically increasing likelihood.**

EM: Coordinate Ascent on Lower Bound



- 1 Start at θ^{old} .
- 2 Find q giving best lower bound at $\theta^{\text{old}} \implies \mathcal{L}(q, \theta)$.
- 3 $\theta^{\text{new}} = \arg \max_{\theta} \mathcal{L}(q, \theta)$.

From Bishop's *Pattern recognition and machine learning*, Figure 9.14.

Is ELBO a "good" lowerbound?

$$\begin{aligned}\mathcal{L}(q, \theta) &= \sum_{z \in \mathcal{Z}} q(z) \log \frac{p(x, z \mid \theta)}{q(z)} \\&= \sum_{z \in \mathcal{Z}} q(z) \log \frac{p(z \mid x, \theta) p(x \mid \theta)}{q(z)} \\&= - \sum_{z \in \mathcal{Z}} q(z) \log \frac{q(z)}{p(z \mid x, \theta)} + \sum_{z \in \mathcal{Z}} q(z) \log p(x \mid \theta) \\&= -\text{KL}(q(z) \parallel p(z \mid x, \theta)) + \underbrace{\log p(x \mid \theta)}_{\text{evidence}}\end{aligned}$$

- **KL divergence:** measures "distance" between two distributions (not symmetric!)
- $\text{KL}(q \parallel p) \geq 0$ with equality iff $q(z) = p(z \mid x)$.
- $\text{ELBO} = \text{evidence} - \text{KL} \leq \text{evidence}$

Maximizing over q for fixed θ .

- Find q maximizing

$$\mathcal{L}(q, \theta) = -\text{KL}[q(z), p(z | x, \theta)] + \underbrace{\log p(x | \theta)}_{\text{no } q \text{ here}}$$

- Recall $\text{KL}(p \| q) \geq 0$, and $\text{KL}(p \| p) = 0$.

- Best q is $q^*(z) = p(z | x, \theta)$ and

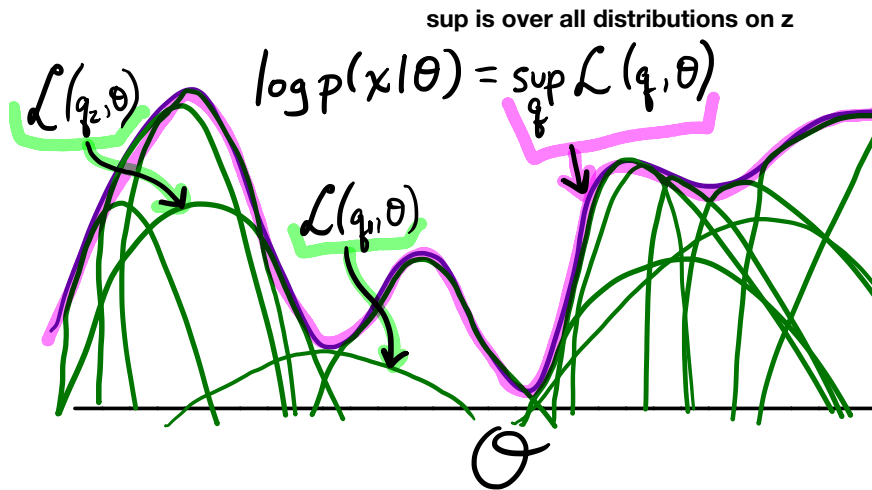
$$\mathcal{L}(q^*, \theta) = -\underbrace{\text{KL}[p(z | x, \theta), p(z | x, \theta)]}_{=0} + \log p(x | \theta)$$

- Summary:

$$\log p(x | \theta) = \sup_q \mathcal{L}(q, \theta) \quad \forall \theta$$

- For any θ , **sup is attained** at $q(z) = p(z | x, \theta)$.

Marginal Log-Likelihood **IS** the Supremum over Lower Bounds



Summary

Latent variable models: clustering, latent structure, missing labels etc.

Parameter estimation: maximum marginal log-likelihood

Challenge: directly maximize the **evidence** $\log p(x; \theta)$ is hard

Solution: maximize the **evidence lower bound**:

$$\text{ELBO} = \mathcal{L}(q, \theta) = -\text{KL}(q(z) \| p(z | x; \theta)) + \log p(x; \theta)$$

Why does it work?

$$q^*(z) = p(z | x; \theta) \quad \forall \theta \in \Theta$$
$$\mathcal{L}(q^*, \theta^*) = \max_{\theta} \log p(x; \theta)$$

EM algorithm

Coordinate ascent on $\mathcal{L}(q, \theta)$

- 1 Random initialization: $\theta^{\text{old}} \leftarrow \theta_0$
- 2 Repeat until convergence
 - i $q(z) \leftarrow \arg \max_q \mathcal{L}(q, \theta^{\text{old}})$

Expectation (the E-step): $q^*(z) = p(z \mid x; \theta^{\text{old}})$
 $J(\theta) = \mathcal{L}(q^*, \theta)$

ii $\theta^{\text{new}} \leftarrow \arg \max_{\theta} \mathcal{L}(q^*, \theta)$

Maximization (the M-step): $\theta^{\text{new}} \leftarrow \arg \max_{\theta} J(\theta)$

1 Expectation Step

- Let $q^*(z) = p(z | x, \theta^{\text{old}})$. [q^* gives best lower bound at θ^{old}]
- Let

$$J(\theta) := \mathcal{L}(q^*, \theta) = \underbrace{\sum_z q^*(z) \log \left(\frac{p(x, z | \theta)}{q^*(z)} \right)}_{\text{expectation w.r.t. } z \sim q^*(z)}$$

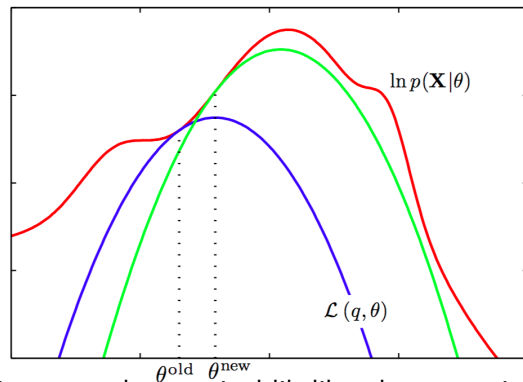
2 Maximization Step

$$\theta^{\text{new}} = \arg \max_{\theta} J(\theta).$$

[Equivalent to maximizing expected complete log-likelihood.]

EM puts no constraint on q in the E-step and assumes the M-step is easy. In general, both steps can be hard.

Monotonically increasing likelihood



Exercise: prove that EM increases the marginal likelihood monotonically

$$\log p(x; \theta^{\text{new}}) \geq \log p(x; \theta^{\text{old}}).$$

Does EM converge to a global maximum?

Variations on EM

EM Gives Us Two New Problems

- The “E” Step: Computing

$$J(\theta) := \mathcal{L}(q^*, \theta) = \sum_z q^*(z) \log \left(\frac{p(x, z | \theta)}{q^*(z)} \right)$$

- The “M” Step: Computing

$$\theta^{\text{new}} = \arg \max_{\theta} J(\theta).$$

- Either of these can be too hard to do in practice.

Generalized EM (GEM)

- Addresses the problem of a difficult “M” step.
- Rather than finding

$$\theta^{\text{new}} = \arg \max_{\theta} J(\theta),$$

find **any** θ^{new} for which

$$J(\theta^{\text{new}}) > J(\theta^{\text{old}}).$$

- Can use a standard nonlinear optimization strategy
 - e.g. take a gradient step on J .
- We still get monotonically increasing likelihood.

EM and More General Variational Methods

- Suppose “E” step is difficult:
 - Hard to take expectation w.r.t. $q^*(z) = p(z \mid x, \theta^{\text{old}})$.
- Solution: Restrict to distributions \mathcal{Q} that are easy to work with.
- Lower bound now looser:

$$q^* = \arg \min_{q \in \mathcal{Q}} \text{KL}[q(z), p(z \mid x, \theta^{\text{old}})]$$