Deep Generative Models

Lecture 3

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Recap of Previous Lecture

Jacobian Matrix

Given a differentiable function $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$,

$$\mathbf{z} = \mathbf{f}(\mathbf{x}), \quad \mathbf{J} = \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_m}{\partial x_1} & \cdots & \frac{\partial z_m}{\partial x_m} \end{pmatrix} \in \mathbb{R}^{m \times m}$$

Change of Variables Theorem (CoV)

Let $\mathbf{x}$ be a random variable with density $p(\mathbf{x})$, and $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ a differentiable invertible mapping. If $\mathbf{z} = \mathbf{f}(\mathbf{x})$ and $\mathbf{x} = \mathbf{f}^{-1}(\mathbf{z}) = \mathbf{g}(\mathbf{z})$, then

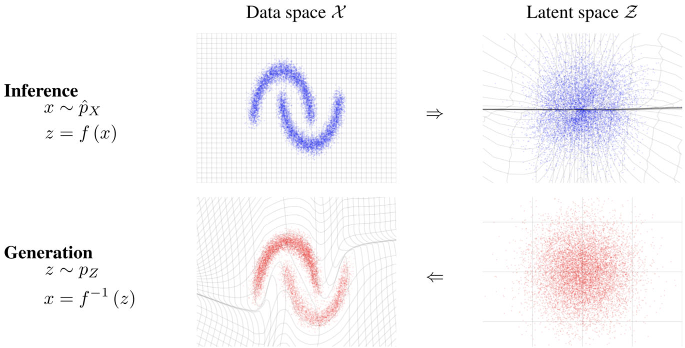
$$p(\mathbf{x}) = p(\mathbf{z}) |\det(\mathbf{J}_\mathbf{f})| = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

$$p(\mathbf{z}) = p(\mathbf{x}) |\det(\mathbf{J}_\mathbf{g})| = p(\mathbf{x}) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = p(\mathbf{g}(\mathbf{z})) \left| \det \left(\frac{\partial \mathbf{g}(\mathbf{z})}{\partial \mathbf{z}} \right) \right|.$$

Recap of Previous Lecture

Definition

A normalizing flow is a *differentiable*, *invertible* transformation that maps data $\mathbf{x}$ to noise $\mathbf{z}$.



Log-Likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_K \circ \cdots \circ \mathbf{f}_1(\mathbf{x})) + \sum_{k=1}^{K} \log |\det(\mathbf{J}_{\mathbf{f}_k})|$$

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

Recap of Previous Lecture

Flow Log-Likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) + \log |\det(\mathbf{J}_{\mathbf{f}})|$$

One significant challenge is efficiently computing the Jacobian determinant.

Linear Flows

$$\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}) = \mathbf{W}\mathbf{x}, \quad \mathbf{W} \in \mathbb{R}^{m \times m}, \quad \boldsymbol{\theta} = \mathbf{W}, \quad \mathbf{J}_{\mathbf{f}} = \mathbf{W}^T$$

- LU Decomposition:
$$\mathbf{W} = \mathbf{P}\mathbf{L}\mathbf{U}.$$
- QR Decomposition:
$$\mathbf{W} = \mathbf{Q}\mathbf{R}.$$

Decomposition is performed only once during initialization. Then the decomposed matrices ($\mathbf{P}, \mathbf{L}, \mathbf{U}$ or $\mathbf{Q}, \mathbf{R}$) are optimized.

Kingma D. P., et al. Glow: Generative Flow With Invertible 1x1 Convolutions, 2018
Hoogeboom E., et al. Emerging Convolutions for Generative Normalizing Flows, 2019

Recap of Previous Lecture

Consider an autoregressive model:

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}), \quad p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}) = \mathcal{N}\left(\mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}), \sigma^2_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})\right).$$

Gaussian Autoregressive Normalizing Flow

$$\mathbf{x} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}) \quad \Rightarrow \quad z_j = (x_j - \mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})}.$$

- This transformation is both **invertible** and **differentiable**, mapping $p(\mathbf{z})$ to $p(\mathbf{x}|\boldsymbol{\theta})$.
- The Jacobian matrix for this transformation is triangular.

The generative function $\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$ is **sequential**, while the inference function $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ is **not sequential**.

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Recap of Previous Lecture

Let us partition $\mathbf{x}$ and $\mathbf{z}$ into two groups:

$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}].$$

Coupling Layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}_1) + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}_1). \end{cases} \quad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_1)) \odot \frac{1}{\boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{x}_1)}. \end{cases}$$

Both density estimation and sampling require just a single pass!

Jacobian

$$\det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) = \det \begin{pmatrix} \mathbf{I}_d & 0_{d \times (m-d)} \\ \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_1} & \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_2} \end{pmatrix} = \prod_{j=1}^{m-d} \frac{1}{\sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_1)}.$$

A coupling layer is a special instance of an gaussian autoregressive normalizing flow.

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

Outline

1. Forward and Reverse KL for NF
2. Latent Variable Models (LVM)
3. Variational Evidence Lower Bound (ELBO)
4. EM-Algorithm

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Forward KL vs. Reverse KL

Forward KL ($\equiv$ Maximum Likelihood Estimation)

$$
\begin{aligned}
\mathrm{KL}(\pi \| p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\boldsymbol{\theta})} d\mathbf{x} \\
&= -\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\boldsymbol{\theta}) + \text{const} \to \min_{\boldsymbol{\theta}}
\end{aligned}
$$

Forward KL for Normalizing Flows

$$
\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) + \log |\det(\mathbf{J}_{\mathbf{f}})|
$$

$$
\mathrm{KL}(\pi \| p) = -\mathbb{E}_{\pi(\mathbf{x})} \Big[\log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) + \log |\det(\mathbf{J}_{\mathbf{f}})| \Big] + \text{const}
$$

- We need to compute $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ and its Jacobian.
- Access to the density $p(\mathbf{z})$ is required.
- The inverse function $\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}) = \mathbf{f}_{\boldsymbol{\theta}}^{-1}(\mathbf{z})$ is required only for sampling from the normalizing flow.

Forward KL vs. Reverse KL

Reverse KL

$$\begin{aligned}\mathrm{KL}(p\|\pi) &= \int p(\mathbf{x}|\boldsymbol{\theta}) \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x})} d\mathbf{x} \\ &= \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \left[\log p(\mathbf{x}|\boldsymbol{\theta}) - \log \pi(\mathbf{x})\right] \to \min_{\boldsymbol{\theta}}\end{aligned}$$

Reverse KL for Normalizing Flows (LOTUS Trick)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{z}) + \log |\det(\mathbf{J_f})| = \log p(\mathbf{z}) - \log |\det(\mathbf{J_g})|$$

$$\mathrm{KL}(p\|\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log |\det(\mathbf{J_g})| - \log \pi(\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}))\right]$$

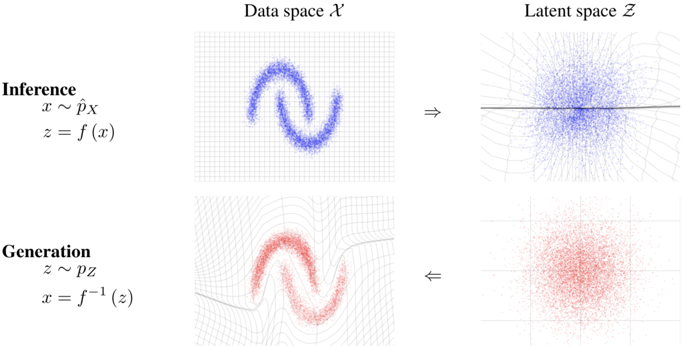
- We need to compute $\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$ and its Jacobian.
- Sampling from $p(\mathbf{z})$ is required (though direct evaluation is not), along with evaluating $\pi(\mathbf{x})$.
- Evaluating $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ is not required.

Normalizing Flows KL Duality

Theorem

Fitting the NF model $p(\mathbf{x}|\boldsymbol{\theta})$ to a target distribution $\pi(\mathbf{x})$ via the forward KL (MLE) is equivalent to fitting the induced distribution $p(\mathbf{z}|\boldsymbol{\theta})$ to the base distribution $p(\mathbf{z})$ via the reverse KL:

$$\arg\min_{\boldsymbol{\theta}} \mathrm{KL}(\pi(\mathbf{x}) \| p(\mathbf{x}|\boldsymbol{\theta})) = \arg\min_{\boldsymbol{\theta}} \mathrm{KL}(p(\mathbf{z}|\boldsymbol{\theta}) \| p(\mathbf{z})).$$



Papamakarios G. et al. Normalizing Flows for Probabilistic Modeling and Inference, 2019

Normalizing Flows KL Duality

Theorem

$$\arg\min_{\boldsymbol{\theta}} \mathrm{KL}(\pi(\mathbf{x}) \| p(\mathbf{x}|\boldsymbol{\theta})) = \arg\min_{\boldsymbol{\theta}} \mathrm{KL}(p(\mathbf{z}|\boldsymbol{\theta}) \| p(\mathbf{z})).$$

Proof

- $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$, so $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$;
- $\mathbf{x} \sim \pi(\mathbf{x})$, $\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$, so $\mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta})$;

$$\log p(\mathbf{z}|\boldsymbol{\theta}) = \log \pi(\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})) + \log |\det(\mathbf{J}_{\mathbf{g}})|;$$
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) + \log |\det(\mathbf{J}_{\mathbf{f}})|.$$

$$\begin{aligned} KL\left(p(\mathbf{z}|\boldsymbol{\theta}) \| p(\mathbf{z})\right) &= \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})}\left[\log p(\mathbf{z}|\boldsymbol{\theta}) - \log p(\mathbf{z})\right] = \\ &= \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})}\left[\log \pi(\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})) + \log |\det(\mathbf{J}_{\mathbf{g}})| - \log p(\mathbf{z})\right] = \\ &= \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log |\det(\mathbf{J}_{\mathbf{f}})| - \log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}))\right] = \\ &= \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log p(\mathbf{x}|\boldsymbol{\theta})\right] = \mathrm{KL}(\pi(\mathbf{x}) \| p(\mathbf{x}|\boldsymbol{\theta})). \end{aligned}$$

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Outline

1. Forward and Reverse KL for NF
2. Latent Variable Models (LVM)
3. Variational Evidence Lower Bound (ELBO)
4. EM-Algorithm

Bayesian Framework

Bayes' Theorem

$$p(\boldsymbol{\theta}|\mathbf{x}) = \frac{p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

- $\mathbf{x}$: observed variables;
- $\boldsymbol{\theta}$: unknown latent variables/parameters;
- $p(\mathbf{x}|\boldsymbol{\theta})$: likelihood;
- $p(\mathbf{x}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$: evidence;
- $p(\boldsymbol{\theta})$: prior distribution;
- $p(\boldsymbol{\theta}|\mathbf{x})$: posterior distribution.

Interpretation

- We begin with unknown variables $\boldsymbol{\theta}$ and a prior belief $p(\boldsymbol{\theta})$.
- Once data $\mathbf{x}$ is observed, the posterior $p(\boldsymbol{\theta}|\mathbf{x})$ incorporates both prior beliefs and evidence from the data.

Bayesian Framework

Consider the case where the unobserved variables $\boldsymbol{\theta}$ are model parameters (i.e., $\boldsymbol{\theta}$ are random variables).

- $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$: observed samples;
- $p(\boldsymbol{\theta})$: prior distribution.

Posterior Distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

If the evidence $p(\mathbf{X})$ is intractable (due to high-dimensional integration), the posterior cannot be computed exactly.

Maximum a Posteriori (MAP) Estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} (\log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}))$$

Latent Variable Models (LVM)

Maximum Likelihood Extimation (MLE) Problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

The distribution $p(\mathbf{x}|\boldsymbol{\theta})$ can be highly complex and often intractable (just like the true data distribution $\pi(\mathbf{x})$).

Extended Probabilistic Model

Introduce a latent variable $\mathbf{z}$ for each observed sample $\mathbf{x}$:

$$p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}); \quad \log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}).$$

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z}.$$

Motivation

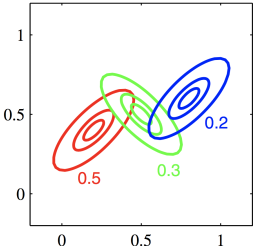
Both $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ and $p(\mathbf{z})$ are usually much simpler than $p(\mathbf{x}|\boldsymbol{\theta})$.

Latent Variable Models (LVM)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

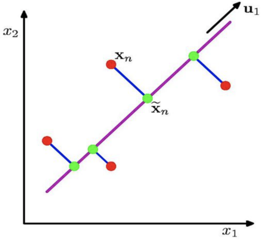
Examples

Mixture of Gaussians



- $p(\mathbf{x}|z, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$
- $p(z) = \mathrm{Categorical}(\boldsymbol{\pi})$

PCA Model

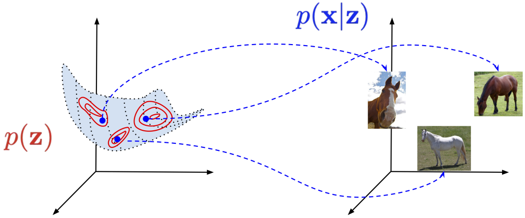


- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{Wz} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$
- $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$

Bishop C. Pattern Recognition and Machine Learning, 2006

MLE for LVM

$$\sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{i=1}^{n} \log \int p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta}) p(\mathbf{z}_i) d\mathbf{z}_i \to \max_{\boldsymbol{\theta}}.$$



Naive Approach

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} = \mathbb{E}_{p(\mathbf{z})} p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) \approx \frac{1}{K} \sum_{k=1}^{K} p(\mathbf{x}|\mathbf{z}_k, \boldsymbol{\theta}),$$

where $\mathbf{z}_k \sim p(\mathbf{z})$.

Challenge: As the dimensionality of $\mathbf{z}$ increases, the number of samples needed to adequately cover the latent space grows exponentially.

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image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

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ELBO Derivation I

Inequality Derivation

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \log \int \frac{q(\mathbf{z})}{q(\mathbf{z})} p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} =$$

$$= \log \mathbb{E}_q \left[\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} \right] \geq \mathbb{E}_q \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} = \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x})$$

Here, $q(\mathbf{z})$ is any distribution such that $\int q(\mathbf{z}) d\mathbf{z} = 1$.

Variational Evidence Lower Bound (ELBO)

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} \leq \log p(\mathbf{x}|\boldsymbol{\theta})$$

This inequality holds for any choice of $q(\mathbf{z})$.

ELBO Derivation II

$$p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) = \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{p(\mathbf{x}|\boldsymbol{\theta})}$$

Equality Derivation

$$\begin{aligned}
\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) &= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\
&= \int q(\mathbf{z}) \log \frac{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) p(\mathbf{x}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\
&= \int q(\mathbf{z}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\
&= \log p(\mathbf{x}|\boldsymbol{\theta}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}))
\end{aligned}$$

Variational Decomposition

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \geq \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}).$$

Here, $\mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \geq 0$.

Variational Evidence Lower Bound (ELBO)

$$
\begin{aligned}
\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) &= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\
&= \int q(\mathbf{z}) \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\
&= \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}))
\end{aligned}
$$

Log-Likelihood Decomposition

$$
\begin{aligned}
\log p(\mathbf{x}|\boldsymbol{\theta}) &= \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \\
&= \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z})) + \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).
\end{aligned}
$$

- Instead of maximizing the likelihood, maximize the ELBO:

$$
\max_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta}) \quad \rightarrow \quad \max_{q, \boldsymbol{\theta}} \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x})
$$

- Maximizing the ELBO with respect to the **variational** distribution q is equivalent to minimizing the KL divergence:

$$
\arg\max_{q} \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) \equiv \arg\min_{q} \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).
$$

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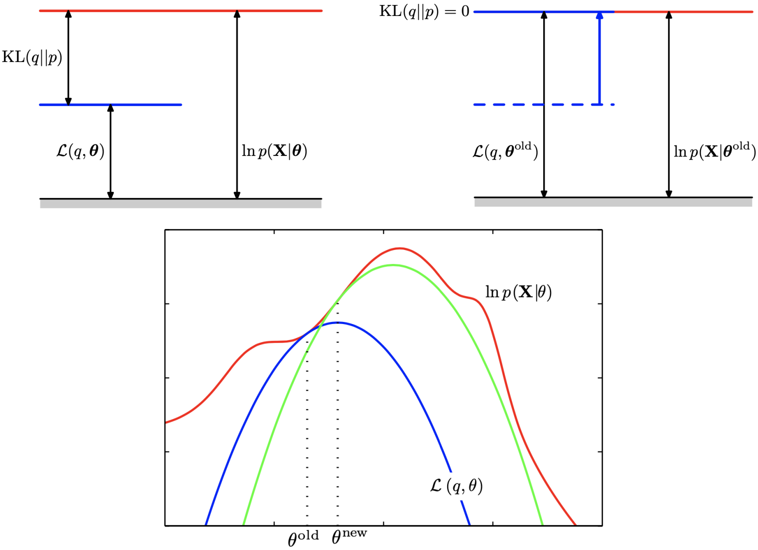
EM-Algorithm

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z})) =$$
$$= \mathbb{E}_q \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \log \frac{q(\mathbf{z})}{p(\mathbf{z})} \right] d\mathbf{z} \rightarrow \max_{q,\boldsymbol{\theta}}.$$

Block-Coordinate Optimization

- Initialize $\boldsymbol{\theta}^*$;
- **E-step** (optimize $\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x})$ over q):
$$q^*(\mathbf{z}) = \arg\max_q \mathcal{L}_{q,\boldsymbol{\theta}^*}(\mathbf{x}) =$$
$$= \arg\min_q \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*);$$
- **M-step** (optimize $\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x})$ over $\boldsymbol{\theta}$):
$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathcal{L}_{q^*,\boldsymbol{\theta}}(\mathbf{x});$$
- Repeat the E-step and M-step until convergence.

EM-Algorithm Illustration



Bishop C. Pattern Recognition and Machine Learning, 2006

Summary

- Flow duality establishes the relationship between the data and latent spaces using forward and reverse KL formulations.
- The Bayesian framework generalizes nearly all standard machine learning methods.
- LVMs introduce latent representations for observed data, enabling more interpretable models.
- LVMs maximize the variational evidence lower bound (ELBO) to obtain maximum likelihood estimates for the parameters.
- The general variational EM algorithm optimizes the ELBO within LVMs to recover the MLE for the parameters $\boldsymbol{\theta}$.