Clustering and Latent Variable Models

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K-means Clustering

Unsupervised learning

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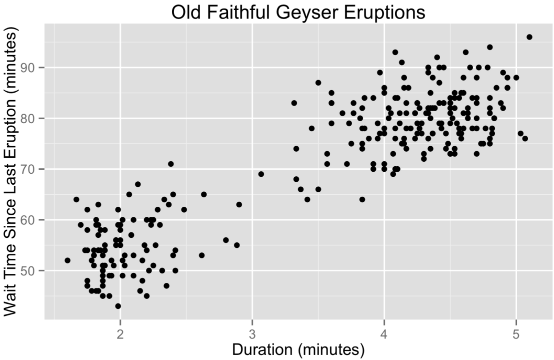
Examples

- 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.

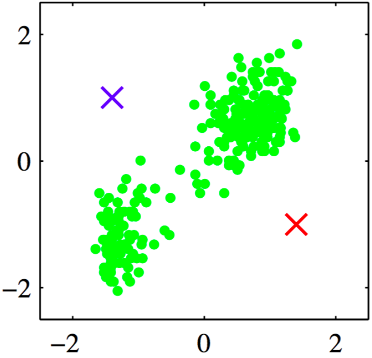
Example: Old Faithful Geyser



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

k-Means: By Example

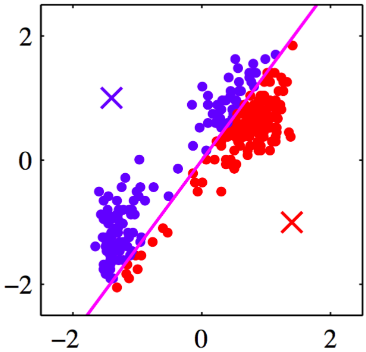
- Standardize the data.
- Choose two cluster centers.



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

k-means: by example

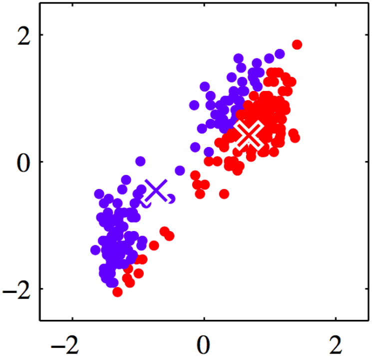
- Assign each point to closest center.



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

k-means: by example

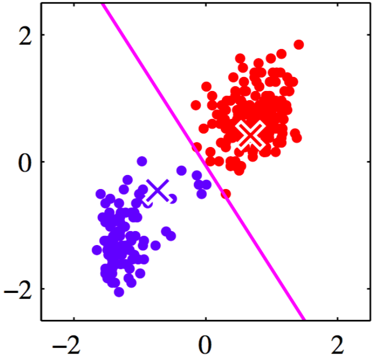
- Compute new cluster centers.



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

k-means: by example

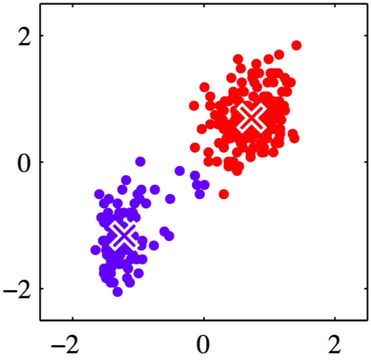
- Assign points to closest center.



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

k-means: by example

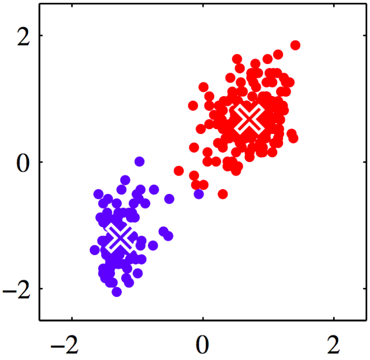
- Compute cluster centers.



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

k-means: by example

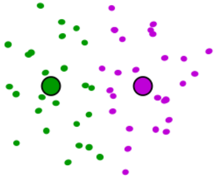
- Iterate until convergence.

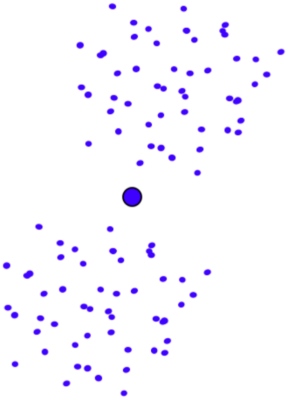


From Bishop's *Pattern recognition and machine learning*, Figure 9.1(i).

Suboptimal Local Minimum

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





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

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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.

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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.
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Next, probabilistic model of clustering.

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

Gaussian Mixture Models

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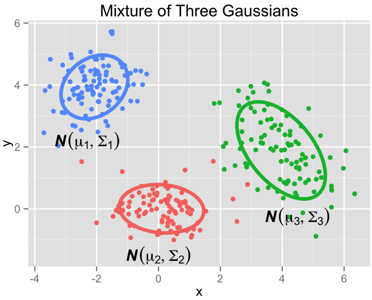
Example:

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.

$$
\begin{aligned}
p(x) &= \sum_z p(x, z) && (5) \\
&= \sum_z p(x \mid z) p(z) && (6) \\
&= \sum_k \pi_k \mathcal{N}(\mu_k, \Sigma_k) && (7)
\end{aligned}
$$

Identifiability Issues for GMM

- Suppose we have found parameters

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

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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:

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

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

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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

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

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Learning GMMs: observable case

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

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

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      - compute soft assignments $p(z \mid x_i)$ for all i.

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2. Run until convergence:
    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:

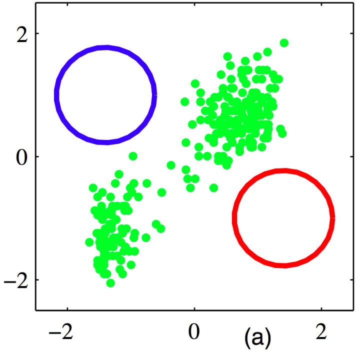
$$\gamma_i^j = \frac{\pi_j^{\text{old}} \mathcal{N}\left(x_i \mid \mu_j^{\text{old}}, \Sigma_j^{\text{old}}\right)}{\sum_{c=1}^{k} \pi_c^{\text{old}} \mathcal{N}\left(x_i \mid \mu_c^{\text{old}}, \Sigma_c^{\text{old}}\right)}.$$

- 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

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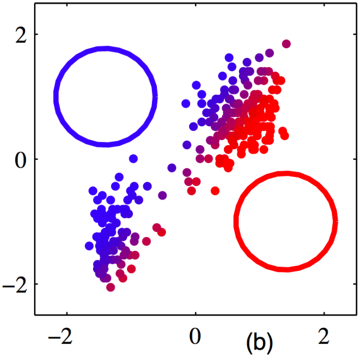

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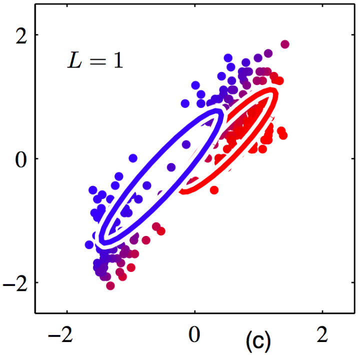

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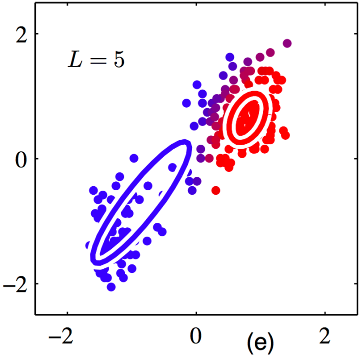
EM for GMM

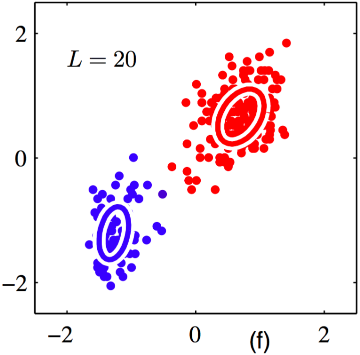
- After 5 rounds of EM:



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.

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- 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

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- Similarly, $\log p(x)$ is the **marginal log-likelihood**.

EM Algorithm

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

Why should this work?

Math Prerequisites

Theorem (Jensen's Inequality)

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

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

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

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- 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 $\mathrm{KL}(p\|p) = 0$)

Theorem (Gibbs Inequality)

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

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

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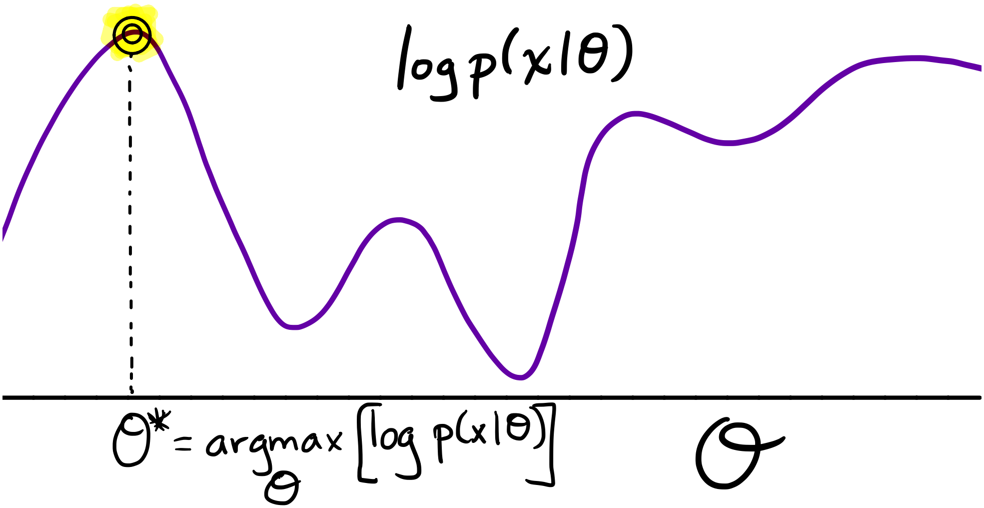
- Since $-\log$ is strictly convex, we have strict equality iff $q(x)/p(x)$ is a constant, which implies $q = p$.

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

The Maximum Likelihood Estimator



Lower bound of the marginal log-likelihood

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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:

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

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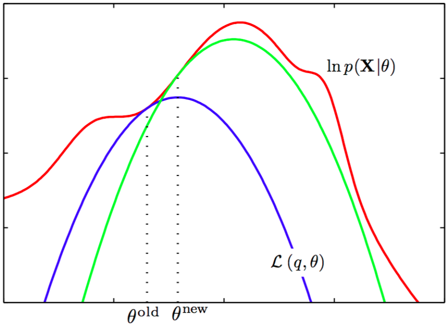
    3. Let $\theta^{\text{new}} = \arg\max_\theta \mathcal{L}(q^*, \theta)$.
    4. Go to step 2, until converged.
- Will show: $p(x \mid \theta^{\textbf{new}}) \geqslant p(x \mid \theta^{\textbf{old}})$
- **Get sequence of θ's with monotonically increasing likelihood.**

EM: Coordinate Ascent on Lower Bound



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

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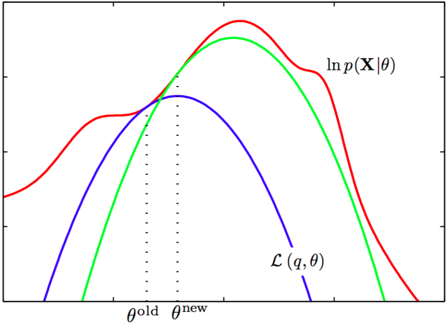

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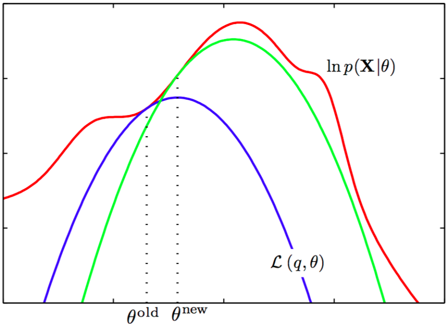

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Is ELBO a "good" lowerbound?

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

- **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

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- Summary:

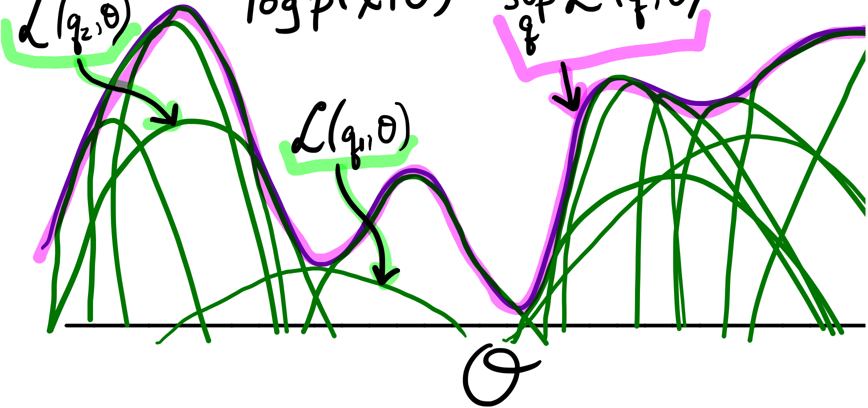
$$\log p(x \mid \theta) = \sup_q \mathcal{L}(q,\theta) \qquad \forall\theta$$

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

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

sup is over all distributions on z

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



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. $q(z) \leftarrow \arg\max_q \mathcal{L}(q, \theta^{\text{old}})$

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

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

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

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

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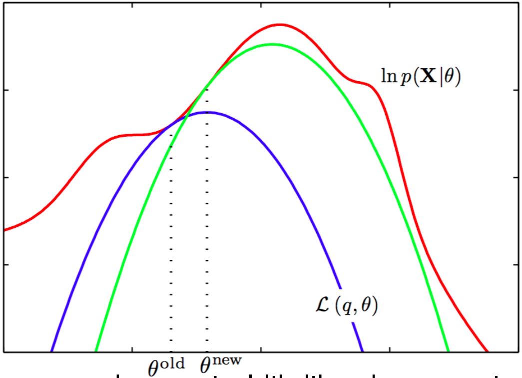
   [Equivalent to maximizing expected complete log-likelihood.]

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

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

Does EM converge to a global maximum?

Variations on EM

EM Gives Us Two New Problems

- The "E" Step: Computing

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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.

EM and More General Variational Methods

- Suppose "E" step is difficult:
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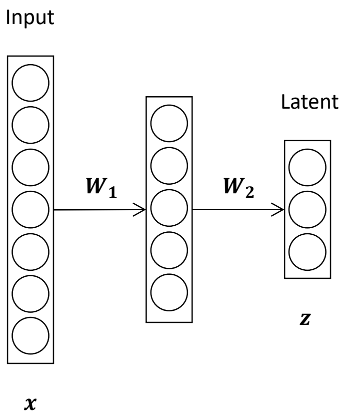
- Solution: Restrict to distributions $\mathcal{Q}$ that are easy to work with.
- Lower bound now looser:

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

Deep Latent Variable Models

- Neural network is a flexible function class to represent transformation between random variables $e.g., q(z)$.



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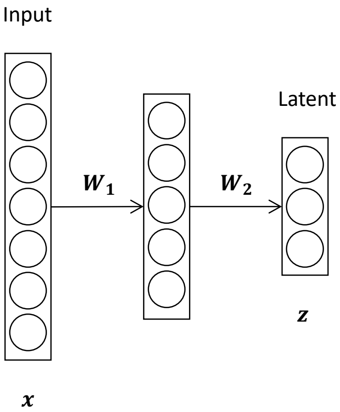

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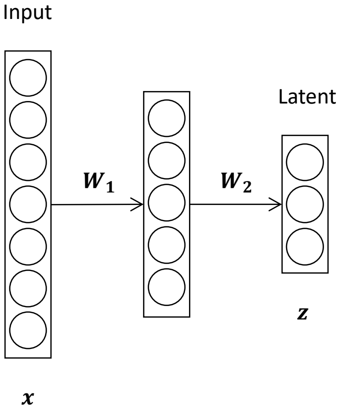
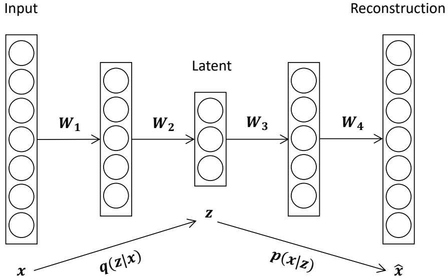
- What if we let the hidden represent some learned latent code?



Variational Autoencoders (VAE) [1]

- An autoencoder (AE) is a neural network that reconstructs the same input.



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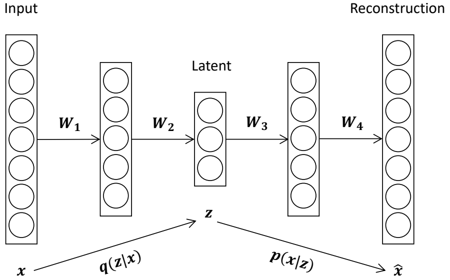

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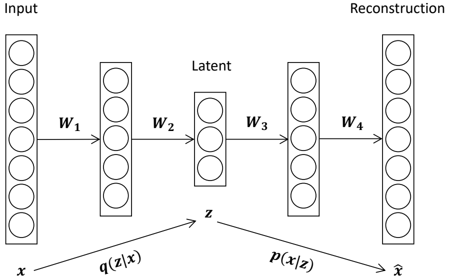

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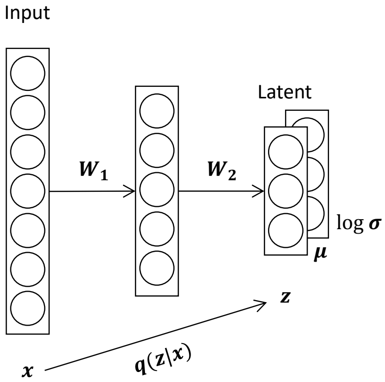

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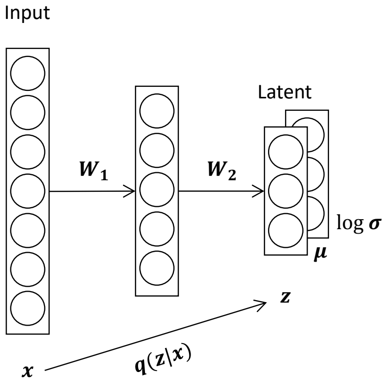

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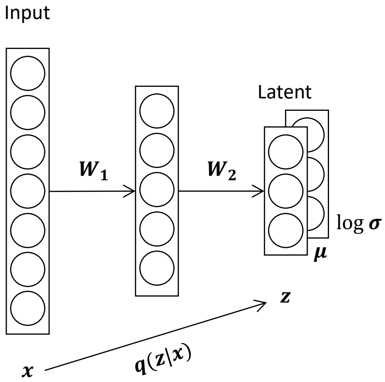
- A stochastic z can be sampled from $\mathcal{N}(\mu, \sigma^2)$: $z = \mu + \sigma \cdot \epsilon$, where $\epsilon \sim \mathcal{N}(0, 1)$.



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&= \underbrace{-KL(q_\phi(z|x)||p_\theta(z))}_{\text{Divergence between } q \text{ and the prior distribution}} + \underbrace{\mathbb{E}_{z\sim q}(\log p_\theta(x|z))}_{\text{Reconstruction based on } z} && (20)
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Stochastic Gradient

- The loss function needs to take expectation over q:

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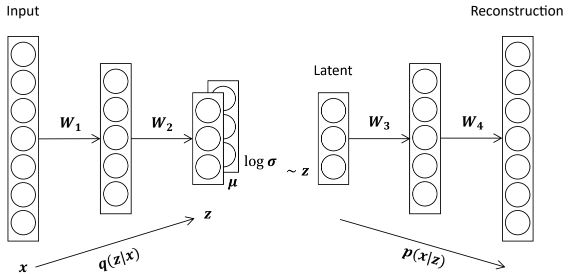

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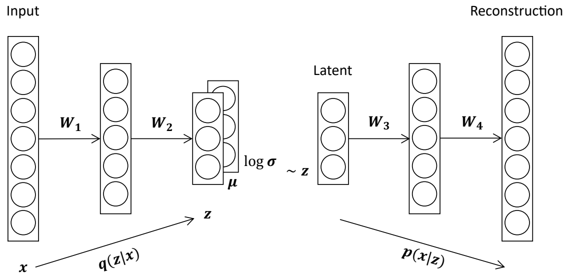

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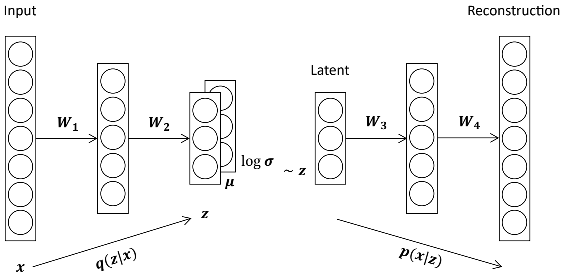
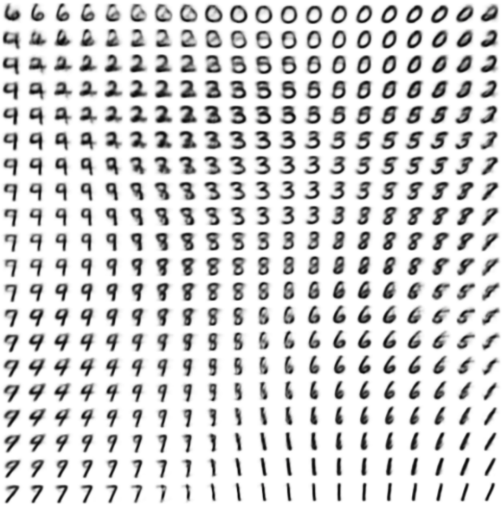
- Backprop through reparameterization.



Learned Manifold



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- VAE: Introducing variational inference to neural networks. A classic starting example for deep generative modeling.

Conclusion and Outlook

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- This is a very challenging grad-level course.
- Congrats, you are almost done.

Next Lecture: Project Presentation

- Dec 12, in-person presentations.
- 24 groups, 120mins.
- Aim for **3 mins** per group, hard stop at 4 mins, and 1 min max for Q&A.
- Send me your slides in PDF with your group number by Dec 11 11:59pm.

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- Trade-offs:
  - approximation error and estimation error (bias and variance),
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- Start from the task requirements, e.g. amount of data, computation resource
- The best lesson is to practice!

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Risk: Expected loss - but expectation over what?

- Frequentist approach: expectation over data.
  - Empirical risk minimization, i.e. average loss on the training data.
  - Regularization: balance estimation error and generalization error.
- Bayesian approach: expectation over parameters.
  - Posterior: prior belief updated by observed data.
  - Bayes action minimizes the posterior risk.

Algorithms

Learning Find model parameters—often an optimization problem.

- (Stocahstic) (sub)gradient descent
- Functional gradient descent (gradient boosting)
- Convex vs non-convex objectives

Inference Answer questions given a learned model.

- Bayesian inference: compute various quantities given the posterior.
- Dynamic programming: compute $\arg\max$ in structured prediction.

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- Classic ML lays down foundation when we innovate DL algorithms.

Other ML Related Advanced Courses in CS

- Computer Vision (Prof. Rob Fergus)
- Deep Learning (Prof. Yann LeCun)
- Deep Reinforcement Learning (Prof. Lerrel Pinto)
- Foundations of Deep Learning Theory (Prof. Matus Telgarsky)
- Inference and Representation (Prof. Joan Bruna)
- Learning with Large Language and Vision Models (Prof. Saining Xie)
- Mathematics of Deep Learning (Prof. Joan Bruna)
- Natural Language Processing (Prof. He He)