From shallow to deep latent variable models

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Overview of todday’s lecture

Super short recap about last lecture

Latent variable models

Non-deep latent variable models

Approximate maximum likelihood for DLVMs

Deep learning as a building block in probabilistic models

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where **the function $\mathbf{x} \mapsto \pi_{\boldsymbol{\theta}}(\mathbf{x})$ is a neural net with parameters θ.** Why it it useful again for classification to use a neural net for $\pi_{\boldsymbol{\theta}}$?

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where **the function $\mathbf{x} \mapsto \pi_{\boldsymbol{\theta}}(\mathbf{x})$ is a neural net with parameters $\boldsymbol{\theta}$.** Why it it useful again for classification to use a neural net for $\pi_{\boldsymbol{\theta}}$?

For many reasons! It can model arbitrarily complex decision boundaries, we can use prior information in the architecure (e.g. for image classification), we can do large-scale maximum likelihood training using stochastic gradient descent, leverage GPUs...

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- if we have images of faces: size of nose, color of hair, glasses or not...
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This assumption is the cornerstone of **latent variable models**, that assume that the data are governed by **unobserved random variables** $\mathbf{z}_1, ..., \mathbf{z}_n$ **that live in a low dimensional space** $\mathcal{Z}$ (for example $\mathbf{R}^2$). We can think of $\mathbf{z}_i$ as a **code** summarizing the essential factors of the data point $\mathbf{x}_i$.

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- $\mathbf{z}_i \sim \mathcal{N}(0, \mathbf{I}_d)$,
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Related models for non-continuous data: topic models (text), Poisson PPCA (count data).
What is the geometric intuition?

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That's the key idea of **deep latent variable models (DLVMs)**, present in particular in both **variational autoencoders (VAEs)**, invented independently by Kingma and Welling (ICLR 2014) and Rezende, Mohamed & Wierstra (ICML 2014), and **generative adversarial networks (GANs)** (Goodfellow et al., NeurIPS 2014).

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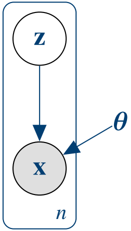
In this lecture, we'll focus on VAEs, but GANs are really quite similar.

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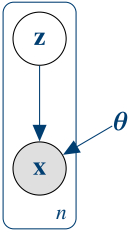
$$\begin{cases} \mathbf{z} \sim p(\mathbf{z}) & \text{(prior)} \\ \mathbf{x} \sim p_{\boldsymbol{\theta}}(\mathbf{x} \mid \mathbf{z}) = \Phi(\mathbf{x} \mid f_{\boldsymbol{\theta}}(\mathbf{z})) & \text{(observation model)} \end{cases}$$



where

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

The role of the prior

As in regular factor analysis, the prior distribution of the latent variable is often an **isotropic Gaussian** $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}_d, \mathbf{I}_d)$.

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More complex, **learnable priors** have also been considered. For example, mixtures of K Gaussians:

$$p(\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k),$$

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Note that **this prior is not a prior in the Bayesian sense** (i.e., about parameter uncertainty).

The role of the observation model

The observation model $(\Phi(\cdot \mid \boldsymbol{\eta}))_{\boldsymbol{\eta} \in H}$ usually **very simple**: unimodal and fully factorised (e.g. multivariate Gaussians or products of multinomials)

Its parameters are the output of the decoder.

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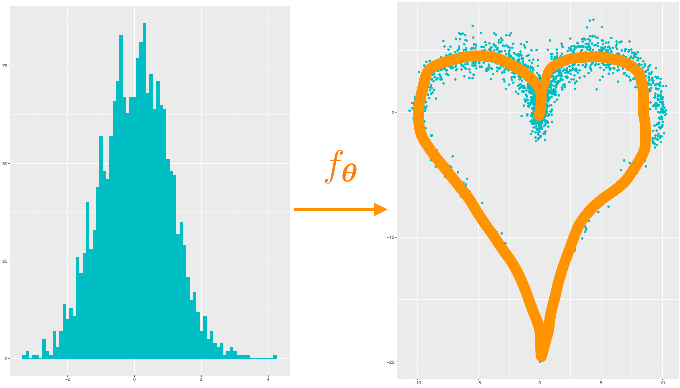
The role of the decoder

The role of the **decoder** $f_{\boldsymbol{\theta}} : \mathbb{R}^d \to H$ is:

- to transform $\mathbf{z}$ (**the code**) into parameters $\eta = f_{\boldsymbol{\theta}}(\mathbf{z})$ of the observation model $\Phi(\cdot \mid \eta)$.
- The weights $\boldsymbol{\theta}$ of the **decoder** are learned.

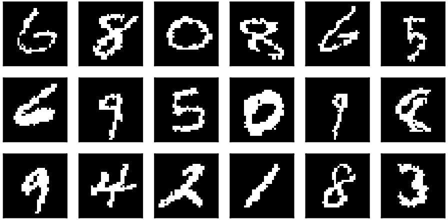
Simple non-linear decoder **($d = 1$, $p = 2$)**: $f_{\boldsymbol{\theta}}(z) = \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\Sigma}_{\boldsymbol{\theta}}(\mathbf{z})$ with, for all $z \in \mathbb{R}$,

$$\boldsymbol{\mu}_{\boldsymbol{\theta}}(z) = \left(10\sin(z)^3, 10\cos(z) - 10\cos(z)^4\right), \; \boldsymbol{\Sigma}_{\boldsymbol{\theta}}(\mathbf{z}) = \text{Diag}\left(\left(\frac{\sin(z)}{3z}\right)^2, \left(\frac{\sin(z)}{z}\right)^2\right).$$



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 $\mathbf{x} \in \{0,1\}^{28\times 28}$

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

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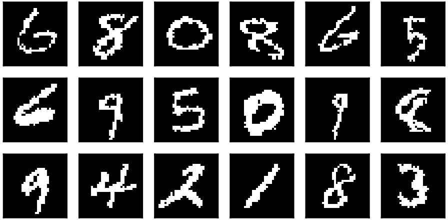

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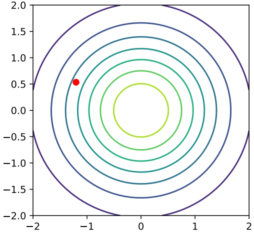
$$\mathbf{z} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

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



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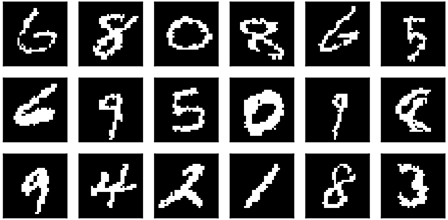

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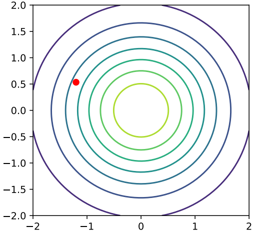

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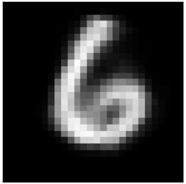

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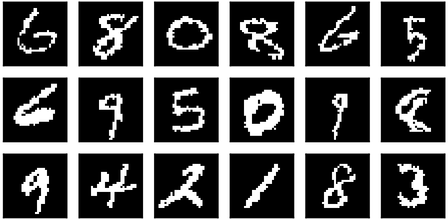

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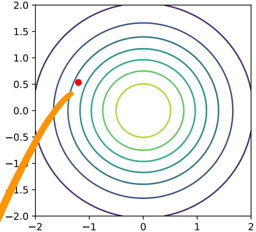
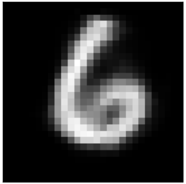
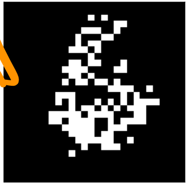


$f(\mathbf{z})$



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



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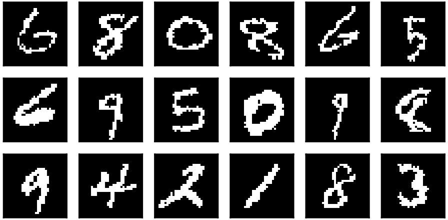

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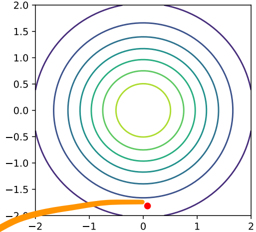
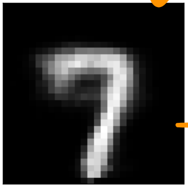
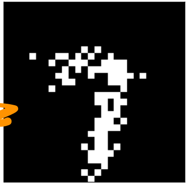


$f(z)$



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



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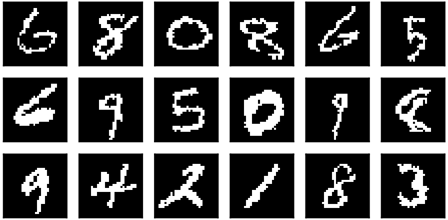

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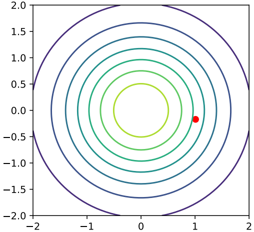
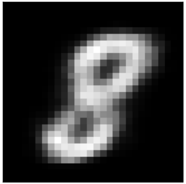
$$\mathbf{z} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

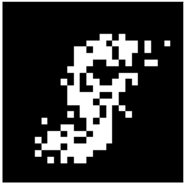
$$\mathbf{z} = (1.0097, -0.1711)$$



$f(z)$



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



DLVMs applications: density estimation on MNIST

Rezende, Mohamed & Wierstra (ICML 2014)

Training data

Model samples

DLVMs applications: clustering on MNIST

Harchaoui, Mattei, Bouveyron & Almansa (2018)

$\mathbf{m}_k$

$\mathbf{m}_k + 0.5\mathbf{S}_k\mathbf{u}$

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$\mathbf{m}_k + 1.5\mathbf{S}_k\mathbf{u}$

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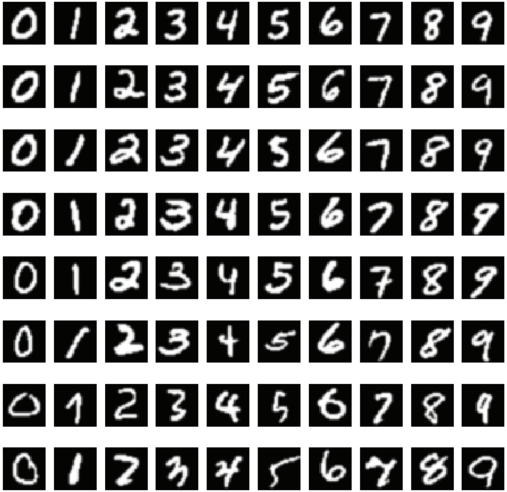
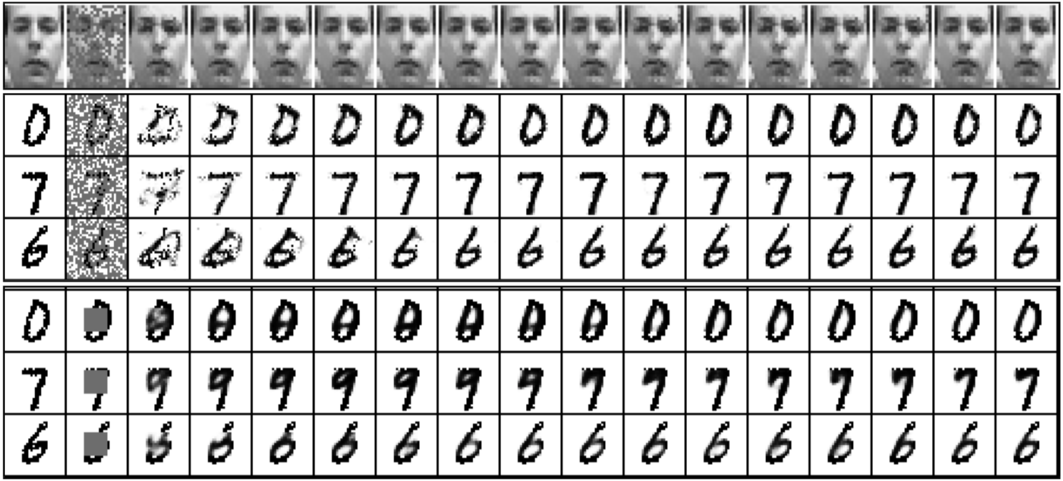


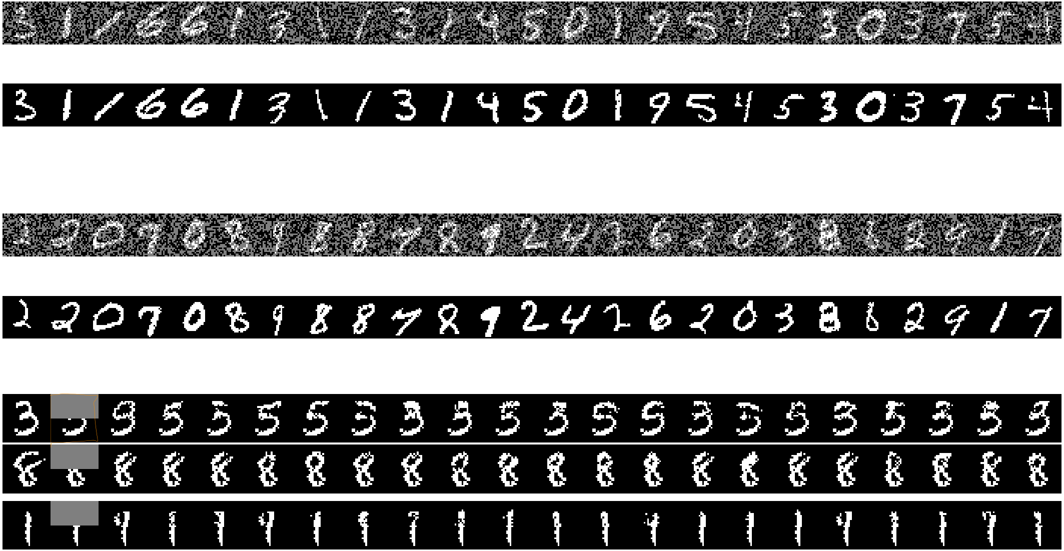
DLVMs applications: Data imputation

Rezende, Mohamed & Wierstra (ICML 2014)



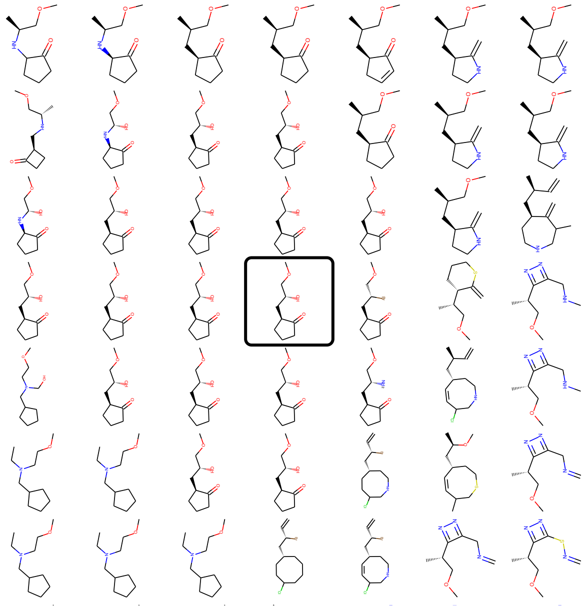
DLVMs applications: Data imputation

Mattei & Frellsen (ICML 2019)



DLVMs applications: Molecular design

Kusner, Paige, and Hernàndez-Lobato (2017)



DLVMs applications: Reinforcement learning

Ha & Schmidhuber (2018)

DLVMs applications: Reinforcement learning

Ha & Schmidhuber (2018)

Overview of todday’s lecture

Super short recap about last lecture

Latent variable models

Non-deep latent variable models

Approximate maximum likelihood for DLVMs

Learning DLVMs

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

Given a data matrix $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\intercal \in \mathcal{X}^n$, 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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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

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

where $f \geq 0$ and p is a density over a space Ω.

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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:

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

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 $x_1, ..., .x_K$ 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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However, this still means that **importance sampling with a good q will work much better than simple MC.**

Back to DLVMs and their likelihood

We want to approximate

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

q*_i (z) = p(z I x_i)

Amortised variational inference

A solution: Amortised variational inference, **all the q_i will be defined together via a neural net!**

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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

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

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It does make sense! For several reasons:

- $\mathcal{L}_K(\boldsymbol{\theta},\boldsymbol{\gamma})$ is a **lower bound of $\ell(\boldsymbol{\theta})$** (exercise !)
- 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).