Latent variable models and variational inference

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AI Winter School 2025

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[0] Slides available at `https://tinyurl.com/22vazp6w`

Outline

Latent Variable Models (LVMs)

- **Definition:** LVMs introduce hidden (latent) variables to model complex data distributions.
- **Motivation:** Observed data can often be better explained by assuming underlying hidden factors.

Mathematical Formulation:

$$p(x) = \int p(x \mid z, \theta) p(z \mid \theta) dz$$

where:

- x is the observed variable
- z is the latent variable
- θ are model parameters

Latent Variable Models (LVMs)

Challenges:

- *Posterior Inference*:

$$p(z \mid x, \theta) = \frac{p(x, z \mid \theta)}{p(x \mid \theta)} = \frac{p(x \mid z, \theta)\, p(z \mid \theta)}{\int p(x \mid z', \theta)\, p(z' \mid \theta)\, dz'}$$

  is often *intractable*.
- The integral or summation over z complicates direct analytical solutions.
- Requires *approximate methods* (e.g., Expectation-Maximization or[1] Variational Inference) to estimate $p(z \mid x, \theta)$.

[1] EM is a special case of VI in fact.

Example: Customer Segmentation in Retail

Scenario:

- A retail store tracks every customer's purchase history over time.
- *Observed data:* Which items each customer buys and how frequently.
- *Latent variable:* Each customer's **segment** or **cluster** (e.g., "budget-conscious," "brand-focused," "tech-savvy," etc.).

Simple Model (Mixture Idea):

$$
\begin{aligned}
z_i &\sim \text{Discrete}(\pi_1, \pi_2, \ldots, \pi_K), \\
\mathbf{x}_i \mid z_i &\sim \mathcal{F}(\theta_{z_i}),
\end{aligned}
$$

where:

- z_i indicates the (hidden) segment of customer i.
- $\mathcal{F}$ is a probability model for purchase behaviors (e.g., Poisson, multinomial), parameterized by θ_{z_i}.
- π_k are segment mixing weights ($\sum_k \pi_k = 1$).

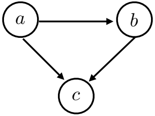
Directed Graphical Models

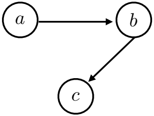
- In LVMs, there is explicit relationship such as $\boldsymbol{z} \to \boldsymbol{x}$.
- Can we generalize this to more complicated relationships like $\boldsymbol{z} \to \boldsymbol{x} \to \boldsymbol{y}$?
- Note that this is different from dependencies.

Directed Graphical Models

- The relation (generative assumption) between random variables can be compactly represented by a directed graph.
  - Nodes: random variables
  - Edges: relations between variables (conditional probabilities).
- Directed edge between two nodes indicates conditional probability.
  - For example, if there is a link from node x to y, the distribution of y depends on x, i.e. $p(y|x)$.
- If node x doesn't have any incoming edge, then, the node is independent of the joint distribution.

Examples





The joint distribution of a, b, c is

$$p(a, b, c) = p(a)p(b|a)p(c|a, b)$$

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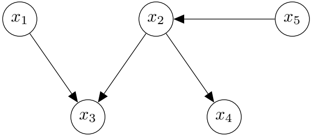
In general, the joint distribution of $p(\boldsymbol{x})$ is given as

$$p(\boldsymbol{x}) = \prod_{k=1}^{K} p(x_k | \mathrm{Pa}_k),$$

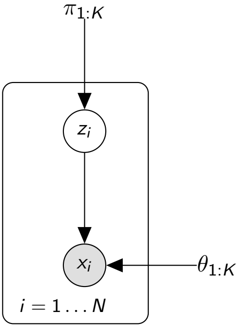
where Pa_k means the parent nodes of x_k.



Given this graph, the joint distribution is defined as:

$$p(\boldsymbol{x}) = p(x_1)p(x_5)p(x_2|x_5)p(x_3|x_1, x_2)p(x_4|x_2)$$

Graphical Model: Customer Segmentation



- Random variables with circle
- Hyperparameters without circle
- Plate repeats everything inside

- Graphical model of the customer segmentation
  - For each customer i:
    - Draw latent $z_i \sim \boldsymbol{\pi}$
    - Observe $x_i \sim \mathcal{F}(\theta_{z_i})$

Outline

Finite Mixture Model

A semi-parametric model in the form of:

$$p(x) = \sum_{k \in [K]} p(x, z = k) = \sum_{k \in [K]} p_k(x) p(z = k)$$

- A point is drawn from one of K component distributions $\{p_k(\cdot)\}_{k \in [K]}$
- z is the latent variable indicating from which component distribution the point is originated.
- $\{\pi_k := p(z = k)\}_{k \in [K]}$ are the mixing parameters such that $\sum_{k \in [K]} \pi_k = 1$ and $\pi_k \in [0, 1]$.

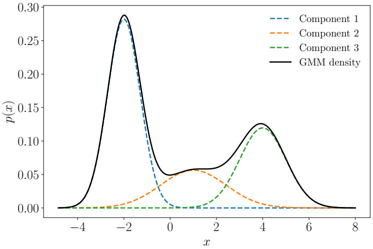
Gaussian Mixture Models: Intuition

- Marginal is a multimodal distribution

$$p_\theta(x) := p(x|\theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$

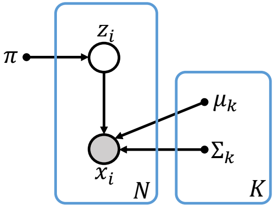
where $\theta = \{\mu_k, \Sigma_k, \pi_k\}_{k=1}^{K}$.

- Flexible than K-means.



$$0.5\mathcal{N}(-2, \frac{1}{2}) + 0.2\mathcal{N}(1, 2) + 0.3\mathcal{N}(4, 1)$$

Gaussian Mixture Model: Graphical Representation



Gaussian Mixture Model (GMM)

- Point x_i's true cluster $z_i \in [K]$ is hidden and independently drawn from

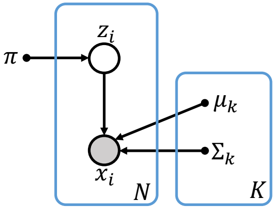
$$p(z_i) = \prod_{k \in [K]} \pi_k^{\mathbb{1}[z_i = k]}, \text{i.e., } p(z_i = k) = \pi_k.$$

- The distribution over observed variables conditioned on the latent variables is

$$p(x_i \mid z_i) = \prod_{k \in [K]} (\mathcal{N}(x_i \mid \mu_k, \Sigma_k))^{\mathbb{1}[z_i = k]}$$

$$\text{or } p(x_i \mid k) = \mathcal{N}(x_i \mid \mu_k, \Sigma_k) \text{ if } z_i = k.$$

Learning GMM



- Compute maximum likelihood estimates of parameters

$$\theta = \{\pi_k, (\mu_k, \Sigma_k)\}_{k \in [K]}$$

- Compute the posterior on latent z_i

$$r_{ik} = p(z_i = k \mid x_i)$$

- Can optimize θ with gradient methods from marginal distribution $p(x|\theta)$?

Parameter estimation via MLE

- Given iid samples $\mathcal{D} = \{x_1, ..., x_N\}$, the log likelihood that we need to maximize is

$$
\begin{aligned}
L(\theta) = \log p(\mathcal{D}|\theta) &= \log \prod_{n=1}^{N} p(x_n|\theta) \\
&= \sum_{n=1}^{N} \log p(x_n|\theta) \\
&= \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)
\end{aligned}
$$

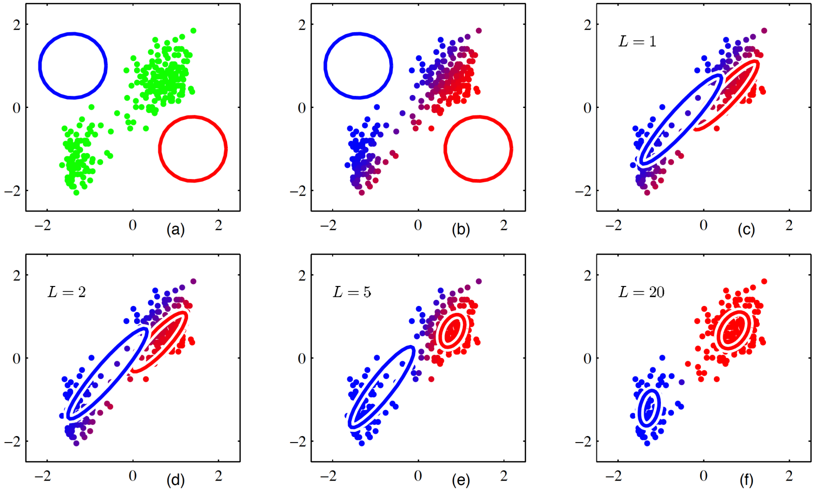
There is no Closed-form Solution

$$L(\theta) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n | \mu_k, \Sigma_k)$$

- Can we compute $\frac{\partial L}{\partial \theta}$?
- Unfortunately, there is no closed-form solution that can find all parameters θ by a single computation.
- For example, setting the partial derivative w.r.t. π_k to zero yields

$$\frac{\partial L}{\partial \mu_k} = \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}\left(x_n \mid \mu_k, \Sigma_k\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(x_n \mid \mu_j, \Sigma_j\right)} \Sigma_k^{-1}(x_n - \mu_k),$$

  which cannot be simplified in a closed form, i.e., $\mu_k =$ something.
- We will apply the expectation-maximization (EM) algorithm.



(a)
(b)
(c)
(d)
(e)
(f)
$L = 1$
$L = 2$
$L = 5$
$L = 20$

EM for isotropic GMM

Define

- $z_i \in [K]$: the cluster to which point x_i belongs.
- θ is a set of hyperparameters, i.e., $\theta = \{\{\pi_k, \mu_k, \sigma_k\}_{k=1}^K\}$
- $\mathcal{L}_c(\theta; \{x_i, z_i\}_{i\in[N]})$: the complete-data log-likelihood, i.e.,

$$\mathcal{L}_c(\theta; \{x_i, z_i\}_{i\in[N]}) = \sum_{i\in[N]} \log p(x_i, z_i \mid \theta)$$

Isotropic GMM

- Letting $z_{ik} = \mathbb{1}[z_i = k]$,

$$p(z_i) = \prod_{k\in[K]} \pi_k^{z_{ik}}, \quad \text{and} \quad p(x_i \mid z_i) = \prod_{k\in[K]} \left(\mathcal{N}(x_i \mid \mu_k, \sigma_k^2 I)\right)^{z_{ik}} .$$

Log-Likelihood for GMM (1)

The complete-data log-likelihood can be calculated as follows:

$$
\begin{aligned}
\mathcal{L}_c(\theta; \{x_i, z_i\}_{i\in[N]}) &= \sum_{i\in[N]} \log p(x_i, z_i \mid \theta) \\
&= \sum_{i\in[N]} \log \left(p(x_i \mid z_i, \theta) p(z_i \mid \theta) \right) \\
&= \sum_{i\in[N]} \log \left(\prod_{k\in[K]} \left(\pi_k \mathcal{N}(x_i \mid \mu_k, \sigma_k^2 I) \right)^{z_{ik}} \right) \\
&= \sum_{i\in[N]} \sum_{k\in[K]} z_{ik} \log \left(\pi_k \mathcal{N}(x_i \mid \mu_k, \sigma_k^2 I) \right) .
\end{aligned}
$$

Log-Likelihood for GMM (2)

For given θ', define the responsibility[2] r_{ik} of cluster k to data point x_i,

$$r_{ik} := p(z_i = k \mid x_i; \theta') = \mathbb{E}_{z_i \mid x_i, \theta'}[z_{ik}] \ .$$

Then, given θ' or $\{r_{ik}\}$, the marginal log-likelihood of $\theta = \{\mu_k, \sigma_k^2\}$ can be approximated by:

$$\begin{aligned}
\mathcal{Q}(\theta; \theta') &:= \mathbb{E}_{\{z_i\}_{i \in [N]} \mid \{x_i\}_{i \in [N]}, \theta'} \left[\mathcal{L}_c(\theta; \{x_i, z_i\}_{i \in [N]})\right] \\
&= \sum_{i \in [N]} \sum_{k \in [K]} \mathbb{E}_{z_i \mid x_i, \theta'} \left[z_{ik} \log\left(\pi_k \mathcal{N}(x_i \mid \mu_k, \sigma_k^2 I)\right)\right] \\
&= \sum_{i \in [N]} \sum_{k \in [K]} r_{ik} \log\left(\pi_k \mathcal{N}(x_i \mid \mu_k, \sigma_k^2 I)\right) \\
&= \sum_{i \in [N]} \sum_{k \in [K]} r_{ik} \left[\log \pi_k - \frac{D}{2} \log \sigma_k^2 - \frac{1}{2\sigma_k^2} \|x_i - \mu_k\|^2\right] + \text{const} \ .
\end{aligned}$$

[2] A posterior of z given the other parameters.

EM for GMM

Starting from an arbitrary choice of $\theta = \left\{\pi_k, \mu_k, \sigma_k^2\right\}_{k\in[K]}$,

- E-step: Compute responsibilities $\{r_{ik}\}$ for given $\theta' = \theta$:

$$r_{ik} := p(z_i = k \mid x_i; \theta') = \frac{\pi_k p(x_i \mid z_i = k, \mu_k, \sigma_k^2)}{\sum_{\ell\in[K]} \pi_\ell p(x_i \mid z_i = \ell, \mu_\ell, \sigma_\ell^2)} \ .$$

- M-step: Update θ_{new} maximizing the approximated marginal log-likelihood $\mathcal{Q}(\theta; \theta')$:

$$\theta_{\text{new}} = \arg\max_{\theta} \ \mathcal{Q}(\theta; \theta') \ .$$

M-Step: Gaussian Parameters (1)

Using the theory of optimization, we find θ such that $\nabla_\theta \mathcal{Q}(\theta) = 0$:

- Mean

$$\frac{\partial \mathcal{Q}}{\partial \mu_k} = -\frac{1}{\sigma_k^2} \sum_{i \in [N]} r_{ik}(x_i - \mu_k) = 0$$

$$\implies \mu_{k,\text{new}} = \frac{\sum_{i \in [N]} r_{ik} x_i}{\sum_{i \in [N]} r_{ik}} .$$

- Variance

$$\frac{\partial \mathcal{Q}}{\partial \sigma_k^2} = \sum_{i \in [N]} r_{ik} \left[-\frac{D}{\sigma_k} + \frac{1}{\sigma_k^3} \|x_i - \mu_k\|^2 \right] = 0$$

$$\implies \sigma_{k,\text{new}}^2 = \frac{1}{D} \frac{\sum_{i \in [N]} r_{ik} \|x_i - \mu_{k,\text{new}}\|^2}{\sum_{i \in [N]} r_{ik}}$$

M-step: Mixing Parameter (2)

$$\mathcal{Q}(\theta) = \sum_{i \in [N]} \sum_{k \in [K]} r_{ik} \left[\log \pi_k - \frac{D}{2} \log \sigma_k^2 - \frac{1}{2\sigma_k^2} \|x_i - \mu_k\|^2 \right] + \text{const}$$

Note that $\{\pi_k\}$ must verify $\sum_{k \in [K]} \pi_k = 1$. Hence, recalling the theory of constrained optimization, consider the Lagrangian

$$\mathcal{Q}'(\theta, \lambda) = \mathcal{Q}(\theta) + \lambda \left(1 - \sum_{k \in [K]} \pi_k \right) .$$

Solving

$$\frac{\partial \mathcal{Q}'(\theta, \lambda)}{\partial \pi_k} = \sum_{i \in [N]} \frac{r_{ik}}{\pi_k} - \lambda = 0 \, ,$$

one can conclude that the optimal Lagrangian multiplier λ is given by $\lambda = N$, and thus

$$\pi_{k,\text{new}} = \frac{1}{N} \sum_{i \in [N]} r_{ik}$$

EM Algorithm for Isotropic GMM: Summary

Starting from an arbitrary choice of $\theta = \left\{\pi_k, \mu_k, \sigma_k^2\right\}_{k\in[K]}$,

- E-step: Compute responsibilities $\{r_{ik}\}$ for given $\theta' = \theta$:

$$r_{ik} := p(z_i = k \mid x_i; \theta') = \frac{\pi_k p(x_i \mid z_i = k, \mu_k, \sigma_k^2)}{\sum_{\ell\in[K]} \pi_\ell p(x_i \mid z_i = \ell, \mu_\ell, \sigma_\ell^2)} .$$

- M-step: Update θ_{new} maximizing the approximated log-likelihood:

$$\mu_{k,\text{new}} = \frac{\sum_{i\in[N]} r_{ik} x_i}{\sum_{i\in[N]} r_{ik}}$$

$$\sigma^2_{k,\text{new}} = \frac{1}{D} \frac{\sum_{i\in[N]} r_{ik} \|x_i - \mu_{k,\text{new}}\|^2}{\sum_{i\in[N]} r_{ik}}$$

$$\pi_{k,\text{new}} = \frac{1}{N} \sum_{i\in[N]} r_{ik}$$

Estimation with Latent Variables

When there are missing data or latent variables, denoted by z, MLE seeks to find θ maximizing the marginal likelihood of the observed data x:

$$p(x \mid \theta) = \int p(x, z \mid \theta) dz \ .$$

As such, MLE or MAP often require the computationally intractable marginalization or maximization. Variational inference is a family of techniques to approximate the marginalization or maximization, e.g.,

- Belief propagation
- Expectation-maximization
- Mean field approximation
- ...

Outline

Convex Set and Function

- A set $C \subset \mathbb{R}^d$ is convex if

$$\lambda x + (1-\lambda) y \in C \ , \quad \forall x, y \in C \text{ and } \forall \lambda \in [0,1].$$

- For a convex set $C \subset \mathbb{R}^d$, a function $f : C \mapsto \mathbb{R}$ is convex if

$$f(\lambda x + (1-\lambda) y) \le \lambda f(x) + (1-\lambda) f(y) \ , \quad \forall x, y \in C \text{ and } \forall \lambda \in [0,1].$$

Jensen's Inequality

Theorem (Jensen's inequality for random variables)

For a convex set C, if function $f : C \mapsto \mathbb{R}$ is convex and X is a random vector on C, then

$$\mathbb{E}[f(X)] \geq f(\mathbb{E}[X]) \, .$$

In case of concave f, we have $\mathbb{E}[f(X)] \leq f(\mathbb{E}[X])$.

Proof of Jensen's Inequality

For simplicity, consider discrete random vector X with $p_i = p(X = x_i)$ for $\{x_i\}_{i\in[N]} \subset C$. We prove $\sum_{i\in[N]} p_i f(x_i) \geq f(\sum_{i\in[N]} p_i x_i)$ by recursion:

$$
\begin{aligned}
& f\left(\sum_{i\in[N]} p_i x_i\right) = f\left(p_1 x_1 + (1-p_1)\left(\frac{\sum_{i=2}^N p_i x_i}{1-p_1}\right)\right) \\
& \leq p_1 f(x_1) + (1-p_1) f\left(\frac{\sum_{i=2}^N p_i x_i}{1-p_1}\right) \\
& = p_1 f(x_1) + (1-p_1) f\left(\frac{p_2}{1-p_1} x_2 + \left(\frac{1-\sum_{i=1}^2 p_i}{1-p_1}\right)\left(\frac{\sum_{i=3}^N p_i x_i}{1-\sum_{i=1}^2 p_i}\right)\right) \\
& \leq p_1 f(x_1) + (1-p_1)\left(\left(\frac{p_2}{1-p_1}\right) f(x_2) + \left(\frac{1-\sum_{i=1}^2 p_i}{1-p_1}\right) f\left(\frac{\sum_{i=3}^N p_i x_i}{1-\sum_{i=1}^2 p_i}\right)\right) \\
& = p_1 f(x_1) + p_2 f(x_2)\left(1-\sum_{i=1}^2 p_i\right) f\left(\frac{\sum_{i=3}^N p_i x_i}{1-\sum_{i=1}^2 p_i}\right) \ldots
\end{aligned}
$$

Information and Entropy

- Information $I(X)$ of random variable X is defined as

$$I(X) := -\log p(X) ,$$

which is itself a random variable, and quantifies the surprise or uncertainty of the realization of X.

- Entropy $H(X)$ of random variable X is defined as the expected value of information:

$$H(X) := \mathbb{E}[I(X)] = -\sum_{x \in \mathcal{X}} p(x) \log_b p(x) ,$$

which measures the uncertainty of X w.r.t. base $b > 0$, and $\mathcal{X}$ is the set of all possible values of X.

Entropy and Relative Entropy

- Entropy is a measure of uncertainty of a random variable, defined by:

$$H(X) := \mathbb{E}[I(X)] = -\sum_{x \in \mathcal{X}} p(x) \log p(x) \; .$$

- Kullback-Leibler divergence is a measure of relative entropy of distribution p to reference distribution q such that p is absolutely continuous w.r.t. q[3], defined by:

$$\mathrm{KL}(p \| q) := \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)} \; ,$$

where we use the convention of $0 \log(0/0) = 0$.

[3] i.e., $q(x) = 0$ implies $p(x) = 0$

Gibb's Inequality

Theorem (Gibb's Inequality)

For any distributions p, q such that $p \ll q$, i.e., p is absolutely continuous w.r.t. q,

$$KL(p\|q) \geq 0 \,,$$

where the equality holds iff $p = q$.

Proof) Consider discrete distributions $\{p_i\}, \{q_i\}$.

$$\begin{aligned}
\mathrm{KL}(p\|q) = \sum_i p_i \log \frac{p_i}{q_i} &= -\sum_i p_i \log \frac{q_i}{p_i} \\
&\geq -\log\left(\sum_i p_i \frac{q_i}{p_i}\right) \qquad \text{(Jensen's ineq.)} \\
&= -\log\left(\sum_i q_i\right) = 0 \,.
\end{aligned}$$

Gibb's Inequality: Proof of the Equality

In order to find the "distribution" p which minimizes $\mathrm{KL}(p\|q)$, we consider Lagrangian

$$\mathcal{F}(p,\lambda) = \mathrm{KL}(p\|q) + \lambda\left(1 - \sum_i p_i\right) = \sum_i p_i \log\frac{p_i}{q_i} + \lambda\left(1 - \sum_i p_i\right) .$$

Then, the minimal p must have λ verifying:

$$\frac{\partial \mathcal{F}}{\partial p_i} = \log p_i - \log q_i + 1 - \lambda = 0 ,$$

which implies $p_i = q_i \exp(\lambda - 1)$ for each i.

$\Rightarrow \sum_i p_i = 1 = \sum_i q_i \exp(\lambda - 1)$, it follows that $\lambda = 1$.

Hence, the minimal p should be identical to q, and $\mathrm{KL}(p\|q) = 0$ on such choice of p.

A Lower Bound on the Log-Likelihood (1)

The log-likelihood of model parameter θ given observation x is:

$$\begin{aligned} \mathcal{L}(\theta) &= \log p(x \mid \theta) \\ &= \log \int p(x, z \mid \theta) dz \ , \end{aligned}$$

where we marginalize the latent variables z in the second equality.

For any distribution $q(z)$ of the latent variables z, we have

$$\begin{aligned} \mathcal{L}(\theta) &= \log \left(\int q(z) \frac{p(x, z \mid \theta)}{q(z)} dz \right) \\ &\geq \int q(z) \log \left(\frac{p(x, z \mid \theta)}{q(z)} \right) dz \qquad \text{(Jensen's ineq.)} \ . \end{aligned}$$

A Lower Bound on the Log-Likelihood (2)

Denote the lower bound by $\mathcal{F}(q, \theta)$:

$$\begin{aligned}\mathcal{F}(q, \theta) &:= \int q(z) \log \left(\frac{p(x, z \mid \theta)}{q(z)} \right) dz \\ &= \int q(z) \log p(x, z \mid \theta) dz + H(q) \qquad \text{(Def. of entropy)} .\end{aligned}$$

where $H(q)$ is the entropy of q.

One can design an EM algorithm using this lower bound:

- E-step: Maximize $\mathcal{F}(q, \theta)$ over q for tighter lower bound
- M-step: Maximize $\mathcal{F}(q, \theta)$ over θ to update estimates of θ.

EM Algorithm with max-max Interpretation

(for $k = 1, 2, \ldots$)

- E-step: Optimize $\mathcal{F}(q, \theta)$ w.r.t. the distribution q of latent variable z given parameters $\theta^{(k)}$, i.e.,

$$q^{(k+1)} = \arg\max_{q} \quad \mathcal{F}(q, \theta^{(k)}) \ .$$

- M-step: Maximize $\mathcal{F}(q, \theta)$ w.r.t. the parameters θ given the distribution $q^{(k+1)}$ of latent variable z, i.e.,

$$\begin{aligned} \theta^{(k+1)} &= \arg\max_{\theta} \quad \mathcal{F}(q^{(k+1)}, \theta) \\ &= \arg\max_{\theta} \quad \int q^{(k+1)}(z) \log p(x, z \mid \theta) dz \ , \end{aligned}$$

where $p(x, z \mid \theta)$ is the complete-data log-likelihood.

Monotonicity of EM Algorithm

The difference between the log-likelihood and the lower bound is:

$$\begin{aligned}
\mathcal{L}(\theta) - \mathcal{F}(q, \theta) &= \log p(x \mid \theta) - \int q(z) \log \left(\frac{p(x, z \mid \theta)}{q(z)} \right) dz \\
&= \log p(x \mid \theta) - \int q(z) \log \left(\frac{p(z \mid x, \theta) p(x \mid \theta)}{q(z)} \right) dz \\
&= - \int q(z) \log \left(\frac{p(z \mid x, \theta)}{q(z)} \right) dz \\
&= \mathrm{KL}(q(\cdot) \| p(\cdot \mid x, \theta)) \,,
\end{aligned}$$

which is zero only if $q(z) = p(z \mid x, \theta)$ (Gibb's ineq.). This is what E-step finds. Hence,

$$\mathcal{L}(\theta^{(k)}) \underset{\text{E-step}}{=} \mathcal{F}(q^{(k+1)}, \theta^{(k)}) \underset{\text{M-step}}{\leq} \mathcal{F}(q^{(k+1)}, \theta^{(k+1)}) \underset{\text{Jensen}}{\leq} \mathcal{L}(\theta^{(k+1)}) \,.$$

EM Algorithm

The EM algorithm seeks to find the MLE by iteratively applying:
(for $k = 1, 2, ...$)

- E-step: Define $\mathcal{Q}(\theta; \theta^{(k)})$ as the expectation of complete-data log-likelihood w.r.t. z given x and $\theta^{(k)}$:

$$\begin{aligned}\mathcal{Q}(\theta; \theta^{(k)}) &:= \mathbb{E}_{z|x,\theta^{(k)}}[\log p(x, z \mid \theta)] \\ &= \int p(z \mid x, \theta^{(k)}) \log p(x, z \mid \theta) dz \ .\end{aligned}$$

- M-step: Find the parameters that maximize:

$$\begin{aligned}\theta^{(k+1)} &:= \arg\max_{\theta} \mathcal{Q}(\theta; \theta^{(k)}) \\ &= \arg\max_{\theta} \mathcal{F}(q, \theta) - H(q) \\ &\quad \text{(with the choice of } q(z) = p(z|x, \theta^{(k)})) \ ,\end{aligned}$$

  where the term $H(q)$ is ignored since $H(q)$ is constant w.r.t. θ.

Variational Inference: Mean-Field Approximation

- We want to approximate the posterior $p(z \mid x)$ when direct computation is intractable.
- **Mean-field assumption:** Factorize the variational distribution into independent blocks:

$$q(z) \;=\; \prod_{j=1}^{M} q_j\big(z_j\big),$$

  where $\{z_j\}$ are disjoint sets of the latent variables.
- The factorization is often called the *mean-field* assumption (each group of latent variables is treated as independent).
- This drastically reduces the complexity of inference by restricting how latent dimensions can interact.

Evidence Lower BOund (ELBO)

Starting from the log-marginal distribution

$$
\begin{aligned}
\log p(x) &= \log \int p(x,z)\, dz \\
&= \log \int q(z) \frac{p(x,z)}{q(z)}\, dz. \\
&\geq \int q(z) \log \left[\frac{p(x,z)}{q(z)} \right] dz \quad \text{(Jensen's ineq)} \\
&= \mathbb{E}_{q(z)}\big[\log p(x,z)\big] - \mathbb{E}_{q(z)}\big[\log q(z)\big] \\
&= \underbrace{\mathbb{E}_{q(z)}[\log p(x \mid z)]}_{\text{(A) Expected log-likelihood}} + \underbrace{\mathbb{E}_{q(z)}[\log p(z)]}_{\text{(B) Log-prior}} - \underbrace{\mathbb{E}_{q(z)}[\log q(z)]}_{\text{(C) Negative entropy}}.
\end{aligned}
$$

Under mean-field, the optimization often splits into simpler subproblems.

ELBO and KL Divergence

Claim: Minimizing the KL divergence $\mathrm{KL}\big(q(z) \,\|\, p(z \mid x)\big)$ is equivalent to maximizing the *ELBO*:

$$\mathcal{L}(q) = \mathbb{E}_{q(z)}\big[\log p(x, z)\big] \;-\; \mathbb{E}_{q(z)}\big[\log q(z)\big].$$

The difference between the marginal and ELBO becomes

$$\log p(x) - \mathcal{L}(q) = \mathrm{KL}\big(q(z) \,\|\, p(z \mid x)\big).$$

Thus,

$$\max_q \; \mathcal{L}(q) \quad \Longleftrightarrow \quad \min_q \; \mathrm{KL}\big(q(z) \,\|\, p(z \mid x)\big).$$

Coordinate Ascent for Mean-Field VI

Coordinate-Ascent Updates:

- Under the mean-field assumption $q(z) = \prod_j q_j(z_j)$, each factor $q_j(z_j)$ has an analytic update (in exponential-family models):

$$\log q_j(z_j) \leftarrow \mathbb{E}_{\substack{i \neq j \\ q_i(z_i)}} \left[\log p(x, z) \right] + \text{const.}$$

- We iterate over each factor $q_j(z_j)$, update it while holding the others fixed.
- This is repeated until the ELBO converges.

Advantages:

- Relatively straightforward to implement for many graphical models.
- Scales to large datasets if combined with stochastic optimizations.

Tradeoff:

- Mean-field underestimates posterior correlations (factorization).

Bayesian Logistic Regression: Model Setup

Data and Parameters:

- Observations: $\{(x_n, y_n)\}_{n=1}^N$, where $x_n \in \mathbb{R}^D$ and $y_n \in \{0, 1\}$.
- Unknown parameter: $w \in \mathbb{R}^D$.
- **Prior** on w: $p(w) = \mathcal{N}(w \mid 0, I)$.

Likelihood: For each n,

$$p(y_n \mid x_n, w) \;=\; \sigma\left(w^\top x_n\right)^{y_n} \left[1 - \sigma\left(w^\top x_n\right)\right]^{1-y_n},$$

where $\sigma(u) = \frac{1}{1+e^{-u}}$ is the logistic function.

Posterior:

$$p(w \mid \{x_n, y_n\}) \;\propto\; p(w) \prod_{n=1}^N p(y_n \mid w, x_n).$$

Challenge: Intractable Posterior

- $\sigma(u)$ is non-conjugate with the Gaussian prior.
- $\implies$ No closed-form expression for $p(w \mid \{x_n, y_n\})$.
- Classic solutions like *Laplace approximation* or *MCMC* can be more expensive.

Idea: Variational Inference (VI)

Approximate the true posterior with a simpler, tractable family $q(w)$ by *optimizing* a divergence measure (often KL).

Mean-Field Approximation

Factorized variational distribution:

$$q(w) \;=\; \prod_{j=1}^{D} q_j(w_j), \quad \text{with each } q_j(w_j) = \mathcal{N}\big(w_j \mid \mu_j, \sigma_j^2\big).$$

- Assumes $\{w_j\}$ are independent under q.
- Reduces complexity: no cross-covariances.
- Variational parameters: $\{\mu_j, \sigma_j^2\}_{j=1}^{D}$.

Tradeoff:

- *Pro:* Simpler updates, easier to scale.
- *Con:* Ignores correlations among components of w.

ELBO of Bayesian Logistic Regression

The ELBO[4] objective of Bayesian Logistic Regression becomes

$$\begin{aligned}
\mathcal{L}(q) &= \underbrace{\mathbb{E}_{q(w)}[\log p(\{y_n\} \mid w)]}_{\text{(A) Expected log-likelihood}} + \underbrace{\mathbb{E}_{q(w)}[\log p(w)]}_{\text{(B) Log-prior}} - \underbrace{\mathbb{E}_{q(w)}[\log q(w)]}_{\text{(C) Negative entropy}}. \\
&= \underbrace{\mathbb{E}_{q(w)}[\log p(\{y_n\} \mid w)]}_{\text{(A) Expected log-likelihood}} - \sum_j \underbrace{\mathrm{KL}(q_j || p_j)}_{\text{KL between } q_j \text{ and } p_j}
\end{aligned}$$

To update variational parameter μ_j, we need to compute $\frac{\partial \mathcal{L}}{\partial \mu_j}$.

First, it is known that $\frac{\partial \mathrm{KL}(q_j || p_j)}{\partial \mu_j} = -\mu_j$

[4]We omit input x_n for compactness.

Partial derivative of (A) w.r.t. μ_j

Recall the Mean-Field Approximation:

$$q(w) \;=\; \prod_{d=1}^{D} \mathcal{N}\big(w_j \mid \mu_j,\, \sigma_j^2\big).$$

Hence, for each j,

$$q_j(w_j) \;=\; \frac{1}{\sqrt{2\pi}\,\sigma_j}\,\exp\Big(-\frac{(w_j-\mu_j)^2}{2\,\sigma_j^2}\Big).$$

Thus,

$$q(w) \;=\; \prod_{j=1}^{D}\Big[\frac{1}{\sqrt{2\pi}\,\sigma_j}\Big]\,\exp\Big(-\frac{1}{2}\sum_{j=1}^{D}\frac{(w_j-\mu_j)^2}{\sigma_j^2}\Big).$$

Target quantity:

$$\mathbb{E}_{q(w)}[\log p(\{y_n\} \mid w)] \;=\; \int_{\mathbb{R}^D} \left(\prod_{j=1}^{D} q_j(w_j) \right) \log p(\{y_n\} \mid w) \;\; dw_1 \, \ldots \, dw_j .$$

We want

$$\frac{\partial}{\partial \mu_j} \mathbb{E}_{q(w)}[\log p(\{y_n\} \mid w)].$$

Two Common Ways to Derive It:

1. **Score-Function Gradient.**
2. **Reparameterization Trick.**

We cover the score-function gradient for now.

Score-Function Gradient

We write the derivative *inside* the integral:

$$\frac{\partial}{\partial \mu_j} \int q(w) \log p(\{y_n\} \mid w)\, dw \;=\; \int \frac{\partial}{\partial \mu_j} \big[q(w) \log p(\{y_n\} \mid w) \big]\, dw.$$

Since $\log p(\{y_n\} \mid w)$ does *not* directly depend on μ_j (only on w),

$$\frac{\partial}{\partial \mu_j} \big[q(w) \log p(\{y_n\} \mid w) \big] \;=\; \log p(\{y_n\} \mid w)\, \frac{\partial\, q(w)}{\partial \mu_j}.$$

Now note

$$\frac{\partial\, q(w)}{\partial \mu_j} \;=\; q(w)\, \frac{\partial}{\partial \mu_j} \Big[\log q(w) \Big].$$

$$\log q(w) \;=\; \sum_{j=1}^{D} \log q_j(w_j) \;=\; \sum_{j=1}^{D} \Big[-\frac{1}{2} \log(2\pi\sigma_j^2) \;-\; \frac{(w_j - \mu_j)^2}{2\,\sigma_j^2} \Big].$$

Hence,

$$\frac{\partial}{\partial \mu_j} \log q(w) \;=\; \frac{\partial}{\partial \mu_j} \Big[-\frac{(w_j - \mu_j)^2}{2\,\sigma_j^2} \Big] \;=\; \frac{(w_j - \mu_j)}{\sigma_j^2}.$$

Therefore,

$$\begin{aligned} \frac{\partial \mathbb{E}_{q(w)}[\log p(\{y_n\} \mid w)]}{\partial \mu_j} \;&=\; \int q(w) \log p(\{y_n\} \mid w) \, \frac{(w_j - \mu_j)}{\sigma_j^2} \, dw \\ &=\; \mathbb{E}_{q(w)} \left[\log p(\{y_n\} \mid w) \, \frac{(w_j - \mu_j)}{\sigma_j^2} \right]. \end{aligned}$$

$\Longrightarrow$ *This is the "score-function" form. It is correct but can have high variance in practice.*

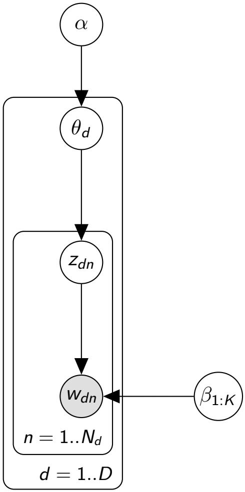
Combine all terms:

Putting all together, we get

$$
\begin{aligned}
\frac{\partial \mathcal{L}(q)}{\partial \mu_j} &= \frac{\partial \mathbb{E}_{q(w)}[\log p(\{y_n\} \mid w)]}{\partial \mu_j} - \frac{\partial \mathrm{KL}(q_j || p_j)}{\partial \mu_j} \\
&= \sum_{n=1}^{N} x_{n,j}\, \mathbb{E}_{q(w)}\big[\, y_n - \sigma(w^\top x_n)\big] - \mu_j. \\
&= \sum_{n=1}^{N} \mathbb{E}_{q(w)}\left[\log p(y_n \mid w)\, \frac{(w_j - \mu_j)}{\sigma_j^2}\right] - \mu_j.
\end{aligned}
$$

Similarly, we can compute $\frac{\partial \mathcal{L}(q)}{\partial \sigma_j}$ as well.

Example: Topic Model (Latent Dirichlet Allocation)



Generative Process (LDA):

1. $\beta_{1:K}$ are the topics, each β_k is a distribution over the vocabulary.
2. For each document d:
   2.1 Draw topic proportions $\theta_d \sim \mathrm{Dirichlet}(\alpha)$.
   2.2 For each word $n \in \{1, \ldots, N_d\}$:
      2.2.1 Draw topic assignment $z_{dn} \sim \mathrm{Discrete}(\theta_d)$.
      2.2.2 Draw word $w_{dn} \sim \mathrm{Discrete}(\beta_{z_{dn}})$.

Outline

Generative Models

Training data ~ $p_{data}(x)$

Generated samples ~ $p_{model}(x)$

Want to learn $p_{model}(x)$ similar to $p_{data}(x)$

- Given training dataset, we want to generate new samples from the same distribution
- In other words, we want to estimate density of data

Applications of Generative Model

- Generative model often provides useful approaches for other machine learning tasks, e.g., density estimation for regression, classification, out-of-distribution detection, ...
- Beside this, there are a number of interesting applications
  - e.g., Image-to-Image translation: super-resolution, style change, colorization, ...

[Isola et al 16]

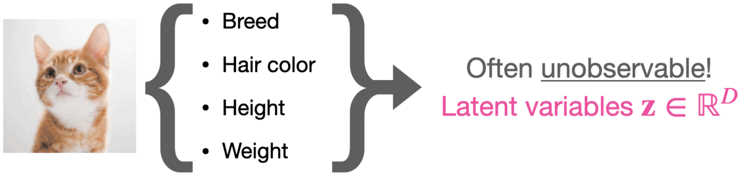
Manifold Hypothesis

- To estimate the density of high-dimensional data, we assume each data point can be characterized by a few properties.
- For example, a cute cat can be (roughly) characterized by

- Breed
- Hair color
- Height
- Weight

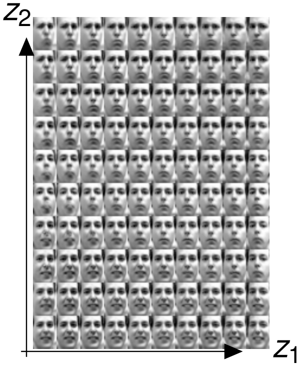
Manifold Hypothesis

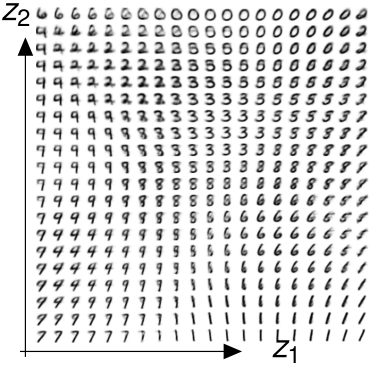
- To estimate the density of high-dimensional data, we assume each data point can be characterized by a few properties.
- For example, a cute cat can be (roughly) characterized by



Manifold Hypothesis

- $x \in \mathbb{R}^M$ is a high dimensional vector
- Data is concentrated around a low dimensional manifold ($z \in \mathbb{R}^D$ with $D \ll M$) $\Rightarrow$ $p(x \mid z)$





[Kingma and Welling 14]

A Probabilistic Approach for Generative Model

Given a single data point x, our objective is to maximize

$$p_\theta(x) = \int p(z) p_\theta(x \mid z) dz$$

where generative model is $p_\theta(x \mid z)$

- Recalling manifold hypothesis, choose prior $p(z)$ to be simple, e.g., Gaussian distribution of reasonable latent attributes z, e.g., pose, degree of smile, ...
- As conditional $p_\theta(x \mid z)$ is anticipated to be complex, a neural network is widely selected
- The marginalization $\int$ is intractable $\rightarrow$ variational inference

Intractability

- Data likelihood is intractable due to the integral:

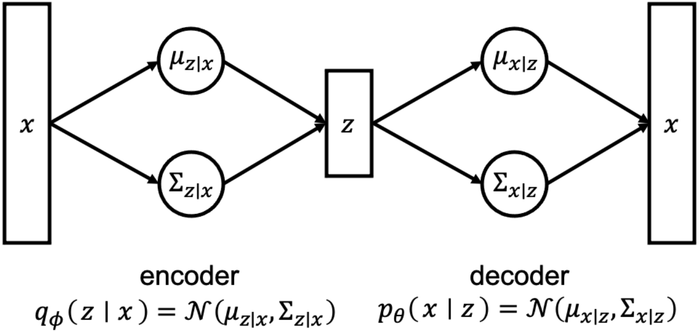
$$p_\theta(x) = \int p(z) p_\theta(x \mid z) dz$$

- Posterior density is also intractable due to the data likelihood:

$$p_\theta(z \mid x) = \frac{p_\theta(x \mid z) p(z)}{p_\theta(x)}$$

- A solution: approximate the posterior $p_\theta(z \mid x)$ using another (encoder) network $q_\phi(z \mid x)$
    - This can overcome the limitation of the mean-field approach.

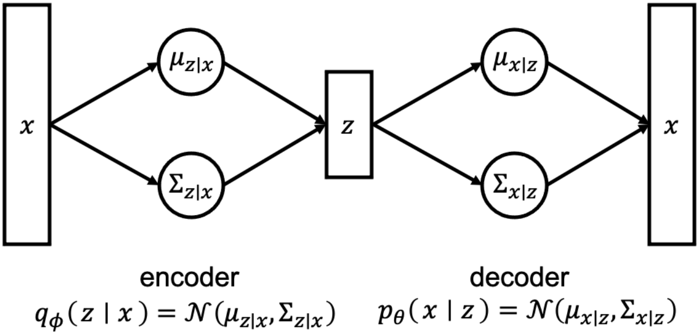
A Probabilistic Framework of Auto-encoder



You can imagine that there is a neural network f_ϕ for encoder, so that

$$f_\phi(x) = \begin{bmatrix} \mu_{z|x} \\ \sigma_{z|x} \end{bmatrix}, \quad \text{and} \quad q_\phi(z|x) = \mathcal{N}\left(f_\phi(x)_1, (f_\phi(x)_2)^2\right)$$

A Probabilistic Framework of Auto-encoder



For decoder p_θ,

$$g_\theta(z) = \begin{bmatrix} \mu_{x|z} \\ \sigma_{x|z} \end{bmatrix}, \quad \text{and} \quad p_\theta(x|z) = \mathcal{N}\left(g_\theta(z)_1, (g_\theta(z)_2)^2\right)$$

Variational Autoencoder

Recalling we aim at MLE: for given x [5],

$$
\begin{aligned}
\log p_\theta(x) &= \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[\log p_\theta(x)\right] \\
&= \mathbb{E}_z\left[\log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)}\right] \\
&= \mathbb{E}_z\left[\log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} \frac{q_\phi(z \mid x)}{q_\phi(z \mid x)}\right] \\
&= \mathbb{E}_z\left[\log p_\theta(x \mid z)\right] - \mathbb{E}_z\left[\log \frac{q_\phi(z \mid x)}{p(z)}\right] + \mathbb{E}_z\left[\log \frac{q_\phi(z \mid x)}{p_\theta(z \mid x)}\right] \\
&= \mathbb{E}_z\left[\log p_\theta(x \mid z)\right] - \mathrm{KL}(q_\phi(z \mid x) \| p(z)) + \mathrm{KL}(q_\phi(z \mid x) \| p_\theta(z \mid x))
\end{aligned}
$$

where the KL divergences take the expectation w.r.t. $z \sim q_\phi(\cdot \mid x)$.

[5] $p(x)p(z \mid x) = p(x \mid z)p(z)$

Variational Autoencoder

Recalling we aim at MLE: for given x,

$$\log p_\theta(x) = \underbrace{\mathbb{E}_z\left[\log p_\theta(x \mid z)\right]}_{\text{(A)}} - \underbrace{\mathrm{KL}(q_\phi(z \mid x) \| p(z))}_{\text{(B)}} + \underbrace{\mathrm{KL}(q_\phi(z \mid x) \| p_\theta(z \mid x))}_{\text{(C)}}$$

- Term (A) is tractable as we can sample $z \sim q_\phi(\cdot \mid x)$ from the encoder, and compute $p_\theta(x \mid z)$ from the decoder.
- Term (B) is tractable as the KL divergence between Gaussians has a closed-form
- Term (C) is intractable, while we know it is non-negative thanks to Gibbs' inequality ($KL \geq 0$)
- Hence, define (A)+(B) as variational lower bound $\mathcal{L}(x, \theta, \phi)$ (ELBO: Evidence Lower BOund and maximize it

Training VAE

Training VAE:

$$\arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)}, \theta, \phi)$$

Understanding ELBO:

$$\begin{aligned}\log p_\theta(x) &\geq \mathcal{L}(x, \theta, \phi) \\ &= \mathbb{E}_z \left[\log p_\theta(x \mid z)\right] - \mathrm{KL}(q_\phi(z \mid x) \| p_\theta(z))\end{aligned}$$

- $\mathbb{E}_z \left[\log p_\theta(x \mid z)\right]$ for reconstruction
- $\mathrm{KL}(q_\phi(z \mid x) \| p(z))$ for regularization to make the approximate posterior close to the prior

Training VAE: Monte Carlo Method

Let's simplify the model by assuming $x, z \in \mathbb{R}$,

$$q_\phi(z|x) \sim \mathcal{N}(z \mid f_\phi(x), \sigma_z^2) \quad \text{and} \quad p_\theta(x|z) \sim \mathcal{N}(x|g_\theta(z), \sigma_x^2)$$

where $f_\phi(x)$ is a function of x parameterized by ϕ, and $g_\theta(z)$ is a function of z parameterized by θ.

The first term of ELBO has no analytic solution:

$$\mathbb{E}_z\left[\log p_\theta(x \mid z)\right] = \int q_\phi(z|x) \log p_\theta(x \mid z) dz$$

We can approximate the expectation with Monte-Carlo method:

$$\mathbb{E}_z\left[\log p_\theta(x \mid z)\right] \approx \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)})$$

where $z^{(1)}, z^{(2)}, ..., z^{(N)}$ are samples drawn from $q_\phi(z|x)$.

Training Decoder p

Given the Monte Carlo approximation

$$\mathbb{E}_z\left[\log p_\theta(x \mid z)\right] \approx \frac{1}{N}\sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)})$$
$$= -\log \sigma_x^2 \sqrt{2\pi} - \frac{1}{2N}\sum_{i=1}^{N} \frac{(x - g_\theta(z^{(i)}))^2}{\sigma_x^2}$$

we can approximate the derivative w.r.t θ[6].

For example, if $g_\theta(z) = \theta_1 z + \theta_0$ where $\theta_1, \theta_0 \in \mathbb{R}$,

$$\frac{\partial\, \mathbb{E}_z\left[\log p_\theta(x \mid z)\right]}{\partial \theta_1} \approx \frac{1}{N}\sum_{i=1}^{N} \frac{(x - g_\theta(z^{(i)}))z^{(i)}}{\sigma_x^2}$$

[6] The same procedure can be applied if g_θ is a NN parameterized by θ.

Training Encoder q

Again, given the Monte Carlo approximation

$$\mathbb{E}_z \left[\log p_\theta(x \mid z)\right] \approx \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)})$$
$$= -\log \sigma_x^2 \sqrt{2\pi} - \frac{1}{2N} \sum_{i=1}^{N} \frac{(x - g_\theta(z^{(i)}))^2}{\sigma_x^2}$$

we cannot approximate the derivative w.r.t ϕ in this case.

Why? the distribution q is replaced by its samples!

$\Rightarrow$ Reparameterization is a key trick to train VAE!

Reparameterization Trick

Some random variables can be represented as a function of another variable. For example, assume $Z \sim \mathcal{N}(\mu, \sigma^2)$.

The distribution of Z can be explained by the standard normal distribution as

$$Z = \sigma\epsilon + \mu, \quad \text{where} \quad \epsilon \sim \mathcal{N}(0, 1)$$

We can also take a sample of Z using the sample from $\mathcal{N}(0, 1)$ via $z^{(i)} = \sigma\epsilon^{(i)} + \mu$

Training Encoder with Reparameterization

Recall $q_\phi(z|x) \sim \mathcal{N}(z \mid f_\phi(x), \sigma_z^2)$.

Using reparam $z^{(i)} = \epsilon^{(i)}\sigma_z + f_\phi(x)$, the expectation can be rewritten as

$$\begin{aligned}
\mathbb{E}_z\left[\log p_\theta(x \mid z)\right] &\approx \frac{1}{N}\sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)}) \\
&= -\log \sigma_x^2\sqrt{2\pi} - \frac{1}{2N}\sum_{i=1}^{N}\frac{(x - g_\theta(z^{(i)}))^2}{\sigma_x^2} \\
&= -\log \sigma_x^2\sqrt{2\pi} - \frac{1}{2N}\sum_{i=1}^{N}\frac{(x - g_\theta(\epsilon^{(i)}\sigma_z + f_\phi(x)))}{\sigma_x^2}
\end{aligned}$$

Then the partial derivative w.r.t. ϕ can be computed via

$$\frac{\partial\, \mathbb{E}_z\left[\log p_\theta(x \mid z)\right]}{\partial \phi} \approx \frac{1}{N}\sum_{i=1}^{N}\frac{(x - g_\theta(z^{(i)}))}{\sigma_x^2}\frac{\partial g_\theta}{\partial \phi}$$

KL Divergence

The second term in ELBO, i.e., $\mathrm{KL}(q_\phi(z \mid x) \| p(z))$, has an analytic solution if both q and p follows the normal distribution:

$$
\begin{aligned}
\int q_\theta(z|x) \log p(z) dz &= \int \mathcal{N}(z; \mu, \sigma^2) \log \mathcal{N}(z; 0, I) dz \\
&= -\frac{J}{2} \log 2\pi - \frac{1}{2} \sum_{j=1}^{J} (\mu_j^2 + \sigma_j^2)
\end{aligned}
$$

where J is a dimensionality of z, μ and σ is a function of x.

We can easily compute the derivatives w.r.t μ and σ.

Training VAE: Summary

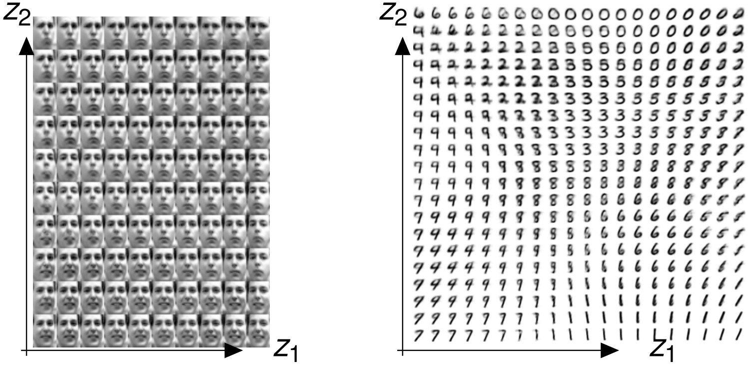
Training VAE via ELBO:

$$
\begin{aligned}
\log p_\theta(x) &\geq \mathcal{L}(x, \theta, \phi) \\
&= \mathbb{E}_z \left[\log p_\theta(x \mid z)\right] - \mathrm{KL}(q_\phi(z \mid x) \| p(z)) \\
&\approx \frac{1}{N} \sum_{n=1}^{N} \left[\log p_\theta(x \mid z^{(n)})\right] - \mathrm{KL}\left(q_\phi(z^{(n)} \mid x) \| p(z^{(n)})\right)
\end{aligned}
$$

- $\partial \mathcal{L}(x, \theta, \phi) / \partial \theta$ is simple given samples from $q(z|x)$
- $\partial \mathcal{L}(x, \theta, \phi) / \partial \phi$ requires reparameterization trick.

Generating Data from VAE

Use the decoder network with z sampled from prior $\mathcal{N}(0, I)$



[Kingma and Welling 14]

- Similar z implies similar output x
- It is interesting to see that in the left, $z_1 \approx$ head pose, and $z_2 \approx$ degree of smile

Summary

- Latent Variable Models (LVMs)
  - introduces causal relation between observed and unobserved variables
- Expectation-Maximization (EM) Algorithm
  - provides a practical solution to the intractable posterior
- Variational inference
  - generalized from the expectation maximization
- Variational Auto Encoders (VAEs)
  - incorporates the power of NNs in VI