Clustering and Latent Variable Models

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(Slides credit to David Rosenberg, He He, et al.)

NYU

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Lecture Slides

K-means Clustering

Unsupervised learning

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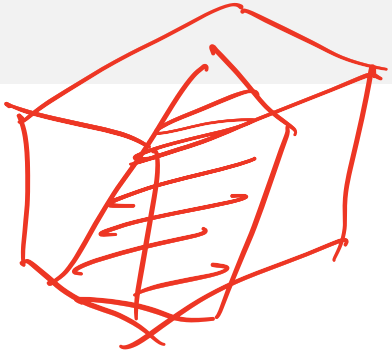
Formulation Density estimation: $p(x; \theta)$ (often with *latent* variables).

Unsupervised learning



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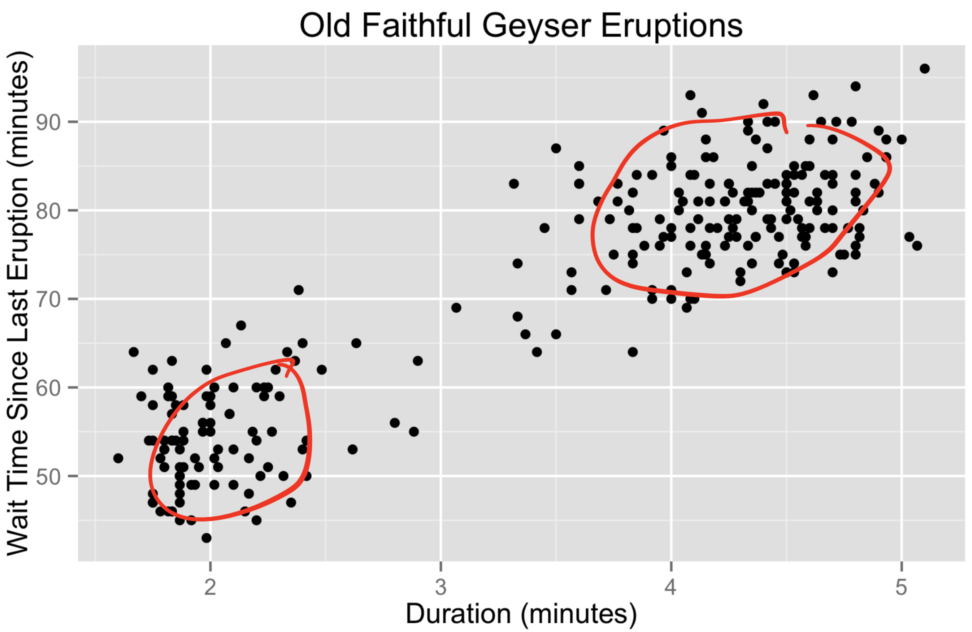
Examples

- 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.

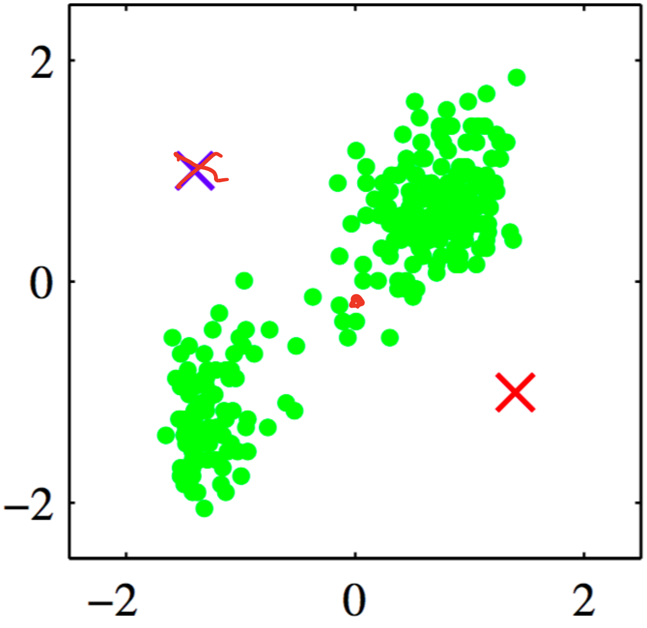
Example: Old Faithful Geyser



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

k-Means: By Example

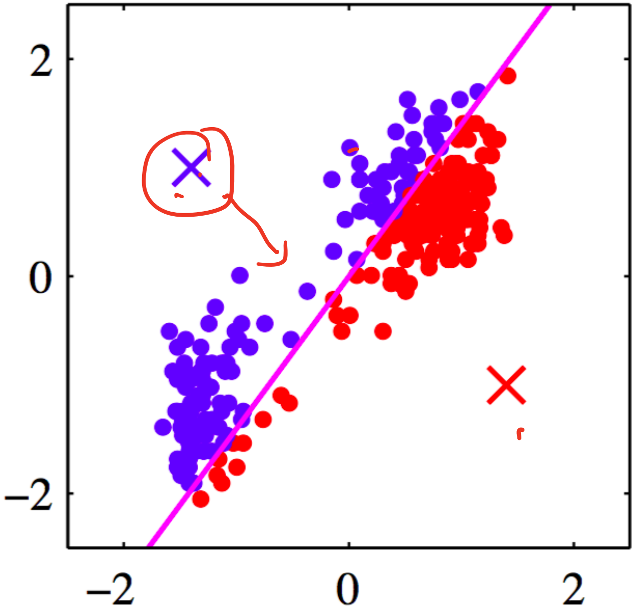
- Standardize the data.
- Choose two cluster centers.



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

k-means: by example

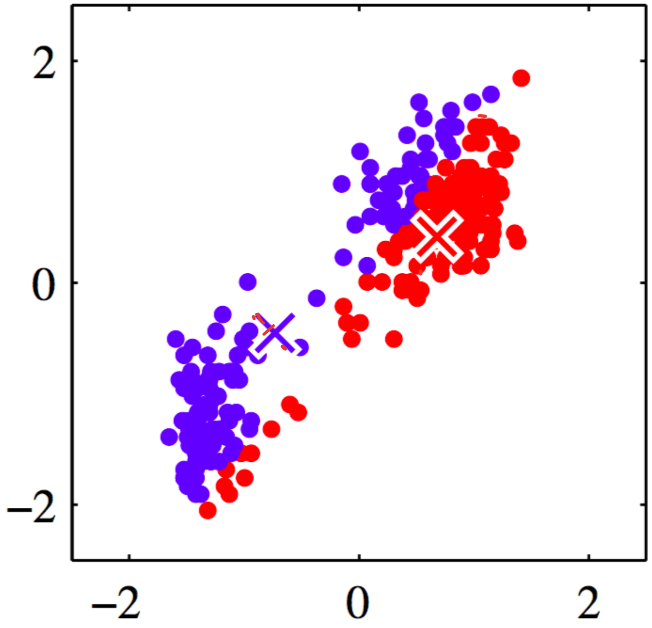
- Assign each point to closest center.



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

k-means: by example

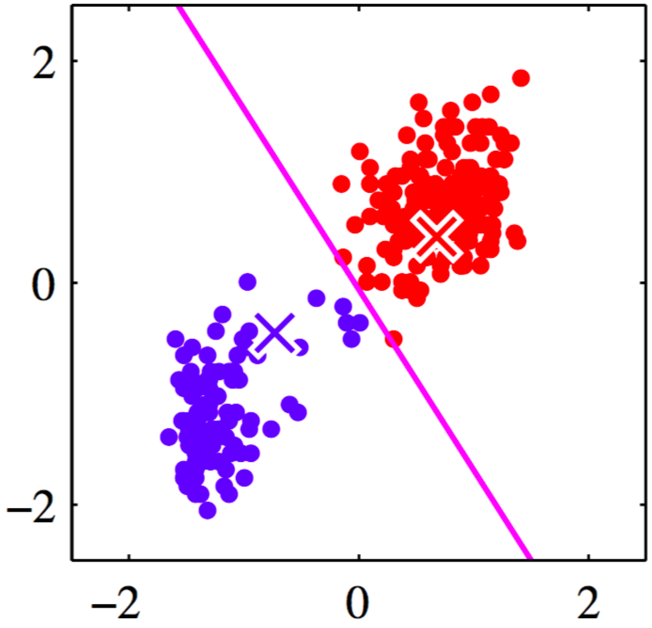
- Compute new cluster centers.



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

k-means: by example

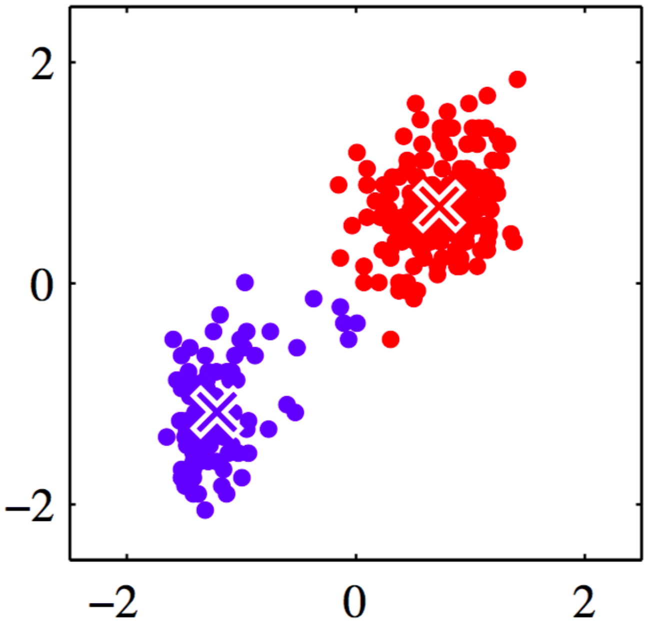
- Assign points to closest center.



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

k-means: by example

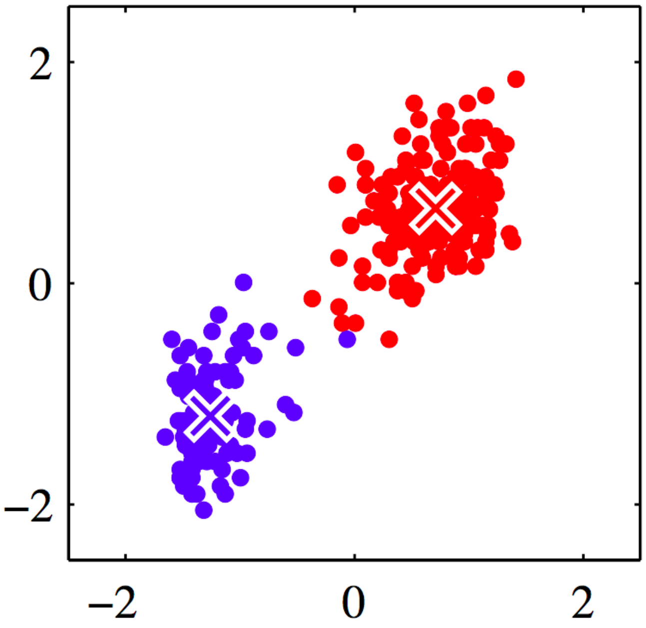
- Compute cluster centers.



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

k-means: by example

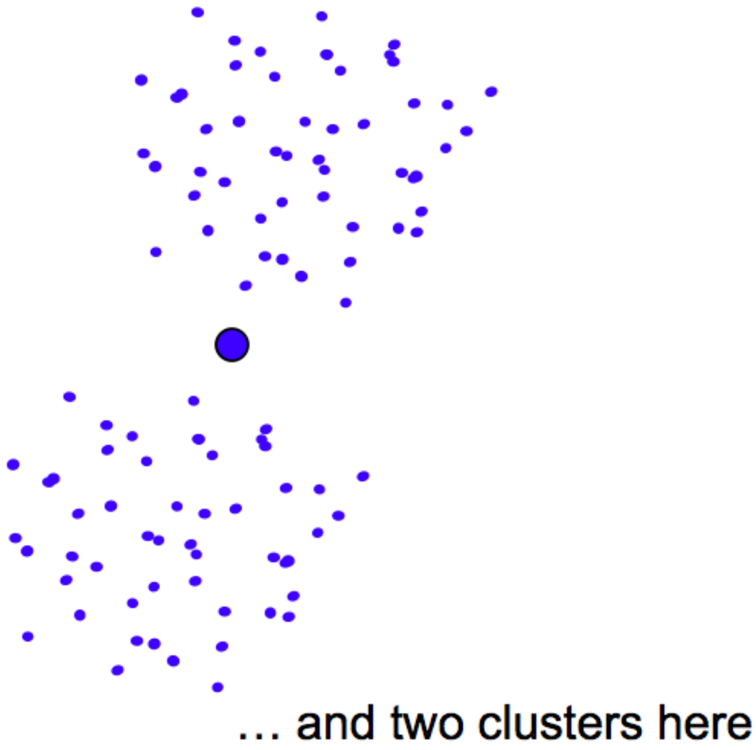
- Iterate until convergence.



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.

Formalize k-Means

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

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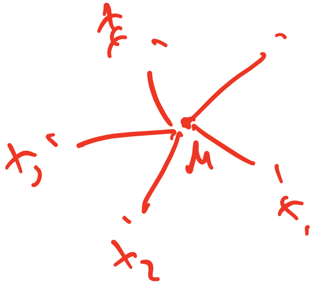

$$\mu_i = \underset{\mu \in X}{\arg\min} \sum_{x \in C_i} \|x - \mu\|^2$$

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

$$J(\underbrace{c}_{\text{assignment}}, \underbrace{\mu}_{\text{Centroid}}) = \sum_i \| x_i - \mu_{c_i} \|^2$$

k-Means: Algorithm

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assignment

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k-means converges to a local minimum.

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Avoid getting stuck with bad local minima:

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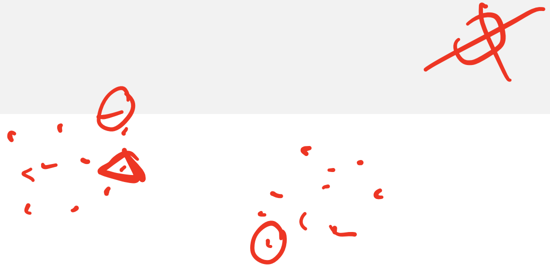

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    - Compute distance between each x_i and the closest already chosen centroids.
    - Randomly choose next centroid with probability proportional to the computed distance squared.

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: minmizing some loss function by coordinate descent.
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Next, probabilistic model of clustering.

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

Gaussian Mixture Models

Gaussian mixture model (GMM)

Generative story of GMM with k mixture components:

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$\pi_1 = 0.2$

$\pi_2 = 0.4$

latent variable

Generative story of GMM with k mixture components:

$p(z)$ ① Choose cluster. $z \sim \underline{\text{Categorical}}(\pi_1, \dots \pi_k)$

$p(x|z)$ [② Choose $x | z \sim N(\mu_z, \Sigma_z)$]

0.4

$\pi_3 =$

Probability density of x:

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

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

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

$$= \sum_{z=k} N(\mu_k, \Sigma_k) \cdot \pi_k.$$

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.

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How to learn the parameters $\{\pi_k, \mu_k, \Sigma_k ?\} = \theta$.

- MLE (also called maximize marginal likelihood).
- Log likelihood of data: $L(\theta) = \sum_{i=1}^{n} \log p(x_i; \theta)$

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

- 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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Learning GMMs: observable case

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

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$$\hat{\mu}_z = \frac{1}{n_z} \sum_{i:z_i=z} x_i \quad \text{empirical cluster mean} \tag{5}$$

$$\hat{\Sigma}_z = \frac{1}{n_z} \sum_{i:z_i=z} (x_i - \hat{\mu}_z)(x_i - \hat{\mu}_z)^T . \quad \text{empirical cluster covariance} \tag{6}$$

Learning GMMs: inference

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

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$$p(z=j \mid x_i) = \frac{p(x, z=j)}{p(x)}$$

$$= \frac{p(z=j)\, p(x \mid z=j)}{\sum_{z=k} p(z=k)\, p(x \mid z=k)}$$

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

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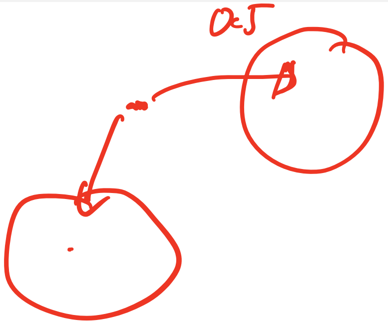
2. Run until convergence:
   1. E-step: fill in latent variables by inference.
      - compute soft assignments $p(z \mid x_i)$ for all i.
   2. M-step: standard MLE for μ, Σ, π given "observed" variables.
      - Equivalent to MLE in the observable case on data weighted by $p(z \mid x_i)$.

M-step for GMM

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

$p(z=j \mid x_i)$

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

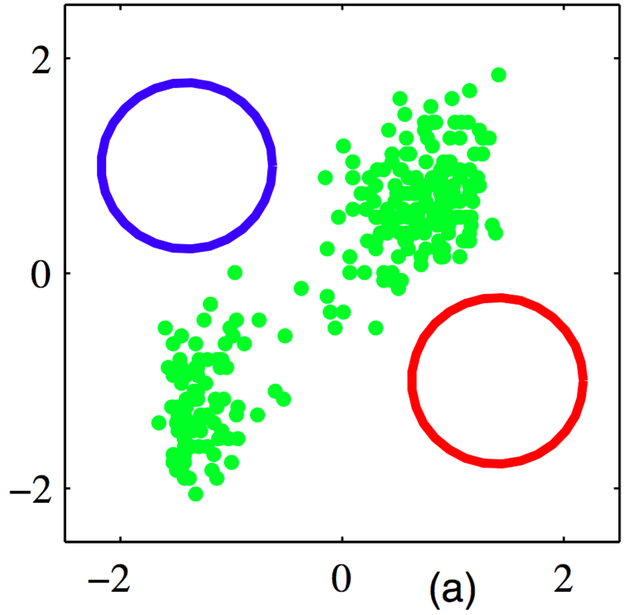


- Exercise: show that

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

EM for GMM

- Initialization



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

EM for GMM

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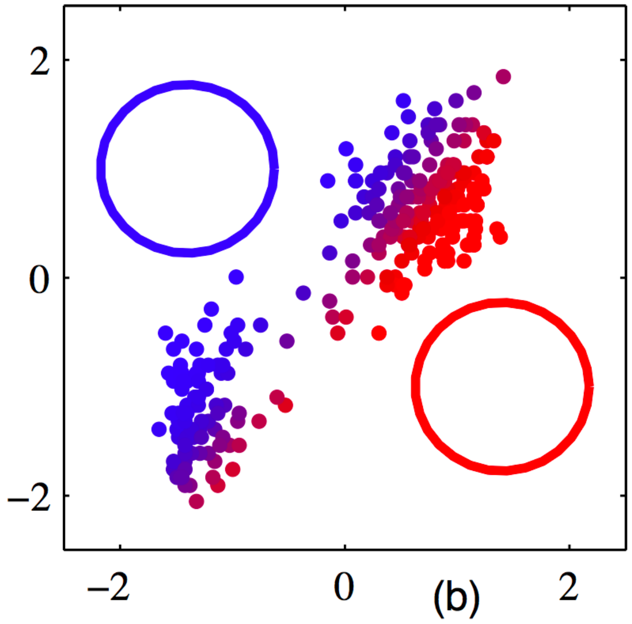

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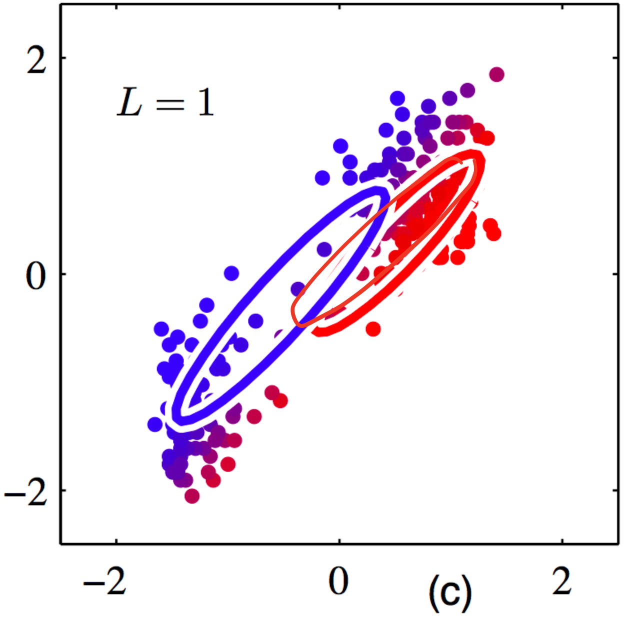

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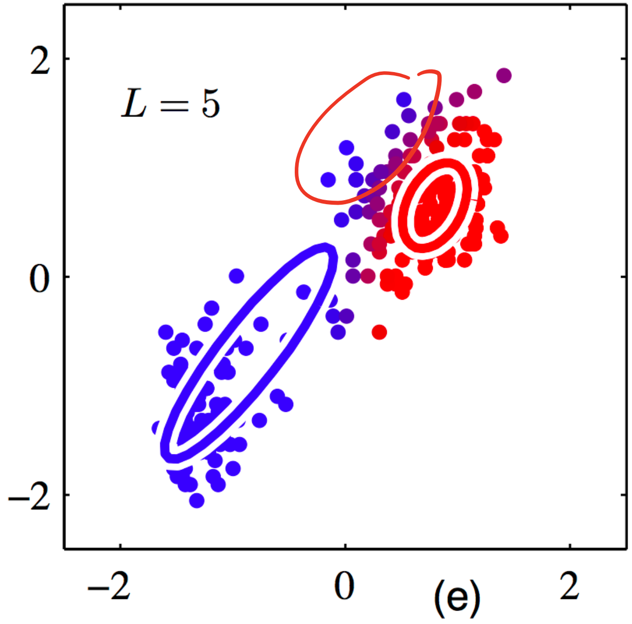
EM for GMM

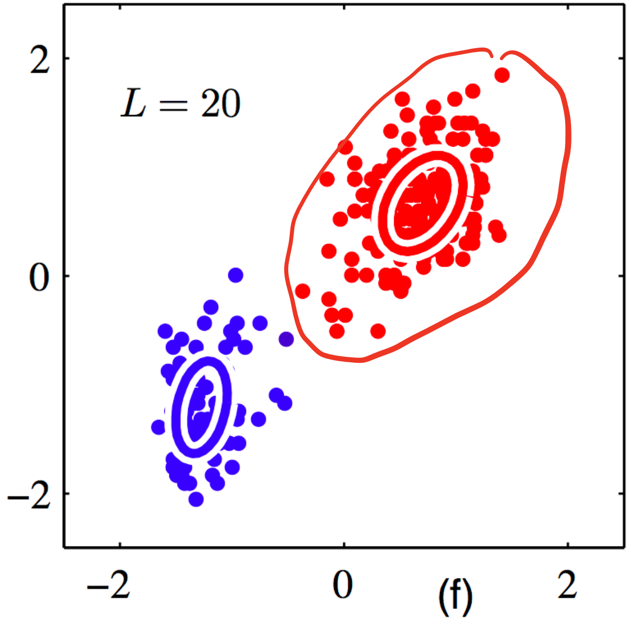
- After 5 rounds of EM:



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

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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

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- For Gaussian mixture model, learning is hard, inference is easy.
- For more complicated models, inference can also be hard.

Log-Likelihood and Terminology

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- We often call $p(x)$ the **marginal likelihood**,
  - because it is $p(x, z)$ with z "marginalized out":

explicit.

$$p(x) = \sum_{z} p(x, z)$$

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

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

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

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*

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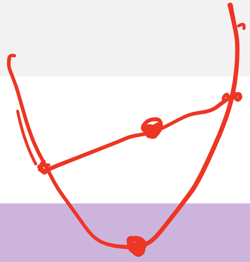

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*Moreover, if f is **strictly convex**, then equality implies that $x = \mathbb{E} x$ with probability 1 (i.e. x is a constant).*

- 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

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

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

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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**.

$KL(p\|q)$ $KL(q\|p)$.

different.

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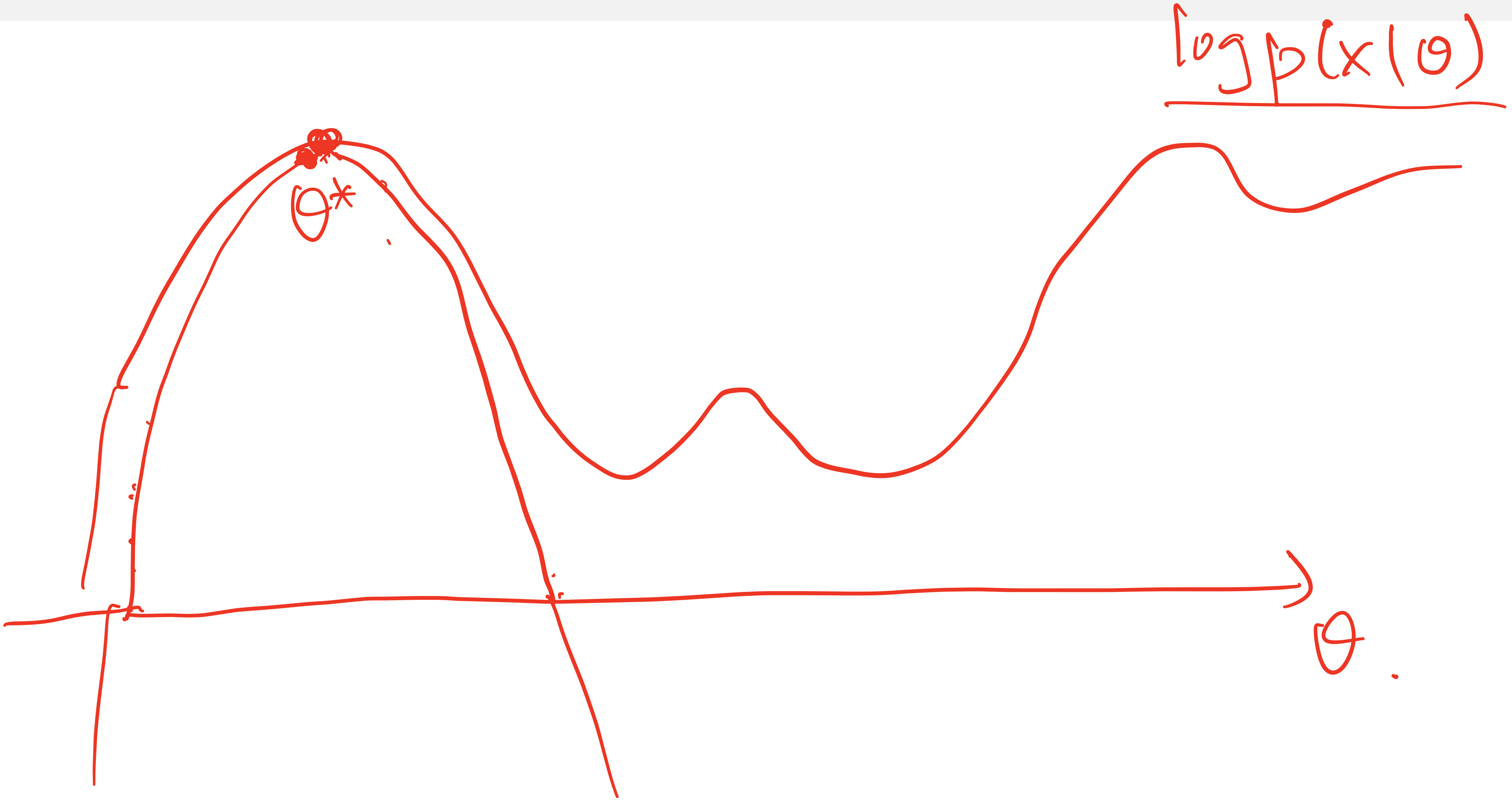
- Since $-\log$ is strictly convex, we have strict equality iff $q(x)/p(x)$ is a constant, which implies $q=p$.

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

The Maximum Likelihood Estimator



Lower bound of the marginal log-likelihood

$$\log p(x;\theta) = \log \sum_z p(x,z;\theta).$$

$$= \log \sum_z q(z) \frac{p(x,z;\theta)}{q(z)}.$$

$$\geq \sum_z q(z) \log \frac{p(x,z;\theta)}{q(z)}. \quad \text{(Jensen)}.$$

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

evidence.

evidence lower bound (ELBO).

MLE, EM, and the ELBO

- The MLE is defined as a maximum over θ:

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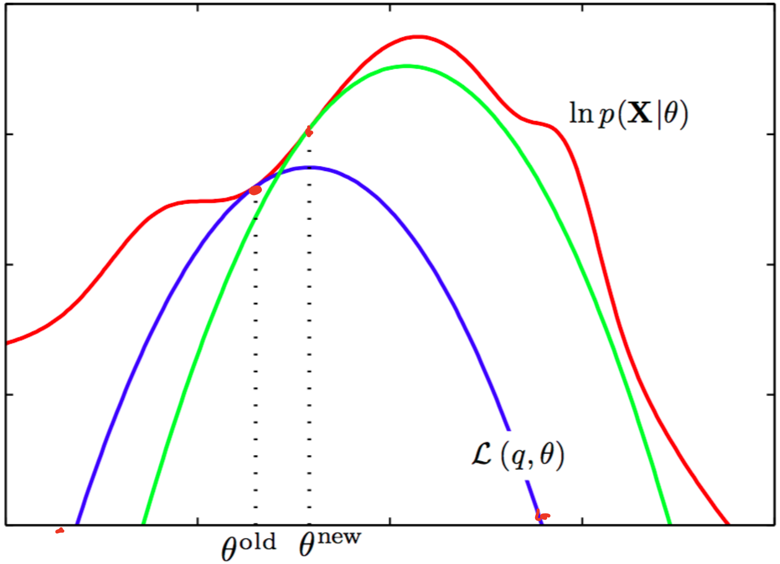
  3. Let $\theta^{\text{new}} = \arg\max_\theta \mathcal{L}(q^*,\theta)$.
  4. Go to step 2, until converged.
- Will show: $p(x \mid \theta^{\textbf{new}}) \geqslant p(x \mid \theta^{\textbf{old}})$
- **Get sequence of θ's with monotonically increasing likelihood.**

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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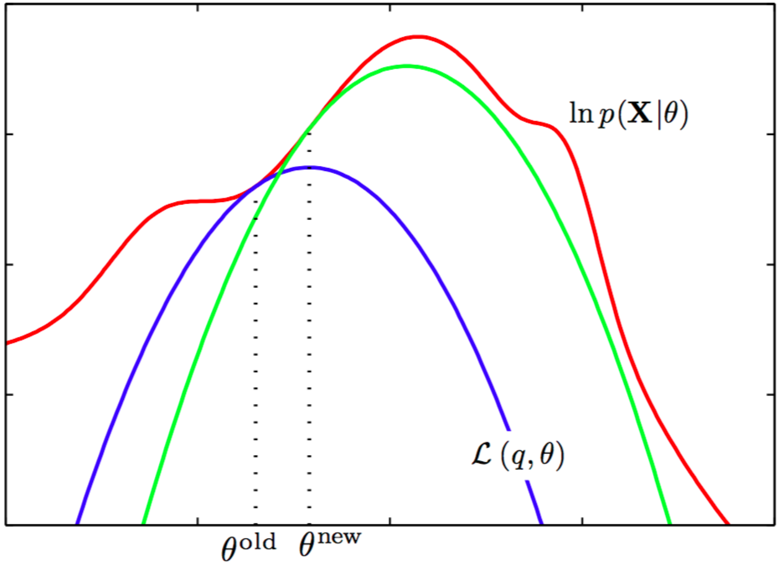

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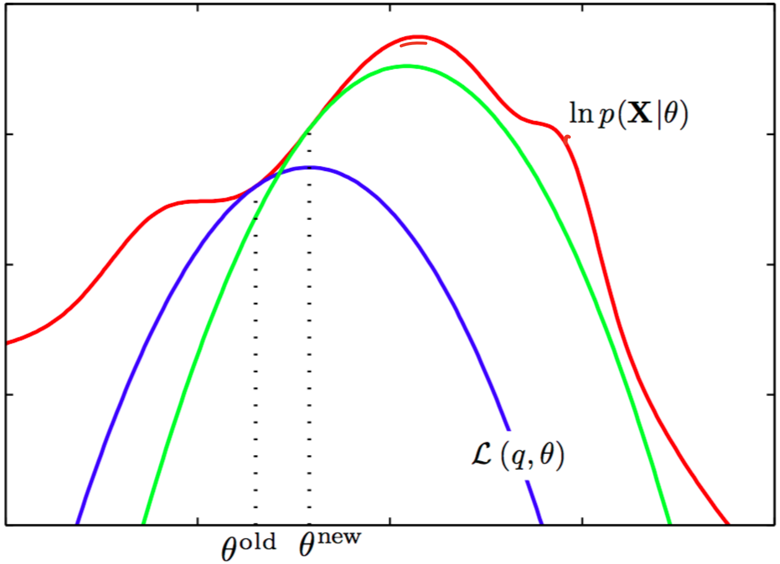

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Is ELBO a "good" lowerbound?

$q(z) \| p(z|x)$ — exact inference.

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

- **KL divergence**: measures "distance" between two distributions (not symmetric!)
- $\mathrm{KL}(q\|p) \geqslant 0$ 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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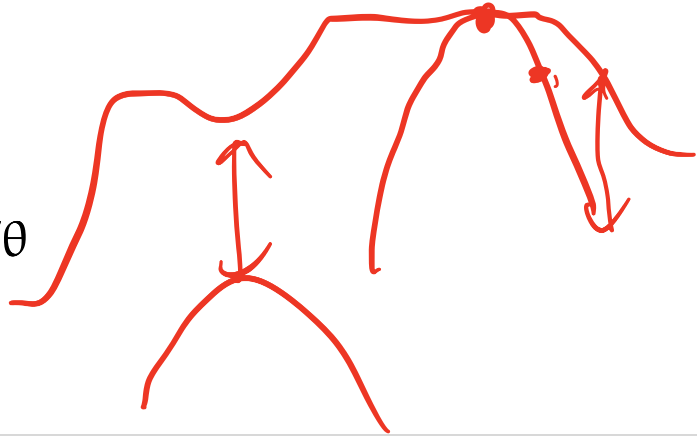
$q(z) = p(z|x)$

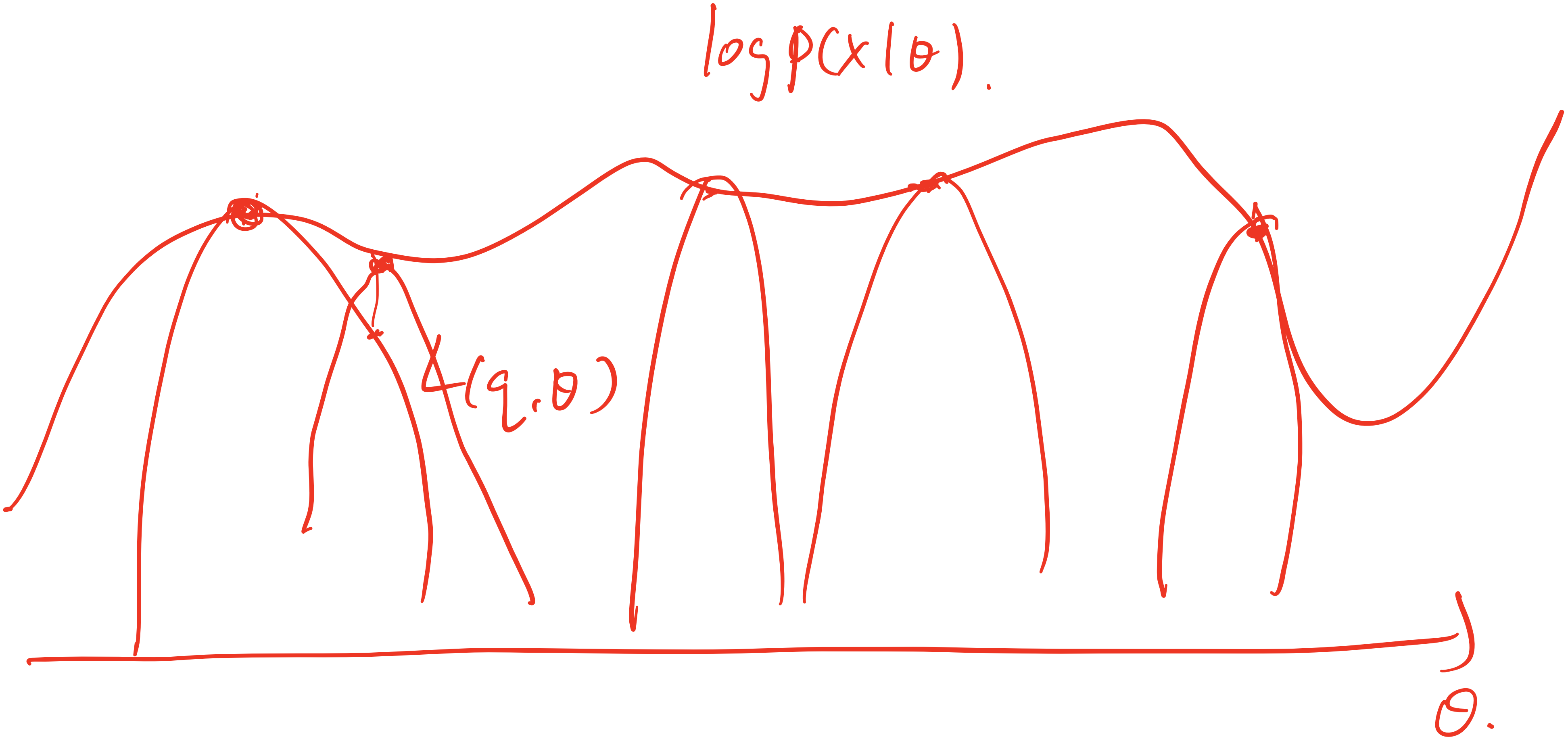


- Summary:

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

- 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?

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

EM algorithm

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

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

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

EM Algorithm

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

2. **Maximization Step**

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

[Equivalent to maximizing expected complete log-likelihood.]

EM Algorithm

1. **Expectation Step**
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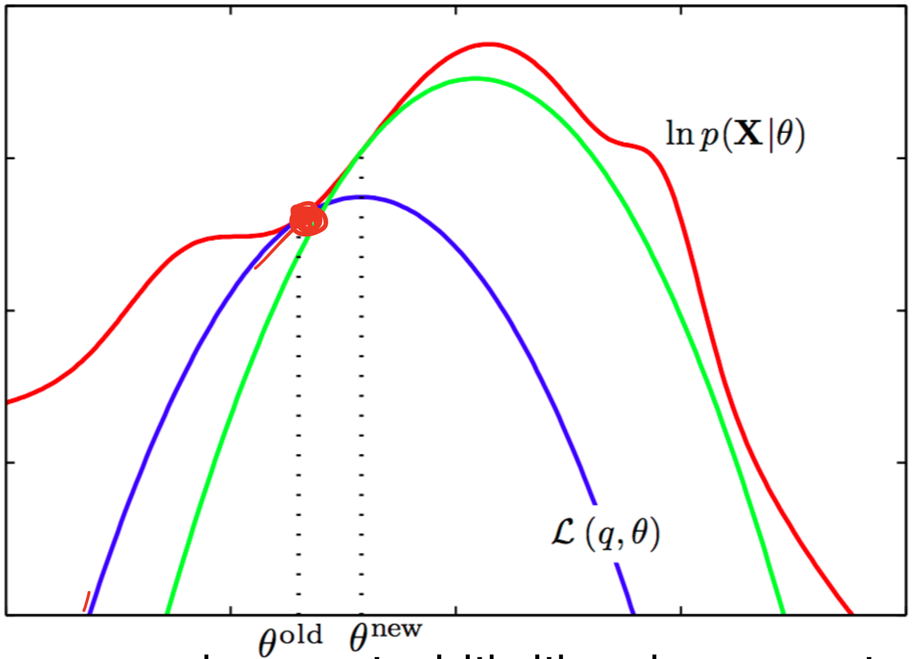
   [Equivalent to maximizing expected complete log-likelihood.]

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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- 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

exact inference.

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EM and More General Variational Methods

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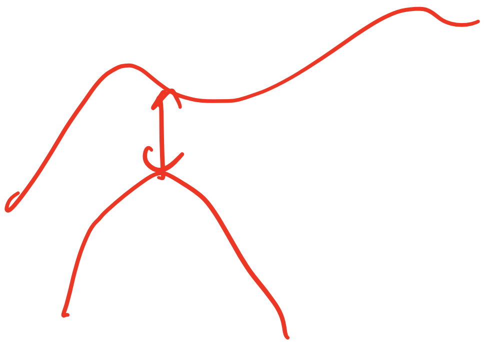
- Solution: Restrict to distributions $\mathcal{Q}$ that are easy to work with.
- Lower bound now looser:

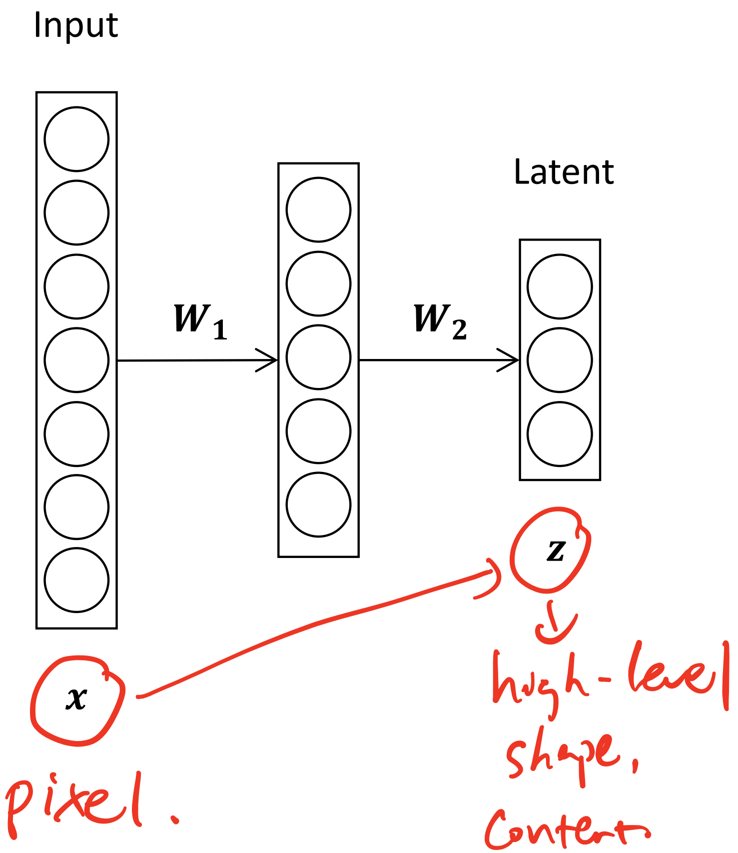
$$q^* = \underset{q \in \mathcal{Q}}{\arg\min}\, \mathrm{KL}[q(z), p(z \mid x, \theta^{\text{old}})]$$



Deep Latent Variable Models

$\underbrace{q(z)}$.

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



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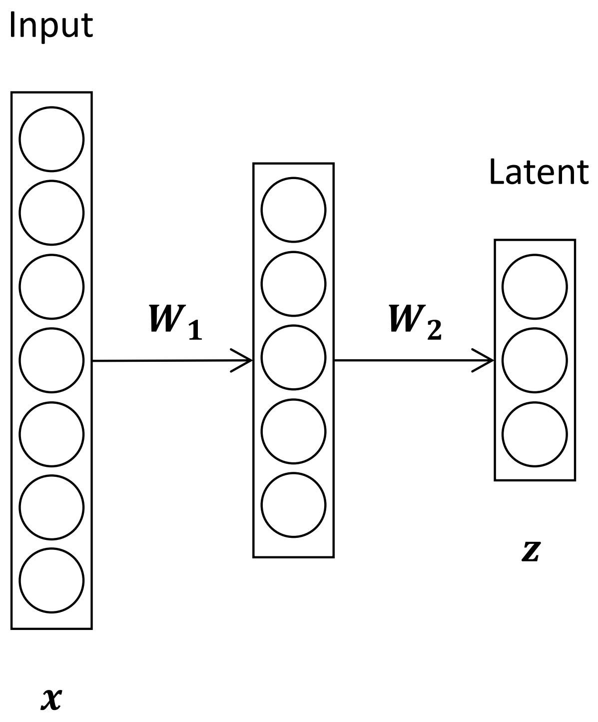

Deep Latent Variable Models

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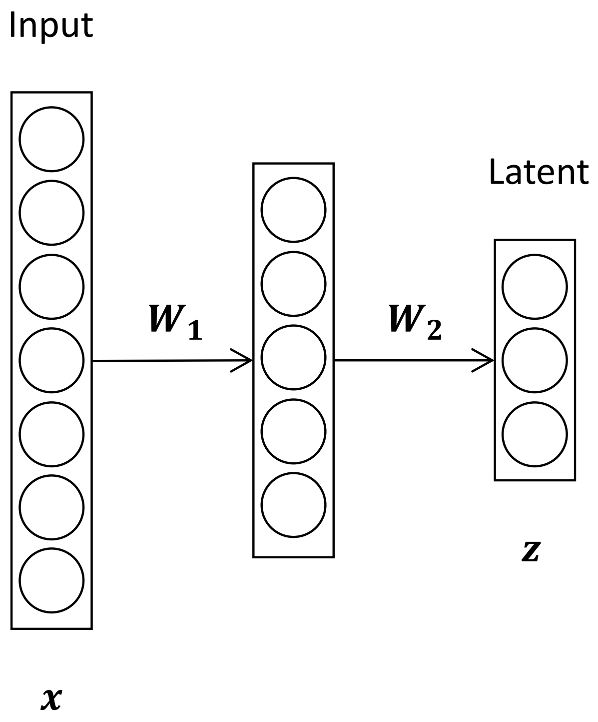
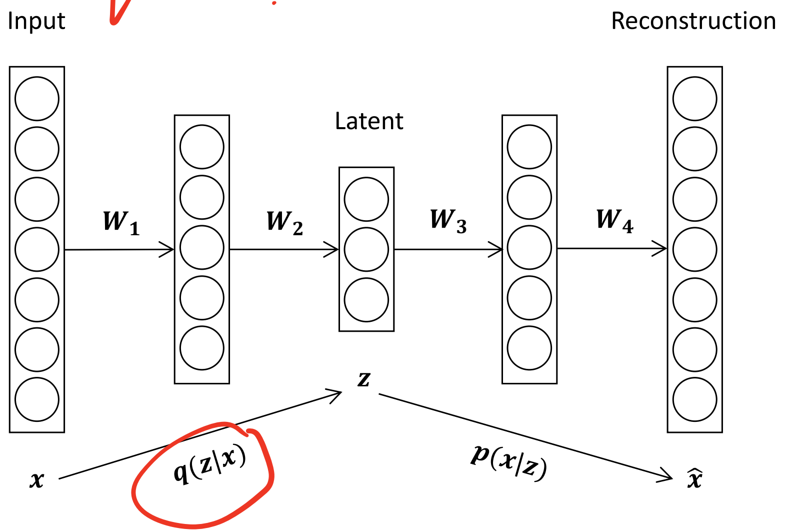
- In neural networks, the hidden activations do not have probabilistic interpretation as they are not random variables.
- What if we let the hidden represent some learned latent code?



Variational Autoencoders (VAE) [1]

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

$q(z|x)$. $p(x|z)$.



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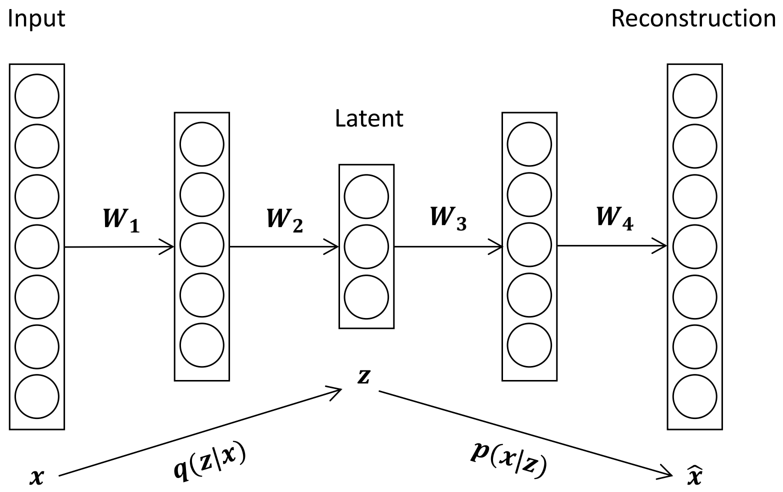

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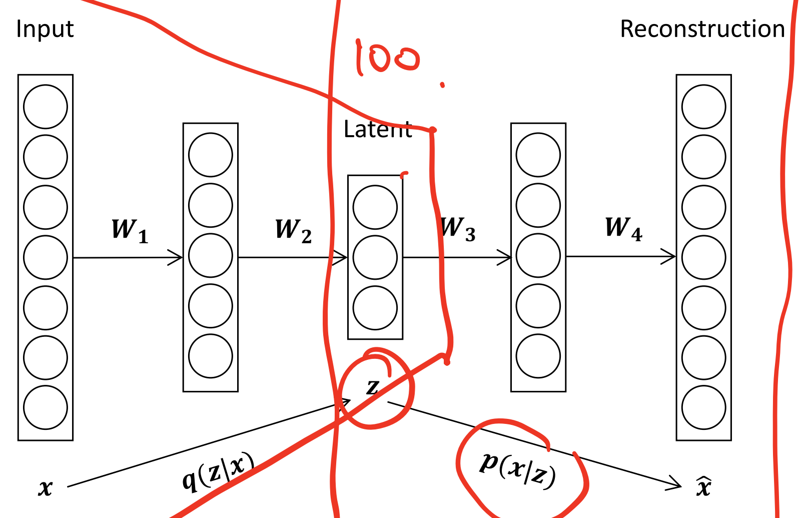
- How to make q a probability distribution?



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

$p(x;\theta)$.

$\sum_{z} p(x|z)\,p(z)$.

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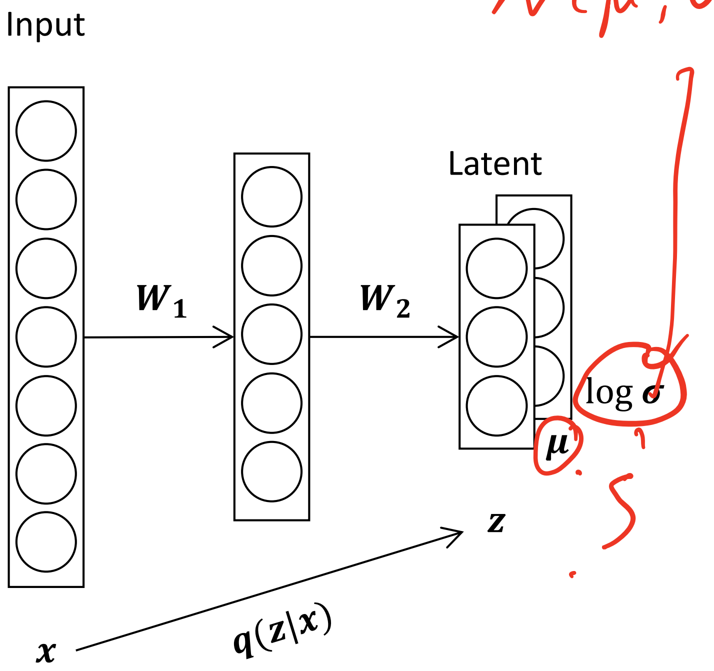
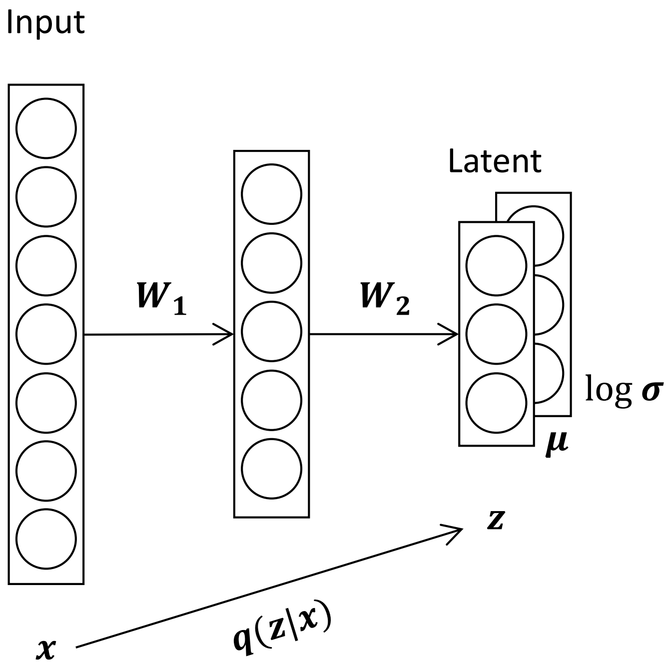
- Let's assume that $q(z|x)$ is a Gaussian distribution.

$\mathcal{N}(\mu;\sigma).$



Reparameterization Trick

- Let's assume that $q(z|x)$ is a Gaussian distribution.
- Instead of letting the neural network to output a stochastic variable, we can let it predict deterministically the distribution parameters μ and σ.



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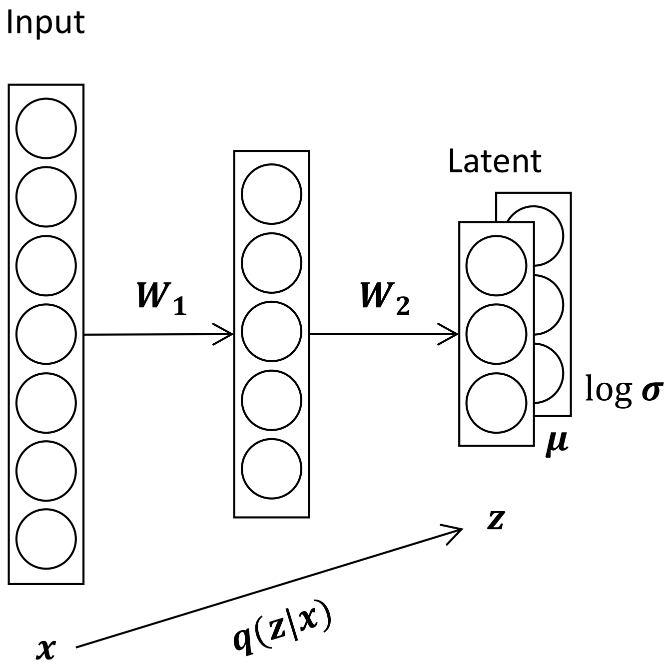

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$$

Square error.

N(0, I).

Stochastic Gradient

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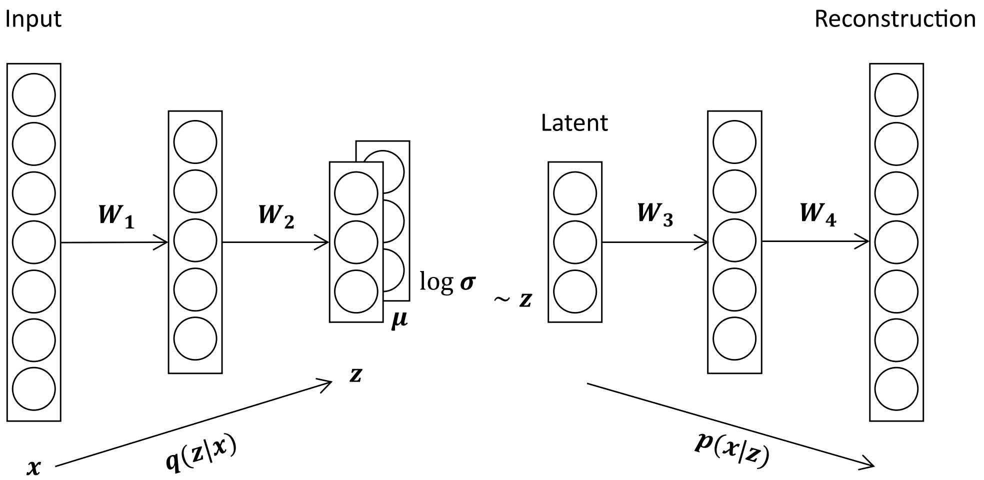

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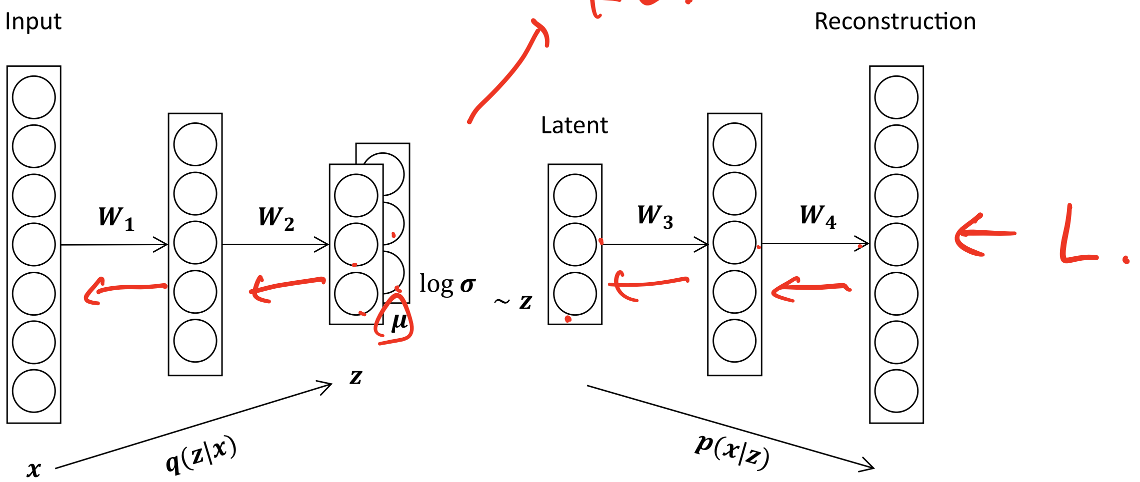
$\frac{\partial L}{\partial z}$.

- Turns out we just need to have a Monte Carlo sample size of 1:
  - For each x, sample one z from $q(z|x)$.

KL ~ prior.



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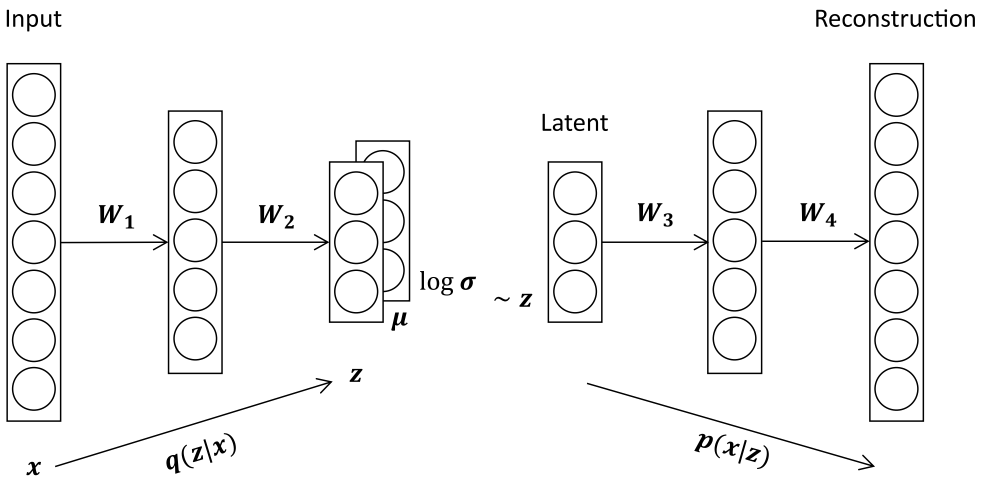
- Backprop through reparameterization.



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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- Later adapted by He He, Tal Linzen, and others.
- This is a very challenging grad-level course.
- Congrats, you are almost done.

Next Lecture: Project Presentation

- Dec 10, in-person presentations.
- 22 groups, 120mins.
- Aim for **3 mins** per group, hard stop at 4 mins, and 1 min max for Q&A.
- Send your slides in PDF with your group number by Dec 9 11:59pm (via Google form).

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Linear Perceptron, conditional probability models, SVMs

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- Trade-offs:
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  - accuracy and efficiency (during both training and inference).

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

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Loss functions How far off a prediction is from the target, e.g. 0-1 loss, margin-based loss, squared loss.

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- 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 sheds new insight into understand DL.
- Classic ML lays down foundation when we innovate in DL algorithms.

Other ML Related Advanced Courses in CS/DS

- Bayesian Machine Learning(Andrew Wilson)
- Computer Vision (Saining Xie)
- Deep Learning (Yann LeCun)
- Deep Reinforcement Learning (Lerrel Pinto)
- Ebodied Learning and Vision (Mengye Ren)
- Foundations of Deep Learning Theory (Matus Telgarsky)
- Inference and Representation (Joan Bruna)
- Learning with Large Language and Vision Models (Saining Xie)
- Mathematics of Deep Learning (Joan Bruna)
- Natural Language Processing (He He)