Deep latent variable models: variational autoencoders and extensions

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Overview of today's lecture

Some bits of information geometry

Approximate inference for DLVMs

What is information geometry about?

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For example, we may want to answer these kinds of questions:

- what does it mean to **find the "model that fits the data best"?**
- what does it mean for a probability distribution p **to be "close" to another probability distribution** q**?** $\text{dist}(p, q) \approx 0$?
- how can we **move around the sets of probability distributions** in a (geometrically) principled way?

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Today, we'll simply talk about the **first question**. There are **many ways to define "distances" over sets of probability distributions.** Today, we'll talk about the **Kullback-Leibler divergence** $\text{KL}(p||q)$.

What's a distance again?

A **distance** (aka metric) over a set $\mathcal{X}$ is a function $d : \mathcal{X}^2 \longrightarrow \mathbb{R}$ such that, for all $x, y, z \in \mathcal{X}$;

- $d(x, y) = d(y, x)$ – *symmetry*
- $d(x, y) = 0 \iff x = y$ – *identity of indiscernibles*
- $d(x, z) \geq d(x, y) + d(y, z)$ – *triangle inequality*

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It's generally hard to satisfy all these axioms. The **Kullback-Leibler** does not! so it's not a "true distance", that's why we call it a **divergence** (in topology, people may call it a premetric, or a pseudometric).

Definition of the KL divergence

Let p and q be two probability densities over a space $\mathcal{X}$, we define

$$\mathbf{KL}(p||q) = \mathbb{E}_{x\sim p}\left[\log \frac{p(x)}{q(x)}\right].$$

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The KL divergence has many interesting properties that we don't have the time to see today, and it's not the only interesting "distance" over probabilities![2]

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Example: how far away are two Gaussians

Usually, computing the KL in closed-form is quite hard. But it is sometimes possible, like for p**-variate Gaussians:**

$$\mathbf{KL}(\mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)||\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)) = \frac{1}{2}\left(\mathbf{tr}(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_0) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) + \log\frac{\det\boldsymbol{\Sigma}_1}{\det\boldsymbol{\Sigma}_0} - p\right).$$

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One can see that it is not symmetric, and "not just the Euclidean distance between the means and covariances".

Application: why do we do maximum likelihood?

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How can we choose $\hat{\theta}$?

It makes sense to choose θ in order to be "as close to the truth as possible". If we measure "closeness" using the KL, this means that we want to find

$$\hat{\theta} \in \text{argmin}_{\theta \in \Theta} \text{KL}(p_{\text{true}}, p_\theta).$$

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Let's play a bit with that KL we want to minimise:

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But **we don't know p_{true}!** How can we try to compute

$$-\mathbb{E}_{x\sim p_{\text{true}}}\left[\log p_\theta(x)\right]$$

anyway?

Application: why do we do maximum likelihood?

Let's use Monte Carlo!

$$-\mathbb{E}_{x\sim p_{\text{true}}}\left[\log p_\theta(x)\right] \approx \frac{-1}{n}\sum_{i=1}^{n}\log p_\theta(x_i) = \frac{-1}{n} \times \textbf{Log-likelihood},$$

so **maximum likelihood is equivalent to minimising a Monte Carlo estimate of the KL between the truth and the model.**

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Maximum likelihood (approximatively) finds the best model with respect to the KL divergence.

This does not means that maximum likelihood is always a good choice. There were a few important assumptions in these two slides (existence of a true model, Monte Carlo approximation...). Sometimes, maximum likelihood works very poorly (but that's another story).

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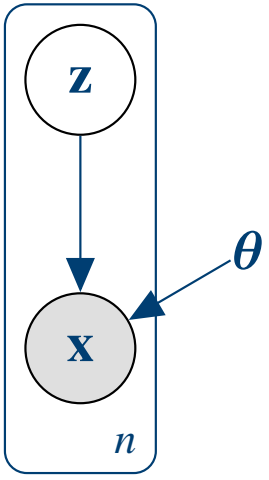
Recap: Deep latent variable models (DLVMs)

Kingma and Welling (ICLR 2014), Rezende, Mohamed & Wierstra (ICML 2014), Goodfellow et al. (NeurIPS 2014)

Assume that $(\mathbf{x}_i, \mathbf{z}_i)_{i \leq n}$ are i.i.d. random variables driven by the model:

$$\begin{cases} \mathbf{z} \sim p(\mathbf{z}) & \text{(prior)} \\ \mathbf{x} \sim p_{\boldsymbol{\theta}}(\mathbf{x} \mid \mathbf{z}) & \text{(observation model)} \end{cases}$$



where

- $\mathbf{z} \in \mathbb{R}^d$ is the **latent** variable,
- $\mathbf{x} \in \mathcal{X}$ is the **observed** variable.

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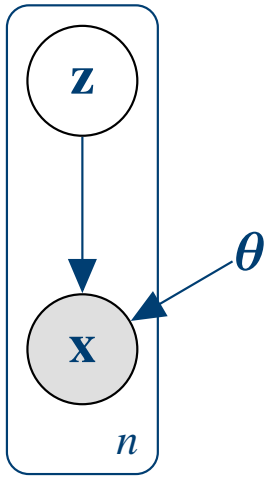
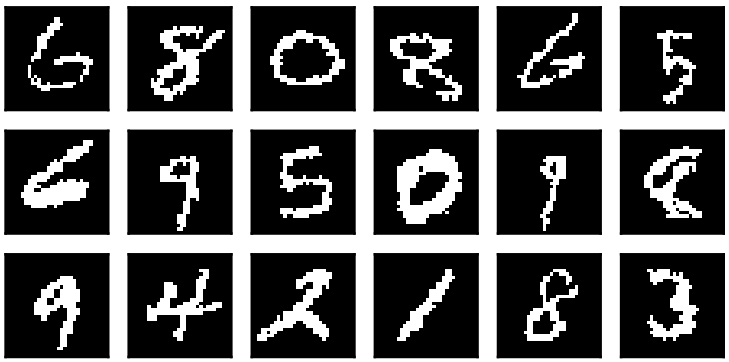


where

- $\mathbf{z} \in \mathbb{R}^d$ is the **latent** variable,
- $\mathbf{x} \in \mathcal{X}$ is the **observed** variable,
- the function $f_{\boldsymbol{\theta}} : \mathbb{R}^d \to H$ is a **(deep) neural network** called the **decoder**
- $(\Phi(\cdot \mid \boldsymbol{\eta}))_{\boldsymbol{\eta} \in H}$ is a parametric family called the **observation model**, usually **very simple**: unimodal and fully factorised (e.g. multivariate Gaussians or products of multinomials)

Recap: Illustrative example of a DLVM

Training data $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ binary MNIST



Generative model for $\mathbf{z} \in \mathbb{R}^2$ and $\mathbf{x} \in \{0,1\}^{28\times 28}$

$$\begin{cases} \mathbf{z} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) \\ x^{j,k} \sim \text{Bernoulli}(p = f^{j,k}(\mathbf{z})) \end{cases}$$

Decoder network

$$f(\mathbf{z}) = \text{Sigmoid}(\mathbf{V}\tanh(\mathbf{W}\mathbf{z} + \mathbf{b}) + \boldsymbol{\beta})$$

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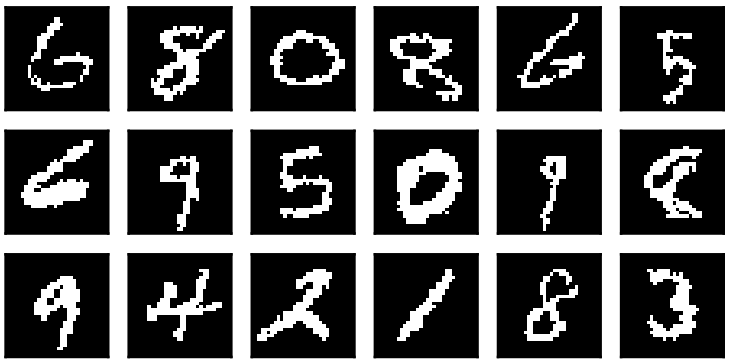
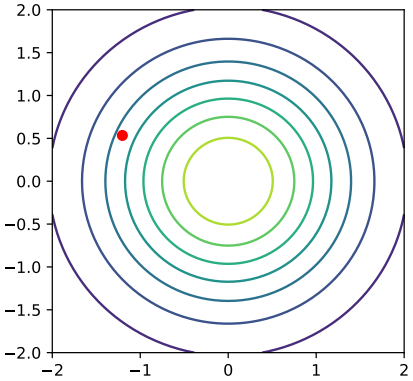


Generation

$$\mathbf{z} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$\mathbf{z} = (-1.2033, 0.5340)$$



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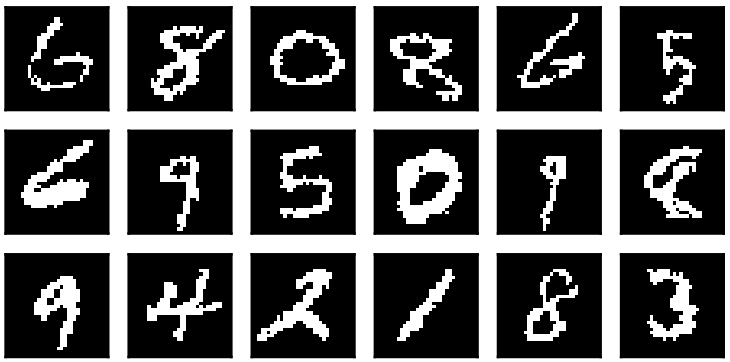

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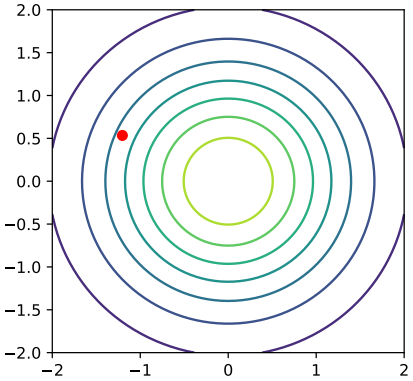

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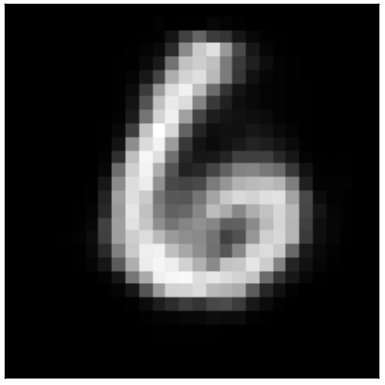

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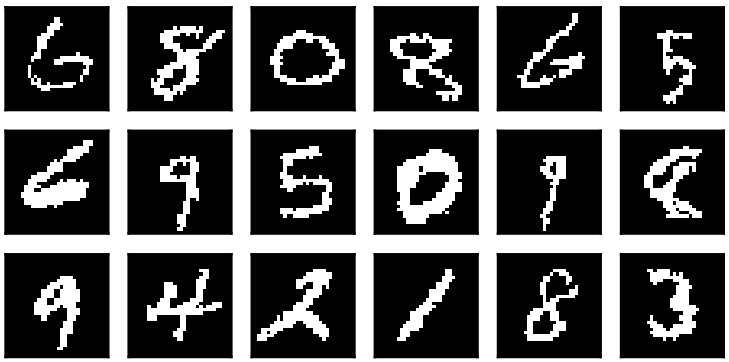

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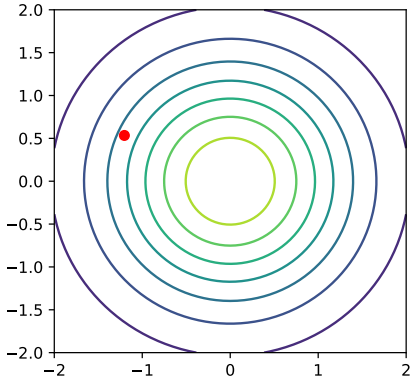

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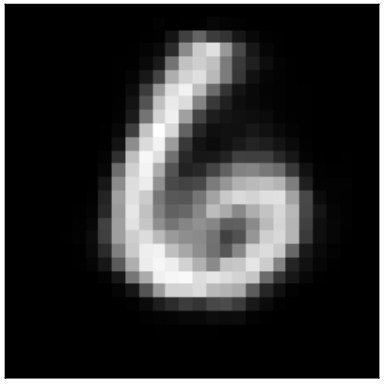

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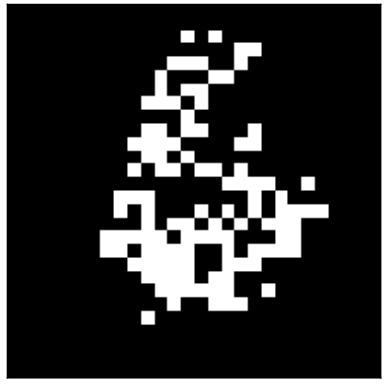

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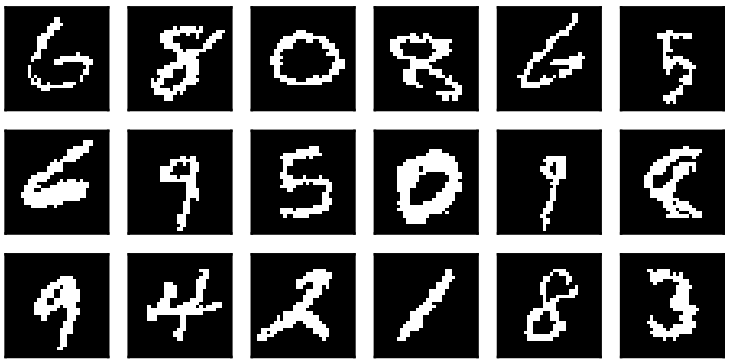

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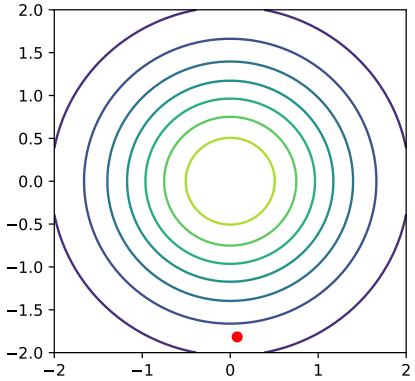

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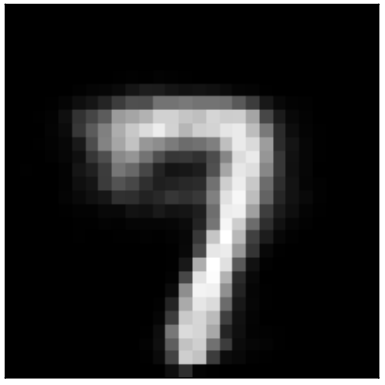

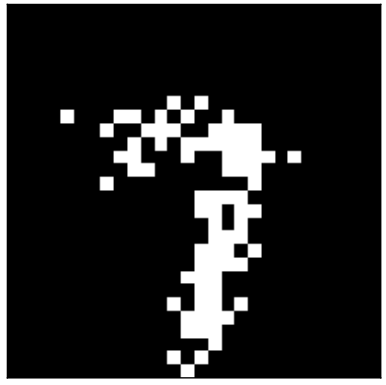

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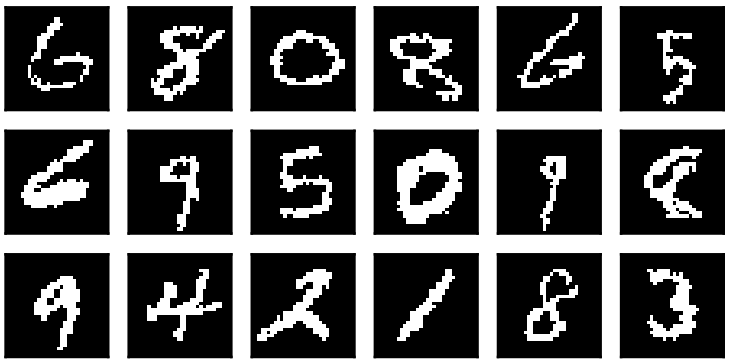

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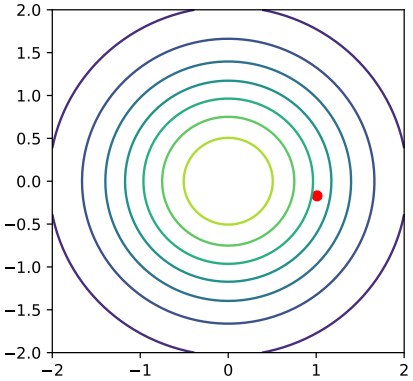
$$\mathbf{z} = (1.0097, -0.1711)$$



Generative model for $\mathbf{z} \in \mathbb{R}^2$ and $\mathbf{x} \in \{0,1\}^{28\times 28}$

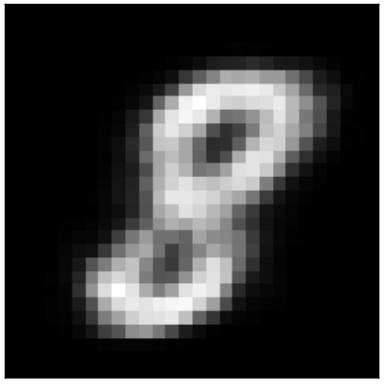
$$\begin{cases} \mathbf{z} \sim \mathcal{N}\left(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\right) \\ x^{j,k} \sim \text{Bernoulli}(p = f^{j,k}(\mathbf{z})) \end{cases}$$

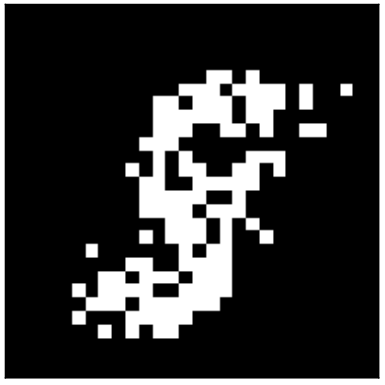
Decoder network

$$f(\mathbf{z}) = \text{Sigmoid}(\mathbf{V}\tanh(\mathbf{W}\mathbf{z} + \mathbf{b}) + \boldsymbol{\beta})$$

$f(z)$

$x^{j,k} \sim \text{Bern}(f^{j,k}(z))$





Learning DLVMs

Kingma & Welling (2014), Rezende et al. (2014)

Given a data matrix $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)^\intercal \in \mathcal{X}^n$, the **log-likelihood function** for a DLVM is

$$\ell(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{X}) = \sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\mathbf{x}_i),$$

where

$$p_{\boldsymbol{\theta}}(\mathbf{x}_i) = \int_{\mathbb{R}^d} p_{\boldsymbol{\theta}}(\mathbf{x}_i \mid \mathbf{z}) p(\mathbf{z}) \mathbf{z}.$$

We would like to find a **MLE** $\hat{\theta} \in \operatorname{argmax}_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta})$.

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- $p_{\boldsymbol{\theta}}(\mathbf{z} \mid \mathbf{x})$ is **intractable** rendering **EM intractable**
- **stochastic EM is not scalable** to large n and moderate d.

The solution: amortised variational inference

A general and scalable framework to tackle these issues was proposed by Kingma & Welling (2014), Rezende et al. (2014), leading to the **variational autoencoder (VAE).**

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Burda, Grosse & Salakhutdinov (2016), *Importance weighted autoencoders*, ICLR 2016

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The main idea is to use **Monte Carlo techniques** to approximate the intractable integrals

$$p_{\boldsymbol{\theta}}(\mathbf{x}_i) = \int_{\mathbb{R}^d} p_{\boldsymbol{\theta}}(\mathbf{x}_i \mid \mathbf{z}) p(\mathbf{z}) d\mathbf{z}.$$

Aparté: Monte Carlo and importance sampling

Let's say we want to estimate an integral of the form

$$I = \int_{\Omega} f(x)p(x)dx,$$

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Simple Monte Carlo estimate: We sample $x_1, ..., .x_K \sim p$ and approximate

$$I \approx \frac{1}{K}\sum_{k=1}^{K} f(x_k) = \hat{I}_K.$$

A few properties:

$$\hat{I}_K \xrightarrow{a.s.} I, \ \mathbb{E}[\hat{I}_K] = I, \ \mathbb{V}[\hat{I}_K] = \frac{1}{K}\mathbb{V}[f(x_1)],$$

which sounds nice, but **the variance may be very large.**

Aparté: Monte Carlo and importance sampling

Importance sampling tries to improve this estimate by **sampling** $x_1, \ldots, .x_K$ **from another density** q **rather than** p**.** The trick is the following:

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\begin{aligned}
I &= \int_\Omega f(x)p(x)dx \\
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As before, the estimate is **consistent and unbiased** (under the condition that q has heavier tails than p). **What about the variance?**

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However, this still means that **importance sampling with a good** q **will work much better than simple MC.**

Back to DLVMs and their likelihood

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Exercise: What would be the optimal, zero-variance choices for $q_1, \ldots, q_n$?

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This neural net is called the **inference network** or **encoder**.

Amortised variational inference

All of this leads to the following approximation of the likelihood

$$\ell(\boldsymbol{\theta}) \approx \sum_{i=1}^{n} \mathbb{E}_{\mathbf{z}_{i1},\ldots,\mathbf{z}_{iK} \sim q_{\boldsymbol{\gamma}}(\mathbf{z}|\mathbf{x}_i)} \left[\log \frac{1}{K} \sum_{k=1}^{K} \frac{p_{\boldsymbol{\theta}}(\mathbf{x}_i|\mathbf{z}_{ik}) p(\mathbf{z}_{ik})}{q_{\boldsymbol{\gamma}}(\mathbf{z}_{ik}|\mathbf{x}_i)} \right] = \mathcal{L}_K(\boldsymbol{\theta}, \boldsymbol{\gamma}).$$

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It does make sense! For several reasons:

- $\mathcal{L}_K(\boldsymbol{\theta}, \boldsymbol{\gamma})$ is a **lower bound of $\ell(\theta)$** (exercise !). Which means that we know that the likelihood is at least as big as $\mathcal{L}_K(\boldsymbol{\theta}, \boldsymbol{\gamma})$.
- The bounds get **tighter and tighter!**

$$\mathcal{L}_1(\boldsymbol{\theta}, \boldsymbol{\gamma}) \leq \mathcal{L}_2(\boldsymbol{\theta}, \boldsymbol{\gamma}) \leq \ldots \leq \mathcal{L}_K(\boldsymbol{\theta}, \boldsymbol{\gamma}) \xrightarrow[K\to\infty]{} \ell(\boldsymbol{\theta}).$$

$\mathcal{L}_K(\boldsymbol{\theta}, \boldsymbol{\gamma})$ is called the **importance weighted autoencoder (IWAE)** bound, and was introduced by Burda et al. (2016).

What about the VAE?

The VAE bound of Kingma & Welling (2014) and Rezende et al. (2014) is actually $\mathcal{L}_1(\boldsymbol{\theta}, \boldsymbol{\gamma})$, which is the loosest bound!

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The VAE bound can be interestingly rewritten

$$\mathcal{L}_1(\boldsymbol{\theta}, \boldsymbol{\gamma}) = \ell(\boldsymbol{\theta}) - \mathrm{KL}\left(\prod_{i=1}^{n} q_{\boldsymbol{\gamma}}(\mathbf{z}_i|\mathbf{x}_i) \middle\| \prod_{i=1}^{n} p_{\boldsymbol{\theta}}(\mathbf{z}_i|\mathbf{x}_i) \right).$$

which means that, for a given $\boldsymbol{\theta}$, **the optimal $q_{\boldsymbol{\gamma}}(\mathbf{z}_i|\mathbf{x}_i)$ will be as close as possible (in a KL sense) to the true posterior $p_{\boldsymbol{\theta}}(\mathbf{z}_i|\mathbf{x}_i)$.**

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Concrete consequence: after training, **we may interpret the $q_{\boldsymbol{\gamma}}(\mathbf{z}_i|\mathbf{x}_i)$ as an (approachable) approximation of the (intractable) $p_{\boldsymbol{\theta}}(\mathbf{z}_i|\mathbf{x}_i)$.**

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Is it still true when $K > 1$? **Kind of, but it gets more complicated.** Domke & Sheldon (2019) showed that, when $K \to \infty$, the the "closeness" is no longer in KL sense but in the sense of the χ divergence.

Playing with the VAE bound

The VAE bound can be also rewritten

$$\mathcal{L}_1(\boldsymbol{\theta}, \boldsymbol{\gamma}) = \mathbb{E}_{\mathbf{z}_i \sim q_{\boldsymbol{\gamma}}(\mathbf{z}_i|\mathbf{x}_i)}[p_{\boldsymbol{\theta}}(\mathbf{x}_i|\mathbf{z}_i)] - \mathrm{KL}\left(\prod_{i=1}^{n} q_{\boldsymbol{\gamma}}(\mathbf{z}_i|\mathbf{x}_i) \middle|\middle| \prod_{i=1}^{n} p_{\boldsymbol{\theta}}(\mathbf{z}_i)\right).$$

- $\mathbf{E}_{\mathbf{z}_i \sim q_{\boldsymbol{\gamma}}(\mathbf{z}_i|\mathbf{x}_i)}[p_{\boldsymbol{\theta}}(\mathbf{x}_i|\mathbf{z}_i)]$ can be interpreted as (the opposite of) a **reconstruction error.**
- the **KL between the approximate posterior and the prior** can be interpreted as a regulariser. If $q_{\boldsymbol{\gamma}}(\mathbf{z}|\mathbf{x})$ is Gaussian, then this can be computed in **closed-form.**

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This version of the bound resembles the opposite of the loss of a **KL-regularised autoencoder**, hence the name **variational autoencoder (VAE)**, coined by Kingma and Welling (ICLR 2014).