CS-E4891 Deep Generative Models
Lecture 3: Variational autoencoders

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Outline

- Variational autoencoders (recap)
- Applications of VAE (continued)
- VAE generalizations
- Identifiability of VAEs
- Amortization gap

- Reading: parts of Sec. 20-21 from (Murphy, 2023), Sec. 17 from (Prince, 2023), and other literature (see references at the end)

Variational autoencoder

Variational autoencoder (VAE) is a neural architecture that consists of a deep latent variable model (deep generative model) of the form

$$\boldsymbol{z} \sim p_{\boldsymbol{\theta}}(\boldsymbol{z})$$
$$\boldsymbol{x} \mid \boldsymbol{z} \sim p(\boldsymbol{x} \mid d_{\boldsymbol{\theta}}(\boldsymbol{z}))$$

that is trained using (reparameterized) amortized variational inference with an inference model $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}) = q(\boldsymbol{z} \mid f_{\boldsymbol{\phi}}(\boldsymbol{x}))$

- Data $\boldsymbol{x}$ can be continuous or discrete, or both, typically modeled using distribution from the exponential family
- Decoder $d_{\boldsymbol{\theta}}(\cdot)$ and encoder (inference network) $f_{\boldsymbol{\phi}}(\cdot)$ are commonly neural networks
- For general statistical latent variable models, this can be called as autoencoding variational Bayes method
- Variational approximation $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})$ needs to admit reparametrization

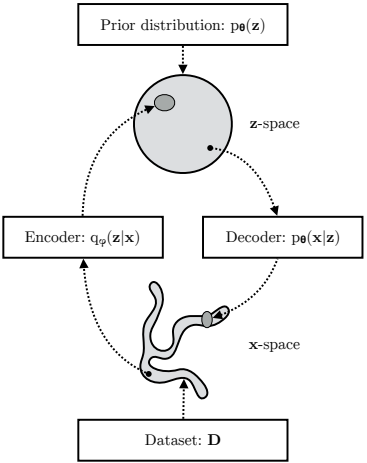

Figure from (Kingma & Welling, 2019)

Applications of variational autoencoders

Variational autoencoders can be used for various tasks

- Statistical modeling[a]
- Generation[a], conditional generation[b]
- Amortized variational inference[a]
- Representation learning[a]
- Reconstruction, missing value estimation[b]
- Latent space interpolation[b]
- Out-of-distribution detection[b]

[a] In the previous lecture.
[b] In this lecture.

Variational autoencoder for reconstruction and data imputation

Consider a test data point $\boldsymbol{x} = (\boldsymbol{x}_\text{o}, \boldsymbol{x}_\text{m})$, where $\boldsymbol{x}_\text{o}$ denotes observed features and $\boldsymbol{x}_\text{m}$ denotes unobserved (missing) features

Observed and missing features can vary between different test data points $\boldsymbol{x}$ and $\boldsymbol{x}'$

For a VAE model $\boldsymbol{x}_\text{o}$ and $\boldsymbol{x}_\text{m}$ are conditionally independent given $\boldsymbol{z}$ (assuming diagonal likelihood covariance), therefore

$$\begin{aligned} p(\boldsymbol{x}_\text{m} \mid \boldsymbol{x}_\text{o}) &= \int p(\boldsymbol{x}_\text{m} \mid \boldsymbol{z}) p(\boldsymbol{z} \mid \boldsymbol{x}_\text{o}) d\boldsymbol{z} \\ &\approx \int p_{\boldsymbol{\theta}}(\boldsymbol{x}_\text{m} \mid \boldsymbol{z}) q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}_\text{o}) d\boldsymbol{z} \end{aligned}$$

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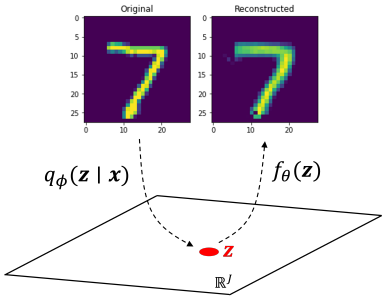

https://mbernste.github.io/posts/vae/

→ VAE architecture automatically implements a statistical data imputation method

Encoder model $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})$ needs to be able to handle missing values in $\boldsymbol{x}$

Variational autoencoder for reconstruction and data imputation

Posterior matching technique (Strauss and Oliva, 2022)

- Artificially mask complete training data points as $\boldsymbol{x} = (\boldsymbol{x}_\text{o}, \boldsymbol{x}_\text{m})$
- Train an additional encoder model with parameters $\boldsymbol{\phi}'$ such that $q_{\boldsymbol{\phi}'}(\boldsymbol{z} \mid \boldsymbol{x}_\text{o}) \approx q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})$ by maximizing

$$\mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}[\log q_{\boldsymbol{\phi}'}(\boldsymbol{z} \mid \boldsymbol{x}_\text{o})]$$

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Variationally optimal approach: use non-amortized variational inference to maximize (Agarwal et al., 2023)

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\psi} \mid \boldsymbol{x}) = &\mathbb{E}_{q_{\boldsymbol{\psi}}(\boldsymbol{z})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_\text{o} \mid \boldsymbol{z})\right] \\ &- D_{\mathbb{KL}}(q_{\boldsymbol{\psi}}(\boldsymbol{z}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}))\end{aligned}$$

w.r.t. $\boldsymbol{\psi}$ and estimate with previously trained decoder

$$p(\boldsymbol{x}_\text{m} \mid \boldsymbol{x}_\text{o}) \approx \int p_{\boldsymbol{\theta}}(\boldsymbol{x}_\text{m} \mid \boldsymbol{z}) q_{\boldsymbol{\psi}}(\boldsymbol{z}) d\boldsymbol{z}$$

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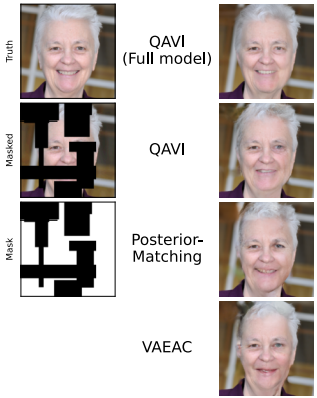

Figure from (Agarval et al., 2023).

Note: above results use additional tricks, such as deep/hierarchical VAEs, more expressive posteriors

Variational autoencoder for reconstruction and data imputation

Some VAE variants can explicitly model missingness together with $\boldsymbol{x}$, e.g., by also modeling missingness mask $\boldsymbol{m}$

Can model

- missing-completely-at-random (MCAR)
- missing-at-random (MAR)
- missing-not-at-random (MNAR)

Latent space interpolation

Explore the generative model via latent space interpolation

Consider two data points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ and the mean of their embeddings $\boldsymbol{z}_1 = f_\phi(\boldsymbol{x}_1)$ and $\boldsymbol{z}_2 = f_\phi(\boldsymbol{x}_2)$

Generate new images via latent space interpolation

$$\boldsymbol{z} = \lambda \boldsymbol{z}_1 + (1 - \lambda)\boldsymbol{z}_2, \quad 0 \leq \lambda \leq 1$$

and decoding $\boldsymbol{x} \sim p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z})$

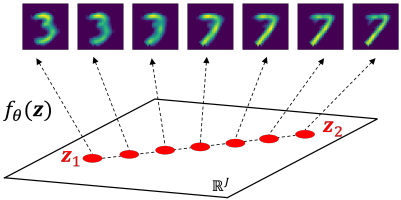

Figure from `https://mbernste.github.io/posts/vae/`

Note that the notation differs.

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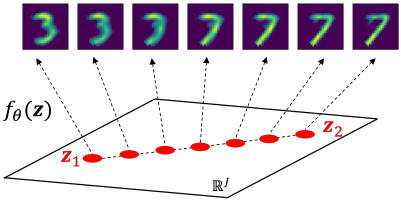

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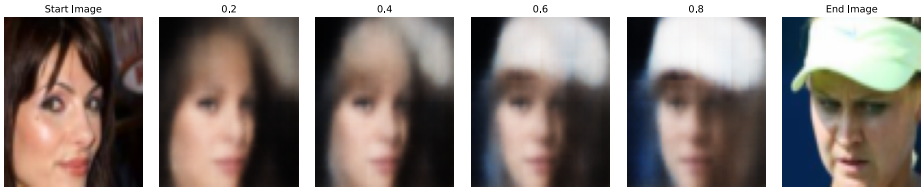

Figure 20.9 from (Murphy, 2023)

Latent space interpolation (and extrapolation)

Example: consider groups of images labeled as

- "neutral": $\{\boldsymbol{x}_i : i \in \mathcal{I}_{\text{neutral}}\}$
- "smiling": $\{\boldsymbol{x}_j : j \in \mathcal{I}_{\text{smiling}}\}$
- "mouth closed": $\{\boldsymbol{x}_k : k \in \mathcal{I}_{\text{closed}}\}$
- "mouth open": $\{\boldsymbol{x}_l : l \in \mathcal{I}_{\text{open}}\}$

and define

$$\boldsymbol{\Delta}_1 = \sum_{j \in \mathcal{I}_{\text{smiling}}} f_{\boldsymbol{\phi}}(\boldsymbol{x}_j) - \sum_{i \in \mathcal{I}_{\text{neutral}}} f_{\boldsymbol{\phi}}(\boldsymbol{x}_i)$$

$$\boldsymbol{\Delta}_2 = \sum_{l \in \mathcal{I}_{\text{open}}} f_{\boldsymbol{\phi}}(\boldsymbol{x}_l) - \sum_{k \in \mathcal{I}_{\text{closed}}} f_{\boldsymbol{\phi}}(\boldsymbol{x}_k)$$

A given image $\boldsymbol{x}$ can be manipulated via interpolation as

$$\begin{aligned} \boldsymbol{z} &= f_{\phi}(\boldsymbol{x}) \\ \boldsymbol{z}' &= \boldsymbol{z} + \lambda_1 \boldsymbol{\Delta}_1 + \lambda_2 \boldsymbol{\Delta}_2, \quad \lambda_1, \lambda_2 \in \mathbb{R} \\ \boldsymbol{x}' &\sim p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}') \end{aligned}$$

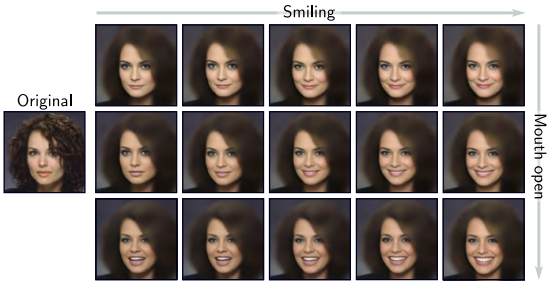

Figure 17.13 from (Prince, 2023)

Note: interpolation above uses non-linear interpolation in spherical coordinates.

Approximating sample probability

Use a trained VAE to approximate sample probability for test data to

- Estimate the quality of the model
- Detect out-of-distribution samples

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Instead of using the ELBO, we can directly estimate probability for a given data point $\boldsymbol{x}$ using Monte Carlo

$$\begin{aligned} p_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \int p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) p_{\boldsymbol{\theta}}(\boldsymbol{z}) d\boldsymbol{z} \\ &= \mathbb{E}_{p_{\boldsymbol{\theta}}(\boldsymbol{z})}[p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z})] \\ &\approx \frac{1}{S} \sum_{s=1}^{S} p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}_s) \end{aligned}$$

where

$$\boldsymbol{z}_s \overset{\text{i.i.d}}{\sim} p_{\boldsymbol{\theta}}(\boldsymbol{z})$$

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This can be improved by importance sampling estimate

$$\begin{aligned} p_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \int p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) p_{\boldsymbol{\theta}}(\boldsymbol{z}) d\boldsymbol{z} \\ &= \int p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) \frac{p_{\boldsymbol{\theta}}(\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})} q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}) d\boldsymbol{z} \\ &= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})} \left[p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) \frac{p_{\boldsymbol{\theta}}(\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})} \right] \\ &\approx \frac{1}{S} \sum_{s=1}^{S} \tilde{w}_s p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}_s), \end{aligned}$$

where

$$\boldsymbol{z}_s \overset{\text{i.i.d}}{\sim} q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}), \quad \tilde{w}_s = \frac{p_{\boldsymbol{\theta}}(\boldsymbol{z}_s)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_s \mid \boldsymbol{x})}, \quad \sup p_{\boldsymbol{\theta}} \subseteq \sup q_{\boldsymbol{\phi}}$$

Posterior collapse

- Consider a powerful decoder (a "super" deep neural net of some sort) such that for every value of latent variable $\boldsymbol{z} \in \mathcal{Z}$ decoder outputs one of the data points
- Then approx. $p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) = p_{\boldsymbol{\theta}}(\boldsymbol{x})$ and $p_{\boldsymbol{\theta}}(\boldsymbol{z} \mid \boldsymbol{x}) = p_{\boldsymbol{\theta}}(\boldsymbol{z})$ because generative model does not really use the latent variable
- We can find inference network parameters $\boldsymbol{\phi}^*$ such that $q_{\boldsymbol{\phi}^*}(\boldsymbol{z} \mid \boldsymbol{x}) = p_{\boldsymbol{\theta}}(\boldsymbol{z} \mid \boldsymbol{x}) = p_{\boldsymbol{\theta}}(\boldsymbol{z})$

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- In this setting, ELBO is maximized because $D_{\mathbb{KL}}(q_{\boldsymbol{\phi}^*}(\boldsymbol{z} \mid \boldsymbol{x}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z} \mid \boldsymbol{x})) = 0$ but the model has not learned any meaningful latent representations
- Then also $D_{\mathbb{KL}}(q_{\boldsymbol{\phi}^*}(\boldsymbol{z} \mid \boldsymbol{x}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z})) = 0$
- This is known as posterior collapse
- Posterior collapse is also due to other aspects, such local maxima in the complex objective function

β-VAE

VAE models can generate samples that may appear too smooth (e.g. blurry images)

β-VAE can improve sample quality (as well as help with posterior collapse) by reducing the penalty on the KL term

$$\mathcal{L}_\beta(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z})\right] - \beta D_{\mathbb{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z})), \quad \beta \geq 0$$

If we set

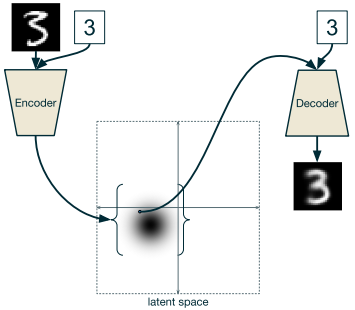
- $\beta = 1$ we obtain the standard objective for VAEs
- $\beta < 1$ we can reconstruct data samples better
- $\beta > 1$ we get more compressed representations (in terms of rate distortion, see Murphy (2023))
- $\beta = 0$ we obtain an objective that is analogous for autoencoder models

Conditional variational autoencoder

Conditional variational autoencoder (CVAE) is a neural architecture that consists of a conditional deep latent variable model of the form

$$\begin{aligned} \boldsymbol{z} &\sim p_{\boldsymbol{\theta}}(\boldsymbol{z}) \\ \boldsymbol{x} \mid \boldsymbol{z} &\sim p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}, \boldsymbol{c}) = p(\boldsymbol{x} \mid d_{\boldsymbol{\theta}}(\boldsymbol{z}, \boldsymbol{c})), \end{aligned}$$

where $\boldsymbol{c}$ contains the explanatory covariates and the model is trained using (reparameterized) amortized variational inference with an inference model $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, \boldsymbol{c})$.



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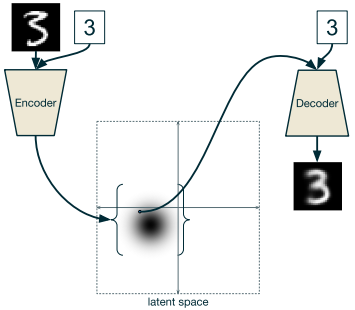

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Alternative CVAE model definitions:

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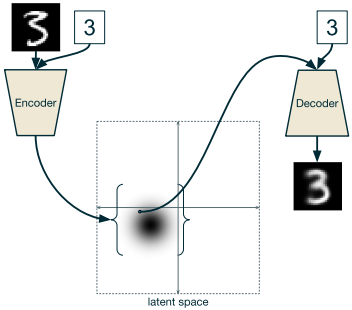

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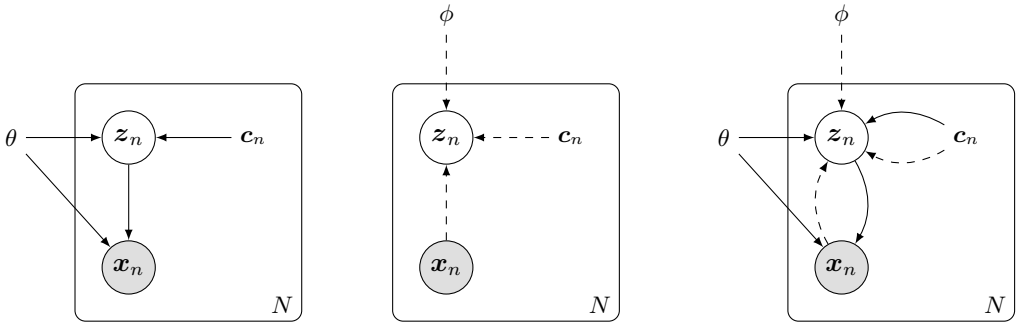
All methodological details remain essentially unchanged, including the ELBO objective

$$\begin{aligned} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}, \boldsymbol{c}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, \boldsymbol{c})} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}, \boldsymbol{c}) \right] \\ - D_{\mathbb{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, \boldsymbol{c}) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{z})) \end{aligned}$$

Conditional variational autoencoder: Probabilistic graphical model

Probabilistic graphical models for CVAE with $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z} \mid \boldsymbol{c}) = p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) p_{\boldsymbol{\theta}}(\boldsymbol{z} \mid \boldsymbol{c})$

- Circled symbols denote random variables
- Non-circled symbols are hyperparameters
- White nodes (circles) are latent
- Shaded nodes are observed



(a) Generative model (b) Inference model (c) Combined

Multimodal variational autoencoder

- Multimodal VAE allows modeling joint distributions over multiple data modalities, e.g. image and text
- Assuming M modalities $\boldsymbol{x}_1 \in \mathcal{X}_1, \ldots, \boldsymbol{x}_M \in \mathcal{X}_M$ and conditional independence given $\boldsymbol{z}$

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_M, \boldsymbol{z}) = p_{\boldsymbol{\theta}}(\boldsymbol{z}) \prod_{m=1}^{M} p_{\boldsymbol{\theta}}(\boldsymbol{x}_m \mid \boldsymbol{z})$$

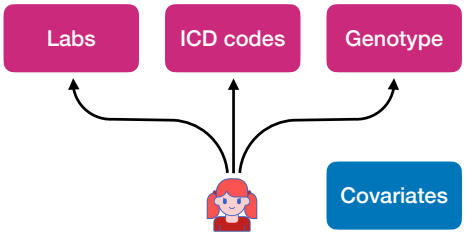


Illustration of multimodal data

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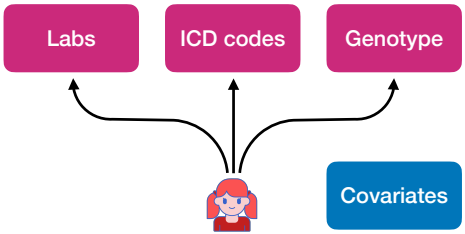

Illustration of multimodal data

- The ELBO for $\mathbf{X} = \{\boldsymbol{x}_1, \ldots \boldsymbol{x}_M\}$ is

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathbf{X}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\mathbf{X})} \left[\sum_{m=1}^{M} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}_m \mid \boldsymbol{z}) \right] - D_{\mathbb{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \mathbf{X}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}))$$

- Likelihood terms may have different ranges
- Weighted ELBO with $\lambda_m \geq 0$

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathbf{X}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\mathbf{X})} \left[\sum_{m=1}^{M} \lambda_m \log p_{\boldsymbol{\theta}}(\boldsymbol{x}_m \mid \boldsymbol{z}) \right] - D_{\mathbb{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \mathbf{X}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}))$$

Multimodal variational autoencoder for unpaired data

- Availability of paired multimodal data across all modalities is often limited
- For example, we may have lots of images, lots of text, but only few image-text pairs
- Let $O_m = 1$ denote that data modality m, $\boldsymbol{x}_m$, is observed, and $O_m = 0$ that modality m is not observed
- ELBO objective for partially paired data is

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathbf{X}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\mathbf{X})} \left[\sum_{m:O_m=1} \lambda_m \log p_{\boldsymbol{\theta}}(\boldsymbol{x}_m \mid \boldsymbol{z}) \right] - D_{\mathbb{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \mathbf{X}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}))$$

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- How to define the amortized VI such that it works for unpaired data?
- For example, if encoder $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}_1, \boldsymbol{x}_2)$ is trained on image-text pairs, how to compute posterior approximation using only images $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}_1)$ or text $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}_2)$, and vice versa?

Multimodal variational autoencoder with product of experts

From the conditional independence we get

$$
\begin{aligned}
p(\boldsymbol{z} \mid \mathbf{X}) &= \frac{p(\boldsymbol{z}) p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m \mid \boldsymbol{z})}{p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m)} \\
&= \frac{p(\boldsymbol{z})}{p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m)} \prod_{m=1}^{M} p(\boldsymbol{x}_m \mid \boldsymbol{z}) \\
&= \frac{p(\boldsymbol{z})}{p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m)} \prod_{m=1}^{M} \frac{p(\boldsymbol{z} \mid \boldsymbol{x}_m) p(\boldsymbol{x}_m)}{p(\boldsymbol{z})} \\
&\propto p(\boldsymbol{z}) \prod_{m=1}^{M} \frac{p(\boldsymbol{z} \mid \boldsymbol{x}_m)}{p(\boldsymbol{z})} \\
&\approx p(\boldsymbol{z}) \prod_{m=1}^{M} q_m(\boldsymbol{z} \mid \boldsymbol{x}_m),
\end{aligned}
$$

where $q_m(\boldsymbol{z} \mid \boldsymbol{x}_m)$ is the "expert" for data modality m

Multimodal variational autoencoder with product of experts

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&= \frac{p(\boldsymbol{z})}{p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m)} \prod_{m=1}^{M} \frac{p(\boldsymbol{z} \mid \boldsymbol{x}_m) p(\boldsymbol{x}_m)}{p(\boldsymbol{z})} \\
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\end{aligned}
$$

where $q_m(\boldsymbol{z} \mid \boldsymbol{x}_m)$ is the "expert" for data modality m

This is known as the product of experts

Posterior approximation can be computed for any subset of modalities which are observed

If prior and experts are Gaussians

$$
\begin{aligned}
p(\boldsymbol{z}) &= \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}_0, \boldsymbol{\Lambda}_0^{-1}) \\
q_m(\boldsymbol{z} \mid \boldsymbol{x}_m) &= \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}_m, \boldsymbol{\Lambda}_m^{-1}),
\end{aligned}
$$

then the approximative posterior is also Gaussian

$$
\prod_{m=0}^{M} \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}_m, \boldsymbol{\Lambda}_m^{-1}) \propto \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}, \boldsymbol{\Lambda})
$$

$$
\boldsymbol{\Sigma} = \left(\sum_{m=0}^{M} \boldsymbol{\Lambda}_m \right)^{-1} \quad \text{and} \quad \boldsymbol{\mu} = \boldsymbol{\Sigma} \left(\sum_{m=0}^{M} \boldsymbol{\Lambda}_m \boldsymbol{\mu}_m \right)
$$

Multimodal variational autoencoder with product of experts: illustration

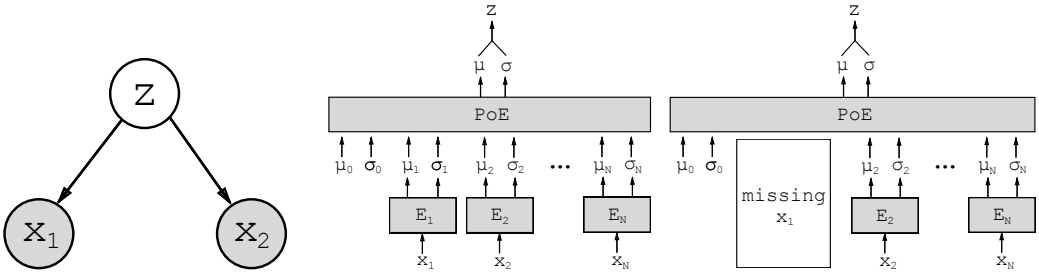

Figure 21.5 from (Murphy, 2023)

Semi-supervised VAEs

Semi-supervised learning methods can be useful when data consists of large amounts of unlabeled data $\mathcal{D}_U = \{(\boldsymbol{x}_n)\}$ and few labeled data points $\mathcal{D}_L = \{(\boldsymbol{x}_n, y_n)\}$

One of the earliest models, called M2, is

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}, y) = p_{\boldsymbol{\theta}}(y)p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid y) = p_{\boldsymbol{\theta}}(y) \int p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid y, \boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})d\boldsymbol{z},$$

where $p_{\boldsymbol{\theta}}(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z} \mid \mathbf{0}, \mathbf{I})$, $p_{\boldsymbol{\theta}}(y) = \mathrm{Cat}(y \mid \boldsymbol{\pi})$ is trainable label prior, and $p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid y, \boldsymbol{z}) = p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid d_{\boldsymbol{\theta}}(y, \boldsymbol{z}))$

Comparison to CVAE:

- $\boldsymbol{c}$ is a fixed covariate/predictor
- here label y is a random variable

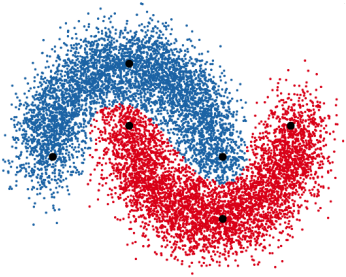

Figure from (Maaloe et al, 2016)

Semi-supervised VAEs

Variational approximation for labeled data

$$\begin{aligned} q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, y) &= q(\boldsymbol{z} \mid f_{\boldsymbol{\phi}}(\boldsymbol{x}, y)) \\ &= \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}_{\boldsymbol{\phi}}(\boldsymbol{x}, y), \operatorname{diag}(\boldsymbol{\sigma}_{\boldsymbol{\phi}}(\boldsymbol{x}, y))) \end{aligned}$$

Standard ELBO for labeled data (by marginalizing $\boldsymbol{z}$)

$$\begin{aligned} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}, y) &\geq \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, y)} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, y, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, y)} \right] \\ &= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, y)} [\log p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid y, \boldsymbol{z}) + \log p_{\boldsymbol{\theta}}(y) \\ &\quad + \log p_{\boldsymbol{\theta}}(\boldsymbol{z}) - \log q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, y)] \\ &= \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}, y) \end{aligned}$$

Semi-supervised VAEs

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Variational approximation for unlabeled data

$$\begin{aligned} q_{\boldsymbol{\phi}}(\boldsymbol{z}, y \mid \boldsymbol{x}) &= q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}) q_{\boldsymbol{\phi}}(y \mid \boldsymbol{x}) \\ q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}) &= \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}_{\boldsymbol{\phi}}(\boldsymbol{x}), \mathrm{diag}(\boldsymbol{\sigma}_{\boldsymbol{\phi}}(\boldsymbol{x}))) \\ q_{\boldsymbol{\phi}}(y \mid \boldsymbol{x}) &= \mathrm{Cat}(y \mid \boldsymbol{\pi}_{\boldsymbol{\phi}}(\boldsymbol{x})) \end{aligned}$$

ELBO for unlabeled data by (marginalizing $\boldsymbol{z}$ and y)

$$\begin{aligned} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}) &\geq \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}, y \mid \boldsymbol{x})} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, y, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}, y \mid \boldsymbol{x})} \right] \\ &= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}, y \mid \boldsymbol{x})} [\log p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid y, \boldsymbol{z}) + \log p_{\boldsymbol{\theta}}(y) \\ &\quad + \log p_{\boldsymbol{\theta}}(\boldsymbol{z}) - \log q_{\boldsymbol{\phi}}(\boldsymbol{z}, y \mid \boldsymbol{x})] \\ &= \mathbb{E}_{q_{\boldsymbol{\phi}}(y \mid \boldsymbol{x})} [\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}, y)] + \mathbb{H}(q_{\boldsymbol{\phi}}(y \mid \boldsymbol{x})) \\ &= \mathcal{U}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}) \end{aligned}$$

Semi-supervised VAEs

Variational approximation $q_{\boldsymbol{\phi}}(y \mid \boldsymbol{x})$ can be considered as discriminative classifier

Because classifier is only used to compute log-likelihood of unlabeled data, a modified objective

$$\mathcal{L}'(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathcal{D}_L, \mathcal{D}_U) = \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathcal{D}_L) + \mathcal{U}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathcal{D}_U) + \mathbb{E}_{(\boldsymbol{x}_n, y_n) \sim \mathcal{D}_L} \log q_{\boldsymbol{\phi}}(y \mid \boldsymbol{x}),$$

where $(\boldsymbol{x}_n, y_n) \sim \mathcal{D}_L$ denotes labeled data distribution

N	NN	CNN	TSVM	CAE	MTC	AtlasRBF	M1+TSVM	M2	M1+M2
100	25.81	22.98	16.81	13.47	12.03	8.10 ($\pm$ 0.95)	11.82 ($\pm$ 0.25)	11.97 ($\pm$ 1.71)	**3.33** ($\pm$ 0.14)
600	11.44	7.68	6.16	6.3	5.13	–	5.72 ($\pm$ 0.049)	4.94 ($\pm$ 0.13)	**2.59** ($\pm$ 0.05)
1000	10.7	6.45	5.38	4.77	3.64	3.68 ($\pm$ 0.12)	4.24 ($\pm$ 0.07)	3.60 ($\pm$ 0.56)	**2.40** ($\pm$ 0.02)
3000	6.04	3.35	3.45	3.22	2.57	–	3.49 ($\pm$ 0.04)	3.92 ($\pm$ 0.63)	**2.18** ($\pm$ 0.04)

Figure from (Kingma et al, 2014)

Semi-supervised VAEs

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$$\mathcal{L}'(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathcal{D}_L, \mathcal{D}_U) = \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathcal{D}_L) + \mathcal{U}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \mathcal{D}_U) + \mathbb{E}_{(\boldsymbol{x}_n, y_n) \sim \mathcal{D}_L} \log q_\phi(y \mid \boldsymbol{x}),$$

where $(\boldsymbol{x}_n, y_n) \sim \mathcal{D}_L$ denotes labeled data distribution

Methods have been further developed e.g. by adding additional latent variables (e.g. Maaloe et al, 2016) among others

N	NN	CNN	TSVM	CAE	MTC	AtlasRBF	M1+TSVM	M2	M1+M2
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Figure from (Kingma et al, 2014)

Hierarchical VAEs

We can define hierarchical VAEs with K stochastic layers $\boldsymbol{z}_{1:K} = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_K)$ as follows

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}_{1:K}) = p_{\boldsymbol{\theta}}(\boldsymbol{z}_K) \prod_{k=1}^{K} p_{\boldsymbol{\theta}}(\boldsymbol{z}_k \mid \boldsymbol{z}_{k+1}) p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}_1)$$

Generative model can be extended into non-Markovian model

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}_{1:K}) = p_{\boldsymbol{\theta}}(\boldsymbol{z}_K) \prod_{k=1}^{K} p_{\boldsymbol{\theta}}(\boldsymbol{z}_k \mid \boldsymbol{z}_{k+1:K}) p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}_{1:K})$$

Similar to using skip connection architecture

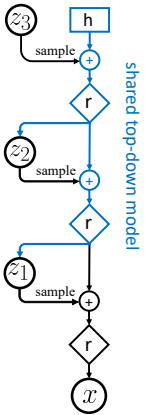

Figure 21.11 from (Murphy et al, 2023)

Hierarchical VAEs: inference model

Variational inference model can be define as bottom-up

$$q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:K}) = q_{\boldsymbol{\phi}}(\boldsymbol{z}_1 \mid \boldsymbol{x}) \prod_{k=2}^{K} q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x}, \boldsymbol{z}_{1:k-1})$$

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or as top-down

$$q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:K}) = q_{\boldsymbol{\phi}}(\boldsymbol{z}_K \mid \boldsymbol{x}) \prod_{k=K-1}^{1} q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x}, \boldsymbol{z}_{k+1:K})$$

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or both

Top-down inference model is generally considered better because it can be shown to more closely approximate the true posterior of a given layer

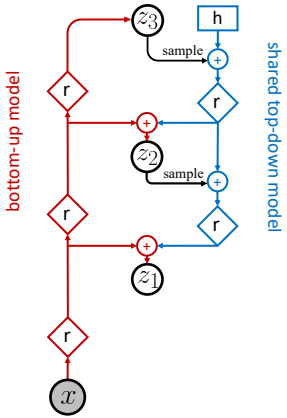

Figure 21.11 from (Murphy et al, 2023)

Hierarchical VAEs: ELBO

Evidence lower-bound for hierarchical VAE with top-down inference model is

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:K} \mid \boldsymbol{x})}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid z_{1:K})] - D_{\mathbb{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z}_K \mid \boldsymbol{x}) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{z}_K)) - \sum_{k=K-1}^{1} \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{k+1:K} \mid \boldsymbol{x})} D_{\mathbb{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x}, \boldsymbol{z}_{k+1:K}) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{z}_k \mid \boldsymbol{z}_{k+1:K})),$$

where $q_{\boldsymbol{\phi}}(\boldsymbol{z}_{k+1:K} \mid \boldsymbol{x}) = \prod_{i=k+1}^{K} q_{\boldsymbol{\phi}}(\boldsymbol{z}_i \mid \boldsymbol{x}, \boldsymbol{z}_{i+1:K})$

Hierarchical VAE example

So-called very deep VAE (VDVAE) model uses hierarchical VAE with bidirectional CNN architecture and nearest neighbour upsampling

Low-resolution (top) latents capture global structure, while the bottom of the hierarchy fills in details

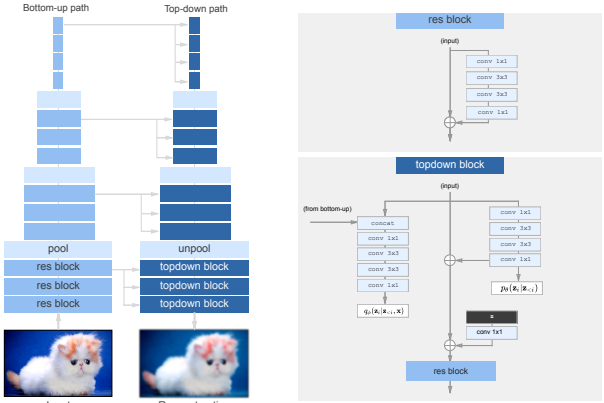

Figure 21.12 from (Murphy et al, 2023)

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Figure 21.13 from (Murphy et al, 2023)

Recap: Marginal likelihood, ELBO, importance sampling

Marginal likelihood and ELBO

$$\log p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \log \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})}\right] \overset{\text{Jensen}}{\geq} \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log\left(\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})}\right)\right] = \mathcal{L}(\boldsymbol{\theta},\boldsymbol{\phi} \mid \boldsymbol{x})$$

and Monte Carlo estimate

$$\mathcal{L}(\boldsymbol{\theta},\boldsymbol{\phi} \mid \boldsymbol{x}) \approx \frac{1}{S}\left(\sum_{s=1}^{S} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{z}_s)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_s \mid \boldsymbol{x})}\right) \quad \text{where} \quad \boldsymbol{z}_s \overset{\text{i.i.d}}{\sim} q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})$$

Recap: Marginal likelihood, ELBO, importance sampling

Marginal likelihood and ELBO

$$\log p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \log \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})}\right] \overset{\text{Jensen}}{\geq} \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log\left(\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})}\right)\right] = \mathcal{L}(\boldsymbol{\theta},\boldsymbol{\phi} \mid \boldsymbol{x})$$

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Importance sampling estimate of $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ and $\log p_{\boldsymbol{\theta}}(\boldsymbol{x})$

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})}\right] \approx \frac{1}{S}\sum_{s=1}^{S} \tilde{w}_s \quad \text{and} \quad \log p_{\boldsymbol{\theta}}(\boldsymbol{x}) \approx \log\left(\frac{1}{S}\sum_{s=1}^{S} \tilde{w}_s\right)$$

where

$$\tilde{w}_s = \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{z}_s)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_s \mid \boldsymbol{x})}, \quad \boldsymbol{z}_s \overset{\text{i.i.d}}{\sim} q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}), \quad \sup p_{\boldsymbol{\theta}} \subseteq \sup q_{\boldsymbol{\phi}}$$

Importance weighted variational autoencoder

Empirical estimate of the importance weighted variational autoencoder (IWAE) objective

$$\tilde{\mathcal{L}}_K^{\text{IWAE}}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}) = \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}_k)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x})} \right) = \log \left(\frac{1}{K} \sum_{k=1}^{K} \tilde{w}_k \right) \approx \log p_{\boldsymbol{\theta}}(\boldsymbol{x})$$

where

$$\boldsymbol{z}_k \overset{\text{i.i.d}}{\sim} q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})$$

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where

$$\boldsymbol{z}_k \overset{\text{i.i.d}}{\sim} q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})$$

By defining $q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:K} \mid \boldsymbol{x}) = \prod_{k=1}^{K} q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x})$, IWAE objective (also called as the multiple-sample ELBO) is

$$\mathcal{L}_K^{\text{IWAE}}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:K} \mid \boldsymbol{x})}\left[\log\frac{1}{K}\sum_{k=1}^{K}\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}_k)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x})}\right] = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:K} \mid \boldsymbol{x})}\left[\log\frac{1}{K}\sum_{k=1}^{K}\tilde{w}_k\right],$$

where

$$\tilde{w}_k = \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}_k)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x})}$$

Importance weighted variational autoencoder: properties

1. IWAE objective reduces to the standard single sample ELBO when $K = 1$

$$\mathcal{L}_1^{\text{IWAE}}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:1} \mid \boldsymbol{x})} \left[\log \frac{1}{1} \sum_{k=1}^{1} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}_k)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_k \mid \boldsymbol{x})} \right] = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x})} \right] = \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x})$$

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2. IWAE objective is a lower bound for $\log p_{\boldsymbol{\theta}}(\boldsymbol{x})$

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3. For any $K \geq 1$, IWAE lower bound satisfies

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4. IWAE lower bound approaches the true log marginal likelihood in the limit

$$\lim_{K \to \infty} \mathcal{L}_K^{\text{IWAE}} = \log p_{\boldsymbol{\theta}}(\boldsymbol{x})$$

Identifiability of VAEs

Consider VAE model with linear parametrization

$$p(\boldsymbol{x} \mid \boldsymbol{z}) = \mathcal{N}(\mathbf{W}\boldsymbol{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$$
$$q(\boldsymbol{z} \mid \boldsymbol{x}) = \mathcal{N}(\mathbf{V}(\boldsymbol{x} - \boldsymbol{\mu}), \mathbf{D}),$$

where $\mathbf{D}$ is diagonal and all parameters are shared with all samples

VAE models are trained via ELBO $\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi} \mid \boldsymbol{x}) \leq \log p_{\boldsymbol{\theta}}(\boldsymbol{x})$

Probabilistic principle component analysis (PPCA) is equivalent with the above decoder model

- Marginal likelihood $\log p(\boldsymbol{x})$ has closed-form
- Posterior $p(\boldsymbol{z} \mid \boldsymbol{x})$ has closed-form
- Maximum likelihood parameter estimates have also closed form (up to rotation), i.e., identifiable

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Identifiability of linear VAE (Lucas et al., 2019)

The global maximum of the ELBO for the linear VAE

- Is identical to the global maximum for the log marginal likelihood of PPCA
- Has the scaled principal components as the columns of the decoder network

Identifiability of VAEs

An unconstrained deep latent variable model $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}) = p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) p_{\boldsymbol{\theta}}(\boldsymbol{z})$ is not in general identifiable

Model identifiability can be proved by assuming specific sparsity in $p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z})$ and additional technical assumptions (Moran et al., 2022)

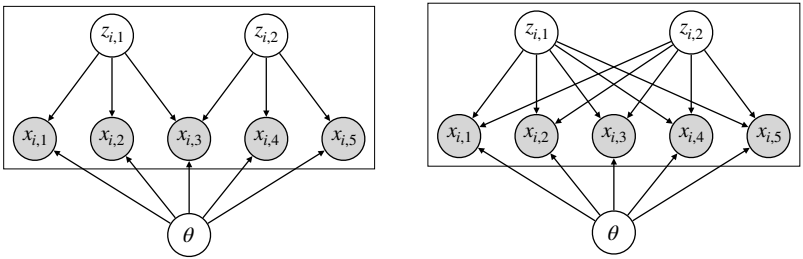

Figure from (Moran et al, 2022)

Identifiability of CVAEs

Consider a CVAE with conditional generative model $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z} \mid \boldsymbol{c}) = p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) p_{\boldsymbol{\theta}}(\boldsymbol{z} \mid \boldsymbol{c})$

- Assume prior $p_{\boldsymbol{\theta}}(\boldsymbol{z} \mid \boldsymbol{c})$ is mean field with exponential family of distributions
- Covariate $\boldsymbol{c}$ has at least $\dim(\boldsymbol{z}) \cdot k + 1$ distinct values, where k denotes the number of sufficient statistics of the prior
- Amortized variational approximation $q_{\boldsymbol{\phi}}(\boldsymbol{z} \mid \boldsymbol{x}, \boldsymbol{c})$ includes the true posterior
- $+$ Additional technical assumptions (Khemakem et al., 2020)

Then the parameters of the CVAE are asymptotically identifiable (Khemakem et al., 2020)

Amortized VI: amortization gap

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