Clustering and EM

CDS, NYU

April 25, 2022

Logistics

Final exam

- Period: May 15 4:00-5:50pm EST
- Format: in person, closed book
- Coverage: mainly about material from week 6 onwards but can overlap with basic concepts before midterm

K-means Clustering

Unsupervised learning

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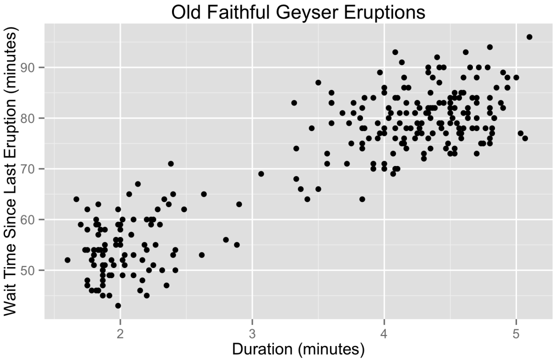
Examples

- 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.

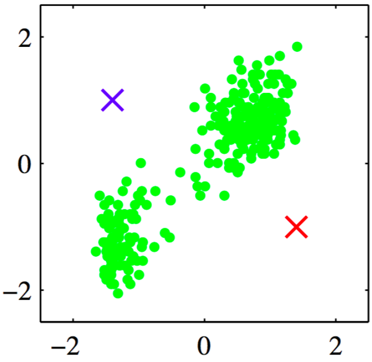
Example: Old Faithful Geyser



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

k-Means: By Example

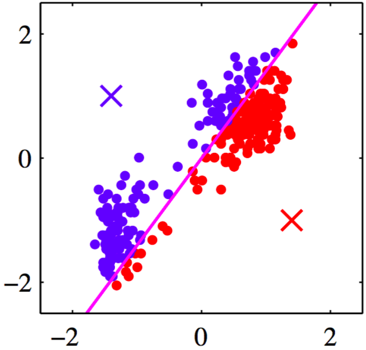
- Standardize the data.
- Choose two cluster centers.



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

k-means: by example

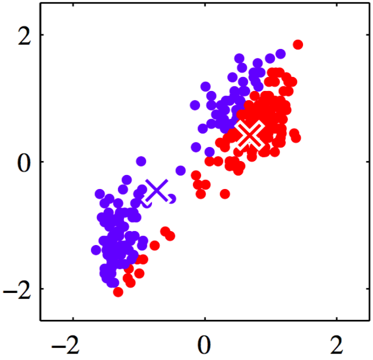
- Assign each point to closest center.



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

k-means: by example

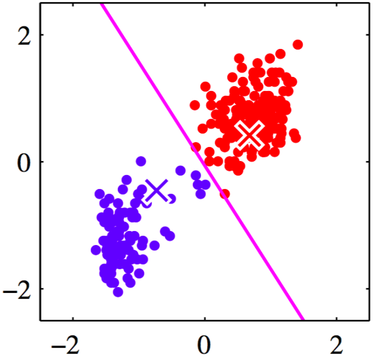
- Compute new cluster centers.



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

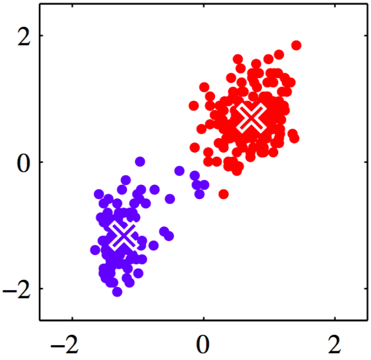
k-means: by example

- Assign points to closest center.



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

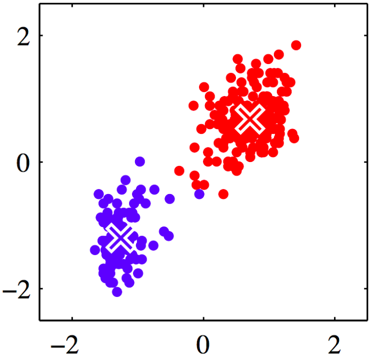
- Compute cluster centers.



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

k-means: by example

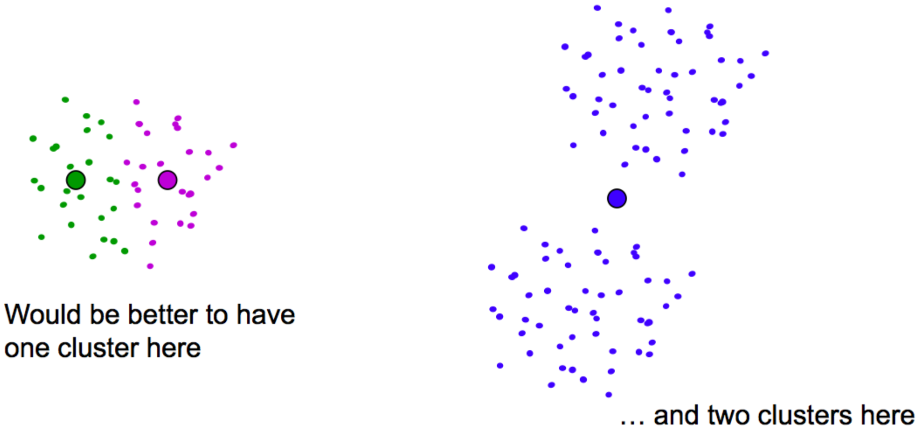
- Iterate until convergence.



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:



From Sontag's DS-GA 1003, 2014, Lecture 8.

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- Dataset $\mathcal{D} = \{x_1, \ldots, x_n\} \subset \mathcal{X}$ where $\mathcal{X} = \mathrm{R}^d$.

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

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

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k-means converges to a local minimum.

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

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    - 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:
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Next, probabilistic model of clustering.

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

Gaussian Mixture Models

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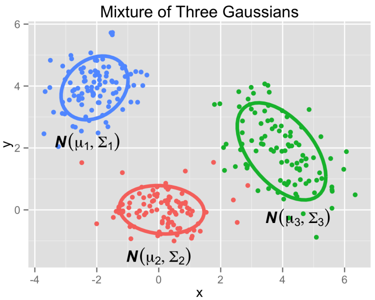
Example:

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:

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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

$$\begin{aligned}\text{Cluster probabilities}: \quad & \pi = (\pi_1, \dots, \pi_k) \\ \text{Cluster means}: \quad & \mu = (\mu_1, \dots, \mu_k) \\ \text{Cluster covariance matrices}: \quad & \Sigma = (\Sigma_1, \dots \Sigma_k)\end{aligned}$$

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- Assuming all clusters are distinct, there are $k!$ equivalent solutions.
- Not a problem *per se*, but something to be aware of.

Learning GMMs

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

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

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

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  - 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]

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Learning GMMs: observable case

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

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

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

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

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

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&= \frac{\pi_j \mathcal{N}(x_i \mid \mu_j, \Sigma_j)}{\sum_k \pi_k \mathcal{N}(x_i \mid \mu_k, \Sigma_k)} && (16)
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- $p(z \mid x)$ is a *soft assignment*.
- If we know the parameters μ, Σ, π, this would be easy to compute.

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   1. E-step: fill in latent variables by inference.
      - compute soft assignments $p(z \mid x_i)$ 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 $p(z \mid x_i)$.

M-step for GMM

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

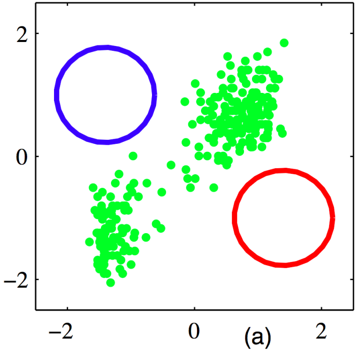
$$\gamma_i^j = \frac{\pi_j^{\text{old}} \mathcal{N}\left(x_i \mid \mu_j^{\text{old}}, \Sigma_j^{\text{old}}\right)}{\sum_{c=1}^k \pi_c^{\text{old}} \mathcal{N}\left(x_i \mid \mu_c^{\text{old}}, \Sigma_c^{\text{old}}\right)}.$$

- Exercise: show that

$$\begin{aligned}
n_z &= \sum_{i=1}^n \gamma_i^z \\
\mu_z^{\text{new}} &= \frac{1}{n_z} \sum_{i=1}^n \gamma_i^z x_i \\
\Sigma_z^{\text{new}} &= \frac{1}{n_z} \sum_{i=1}^n \gamma_i^z \left(x_i - \mu_z^{\text{new}}\right)\left(x_i - \mu_z^{\text{new}}\right)^T \\
\pi_z^{\text{new}} &= \frac{n_z}{n}.
\end{aligned}$$

EM for GMM

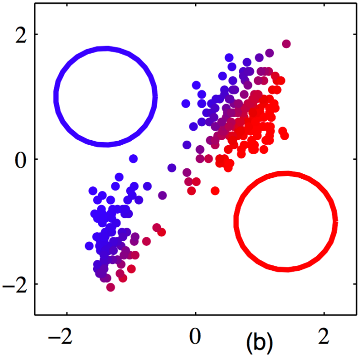
- Initialization



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

EM for GMM

- First soft assignment:



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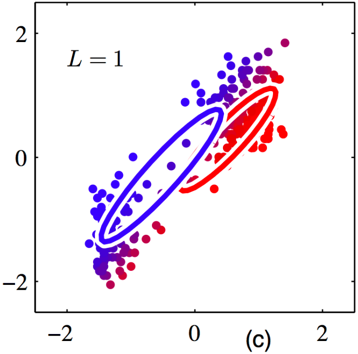
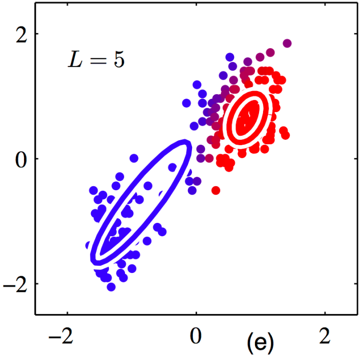


From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

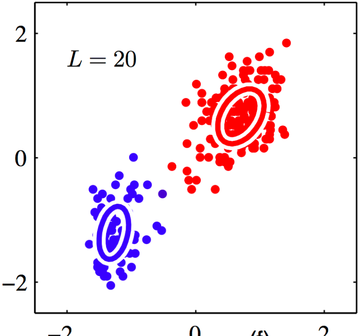
- After 5 rounds of EM:



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

EM for GMM

- After 20 rounds of EM:



(f)

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

Complete and Incomplete Data

- Suppose we observe some data $(x_1, \ldots, x_n)$.

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- To simplify notation, take x to represent the entire dataset

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

and z to represent the corresponding unobserved variables

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

- 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

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- 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

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$$p(x) = \sum_{z} p(x, z)$$
- 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 $f : \mathrm{R} \to \mathrm{R}$ is a ***convex*** *function, and x is a random variable, then*

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

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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 $\mathbb{E}x^2 \geqslant (\mathbb{E}x)^2$. Thus

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

Kullback-Leibler Divergence

- Let $p(x)$ and $q(x)$ be probability mass functions (PMFs) on $\mathcal{X}$.
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- Can also write this as

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

Gibbs Inequality ($\mathrm{KL}(p\|q) \geqslant 0$ and $\mathrm{KL}(p\|p) = 0$)

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

Gibbs Inequality: Proof

$$\mathrm{KL}(p\|q) \quad = \quad \mathbb{E}_p\left[-\log\left(\frac{q(x)}{p(x)}\right)\right]$$

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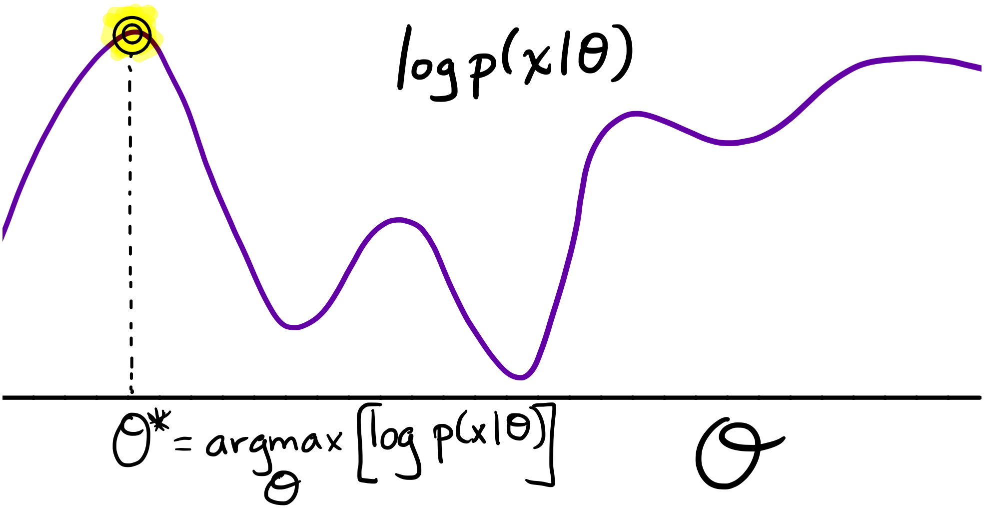
- Since $-\log$ is strictly convex, we have strict equality iff $q(x)/p(x)$ is a constant, which implies $q = p$.

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

The Maximum Likelihood Estimator



Lower bound of the marginal log-likelihood

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

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

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&\geqslant \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:

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

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

$$\log p(x \mid \theta) \geqslant \mathcal{L}(q, \theta).$$

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

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

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- 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 $\mathcal{L}(q, \theta)$.

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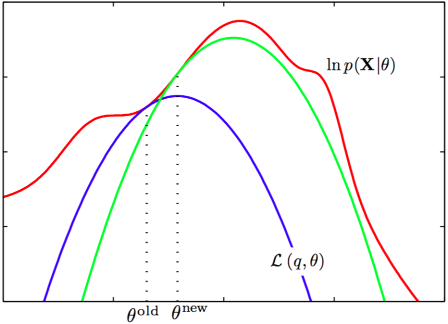
  3. Let $\theta^{\text{new}} = \arg\max_\theta \mathcal{L}(q^*,\theta)$.
  4. Go to step 2, until converged.
- Will show: $p(x \mid \theta^{\textbf{new}}) \geqslant p(x \mid \theta^{\textbf{old}})$
- **Get sequence of θ's with monotonically increasing likelihood.**

EM: Coordinate Ascent on Lower Bound



1. Start at θ^{old}.

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

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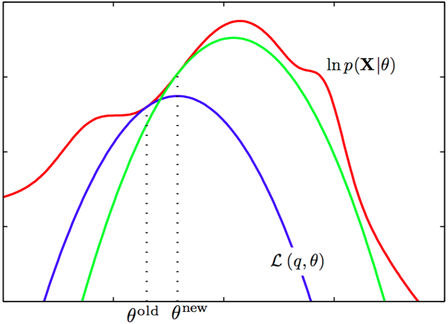

1. Start at θ^{old}.
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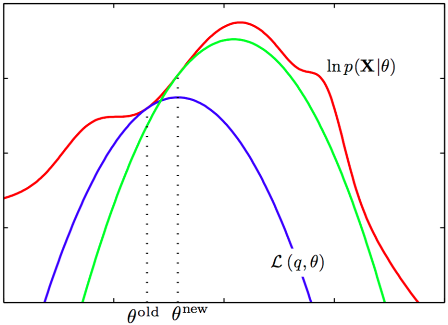

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Is ELBO a "good" lowerbound?

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

- **KL divergence**: measures "distance" between two distributions (not symmetric!)
- $\mathrm{KL}\left(q\|p\right) \geqslant 0$ with equality iff $q(z) = p(z\mid x)$.
- ELBO $=$ evidence - KL $\leqslant$ evidence

Maximizing over q for fixed θ.

- Find q maximizing

$$\mathcal{L}(q,\theta) = -\mathrm{KL}[q(z), p(z \mid x, \theta)] + \log p(x \mid \theta)$$

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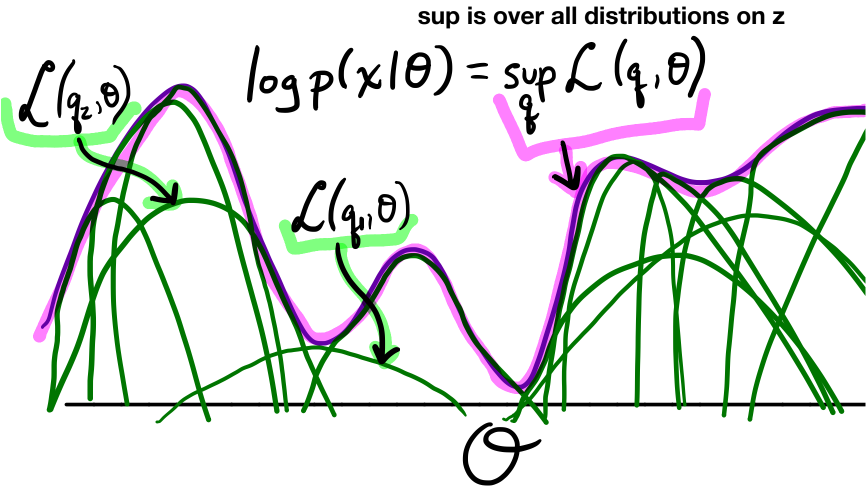
- Summary:

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

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

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



Summary

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

Parameter estimation: maximum marginal log-likelihood

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

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

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

Why does it work?

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

EM algorithm

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

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

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

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

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

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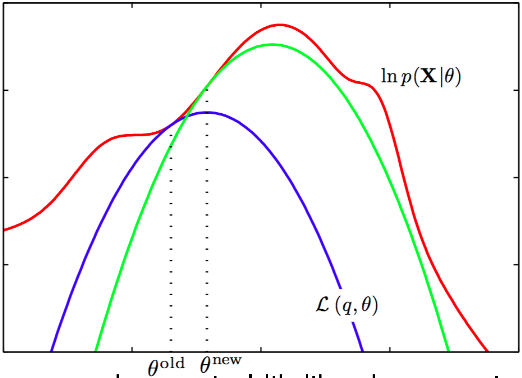
EM puts no constraint on q in the E-step and assumes the M-step is easy. In general, both steps can be hard.

Monotonically increasing likelihood



Exercise: prove that EM increases the marginal likelihood monotonically

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

Does EM converge to a global maximum?

Variations on EM

EM Gives Us Two New Problems

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

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- We still get monotonically increasing likelihood.

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- Solution: Restrict to distributions $\mathcal{Q}$ that are easy to work with.
- Lower bound now looser:

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

Today's Summary

- Motivation: Unsupervised learning
- K-means: A simple algorithm for discovering clusters
- Making k-means probabilistic: Gaussian mixture models
- More generally: Latent variable models
- Learning of latent variable models: EM
- Underlying principle: Maximizing ELBO