More on latent variable models

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Menu for this lecture

1. Recap on VAEs + implementing variational bounds
2. How to optimise variational bounds? + implementation
3. Variational bounds beyond VAEs: Bayesian models, topic models, diffusion models…
4. On d-separation and VAEs

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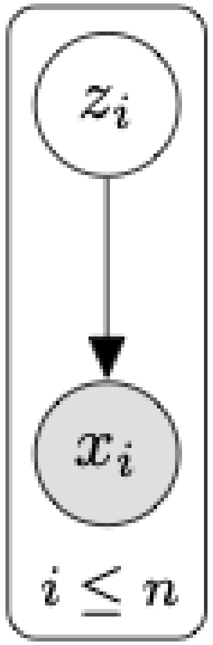
Recap on VAEs/IWAEs

Deep latent variable models

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

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



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)

Deep latent variable models: the role of the prior

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

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

Deep latent variable models: 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.

$$\begin{cases} \mathbf{z} \sim p(\mathbf{z}) & \text{(prior)} \\ \mathbf{x} \sim p_{\boldsymbol{\theta}}(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\Sigma}_{\boldsymbol{\theta}}(\mathbf{z})) & \text{(Gaussian observation model)} \end{cases}$$

$$\begin{cases} \mathbf{z} \sim p(\mathbf{z}) & \text{(prior)} \\ \mathbf{x} \sim p_{\boldsymbol{\theta}}(\mathbf{x} \mid \mathbf{z}) = \mathcal{B}(\mathbf{x} \mid \boldsymbol{\pi}_{\boldsymbol{\theta}}(\mathbf{z})) & \text{(Bernoulli observation model)} \end{cases}$$

$$\begin{cases} \mathbf{z} \sim p(\mathbf{z}) & \text{(prior)} \\ \mathbf{x} \sim p_{\boldsymbol{\theta}}(\mathbf{x} \mid \mathbf{z}) = \mathrm{St}(\mathbf{x} \mid \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\Sigma}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\nu}_{\boldsymbol{\theta}}(\mathbf{z})) & \text{(Student's t observation model)} \end{cases}$$

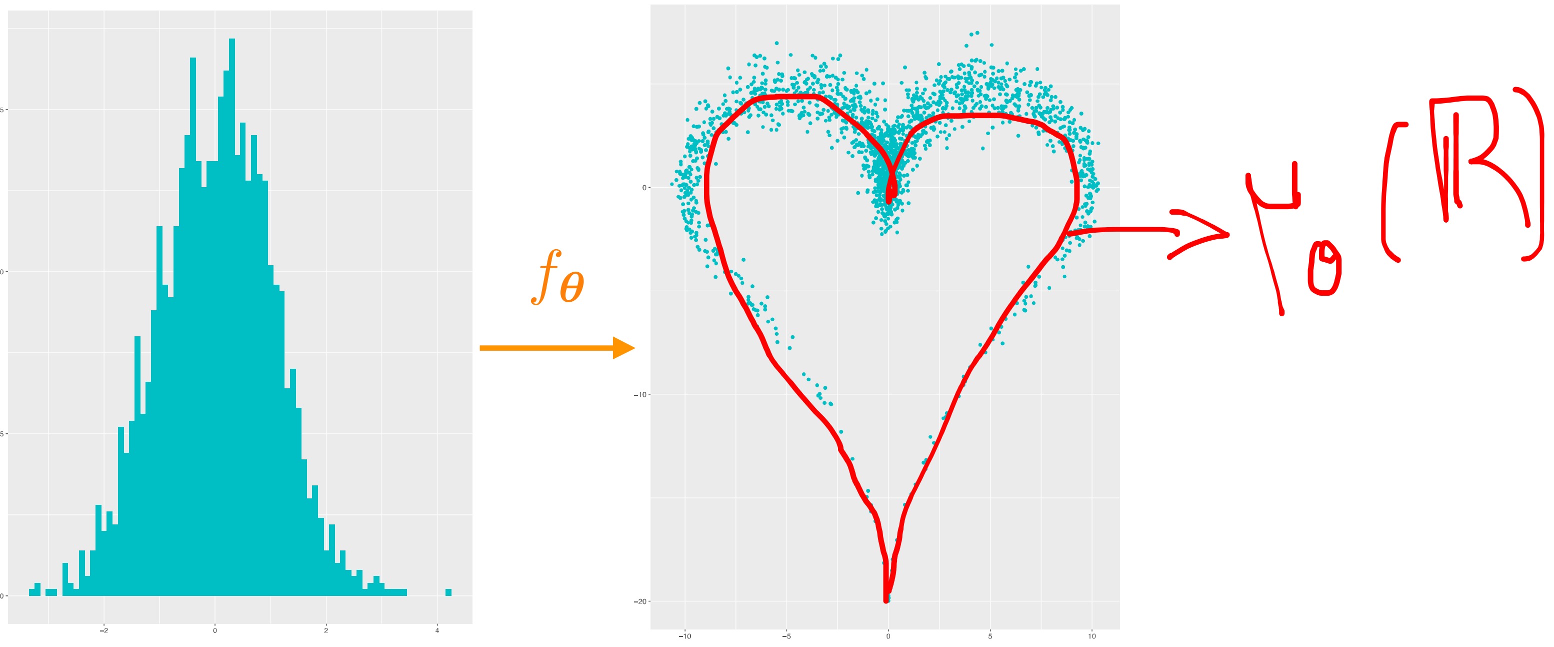
Deep latent variable models: the role of the decoder

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.

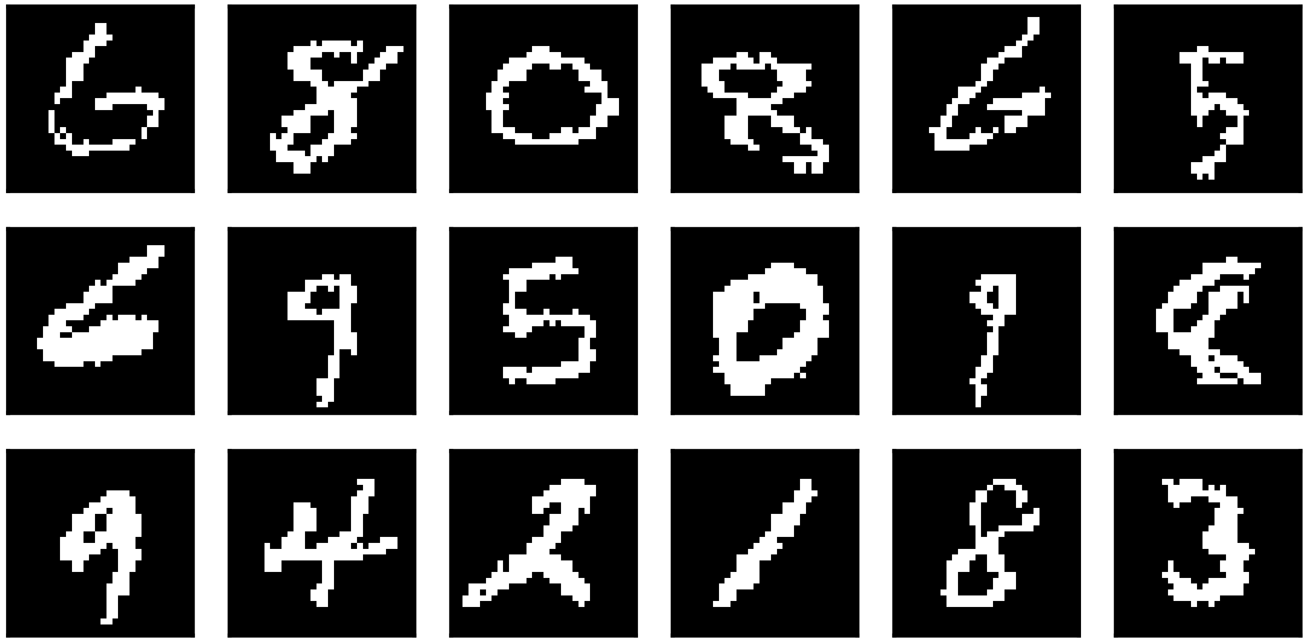
Simple non-linear decoder ($d = 1$**,** $p = 2$): $f_{\boldsymbol\theta}(z) = \boldsymbol\mu_{\boldsymbol\theta}(\mathbf{z}), \boldsymbol\Sigma_{\boldsymbol\theta}(\mathbf{z})$ with, for all $z \in \mathbb{R}$,

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



Illustrative example of a DLVM for binary images

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



Illustrative example of a DLVM for binary images

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

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

Decoder network

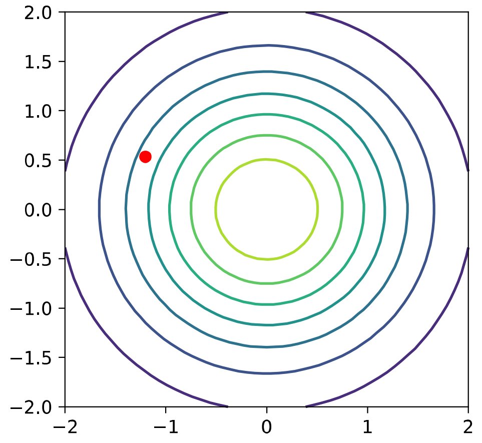
$$f(\mathbf{z}) = \mathrm{Sigmoid}(\mathbf{V} \tanh(\mathbf{W}\mathbf{z} + \mathbf{b}) + \boldsymbol{\beta})$$

$$\mathbb{P}(\theta \mid X)$$

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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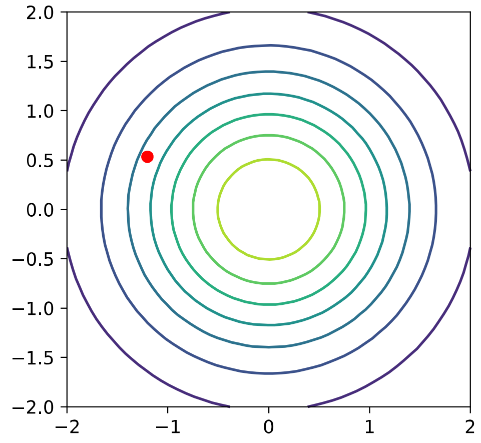
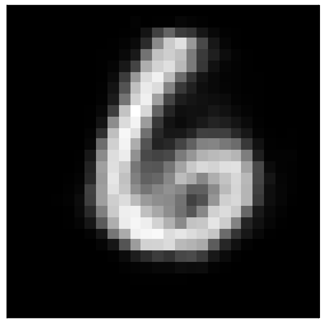


$f(\mathbf{z})$



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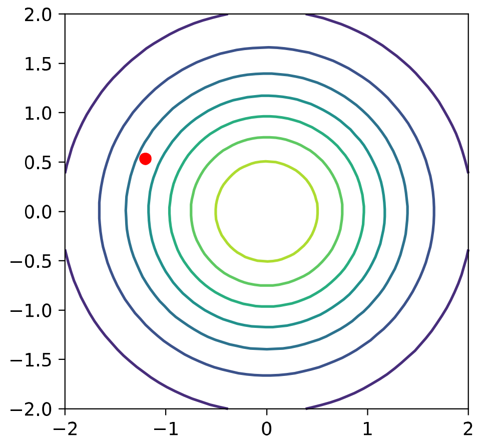

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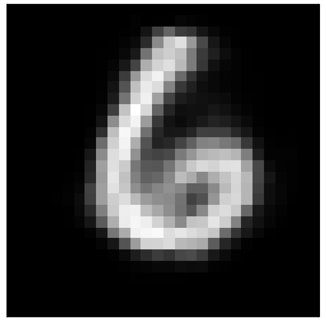
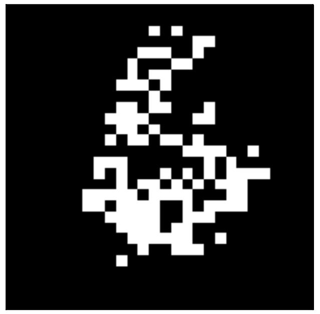


$x^{j,k} \sim \text{Bern}(f^{j,k}(\mathbf{z}))$



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$\mathbb{P}(\theta \mid X)$

Generation

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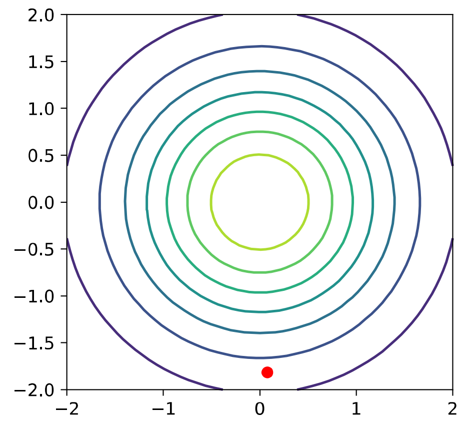
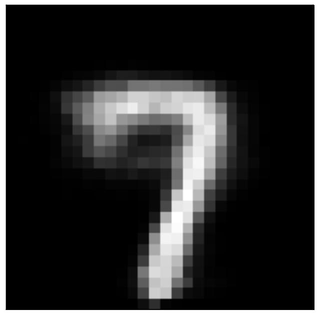
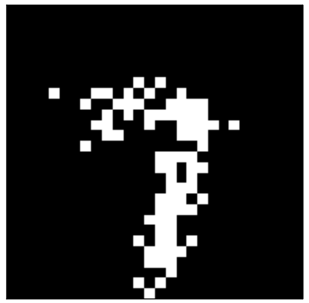
$$\mathbf{z} = (0.0791, -1.8165)$$



$f(z)$



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



Maximum likelihood for DLVM

The log-likelihood function of our dataset $(x_1, \dots, x_n)$ is

$$\ell(\theta) = \sum_{i=1}^{n} \log p(x_i) = \sum_{i=1}^{n} \log \int p(x_i|z)p(z)dz$$

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$p(x_i)$ is actually a difficult integral

Our solution from last lecture : **use importance sampling to attack the integral!**

Aparté: Beyond simple MC: importance sampling

- We have to use Monte Carlo! Our goal is to approximate an integral

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

- We already saw the **simple MC estimate**

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

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- We already saw the **simple MC estimate**

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

- This estimate has nice properties:
  - Unbiasedness: $\mathbb{E}[\hat{I}_K] = I$
  - Consistency: $\hat{I}_K \overset{a.s.}{\to} I$
  - Asymptotic normality

Beyond simple MC: importance sampling

- One way of assessing the accuracy of any unbiased estimate is by looking at its variance. **The lower the variance of an unbiased estimate, the better.**

- If the samples are iid, then the variance of simple MC will be $\mathbb{V}[\hat{I}_K] = \frac{1}{K}\mathbb{V}[f(x_1)]$

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- If the samples are iid, then the variance of simple MC will be $\mathbb{V}[\hat{I}_K] = \frac{1}{K}\mathbb{V}[f(x_1)]$
- So the variance gets smaller and smaller at speed *1/K*, that's good news!
- But it can still be pretty big, depending on the value of $\mathbb{V}[f(x_1)]$
- **Can we reduce the variance of the MC estimate?**

Beyond simple MC: importance sampling

- Key idea: rather than sampling from $p(x)$, we're going to sample from another density $q(x)$ that we'll call a **proposal**

$$x_1, ..., .x_K \sim q$$

- But the integral is an expected value with respect to *p*. **Can we turn an expected value with respect to *p* into an expected value with respect to *q*?**

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- But the integral is an expected value with respect to *p*. **Can we turn an expected value with respect to *p* into an expected value with respect to *q*? Yes!**

$$\begin{aligned} I &= \int_\Omega f(x)p(x)dx \\ &= \int_\Omega \frac{f(x)p(x)}{q(x)} q(x)dx \approx \frac{1}{K}\sum_{k=1}^{K} \frac{f(x_k)p(x_k)}{q(x_k)} = \hat{I}_K^q. \end{aligned}$$

Beyond simple MC: importance sampling

- This new estimate $\hat{I}^q_K$ is called an **importance sampling** estimate.
- Now, is $\hat{I}^q_K$ any better than the simple MC estimate?

$\mathbb{P}(\theta | X)$

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- It's clear that $\hat{I}_K^q$ will aslo be unbiased, consistent, and asymptotically normal.
- The variance will be $\mathbb{V}_{x \sim q}[f(x)p(x)/q(x)]/K$

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- **That seems a bit too good to be true… What's the catch?**

The optimal importance sampling proposal

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$$q^*(x) = \frac{f(x)p(x)}{\int f(x)p(x)dx} = \frac{f(x)p(x)}{I}$$

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- In practice, we won't be able to find this optimal proposal, but this shows that **the improvements of importance sampling can be potentially huge!**
- This simple result is therefore a motivation for looking for good proposals.

Maximum likelihood for DLVM

The likelihood is $\ell(\theta) = \sum_{i=1}^{n} \log p(x_i) = \sum_{i=1}^{n} \log \int p(x_i|z)p(z)dz$

Idea: use importance sampling! Let $\mathbf{z}_{i1}, \ldots, \mathbf{z}_{iK}$ follow some proposal q_i:

$$\int_{\mathbb{R}^d} p_{\boldsymbol{\theta}}(\mathbf{x}_i \mid \mathbf{z}) p(\mathbf{z}_{ik}) d\mathbf{z} \approx \frac{1}{K} \sum_{k=1}^{K} \frac{p_{\boldsymbol{\theta}}(\mathbf{x}_i \mid \mathbf{z}_{ik}) p(\mathbf{z})}{q_i(\mathbf{z}_{ik})}$$

Let's say that we want to choose our **proposal in a parametric family** $(\Psi(\cdot|\kappa))_{\kappa \in \mathcal{K}}$ over $\mathbb{R}^d$ (e.g. Gaussians).

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Let's say that we want to choose our **proposal in a parametric family** $(\Psi(\cdot|\kappa))_{\kappa \in \mathcal{K}}$ over $\mathbb{R}^d$ (e.g. Gaussians).

Problem: we need to choose n **proposals** $q_1, \ldots, q_n$ (and n is usually large in deep learning...).

Maximum likelihood for DLVMs: choosing proposals

For the importance sampling problem

$$p(x_i) = \int p(x_i|z)p(z)dz \approx \frac{1}{K}\sum_{k=1}^{K}\frac{p(x_i|z_{ik})p(z_{ik})}{q_i(z_{ik})}$$

the optimal proposal will be

$$\mathbb{P}(\theta | X)$$

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$$q_i^\star(z) = \frac{p(x_i|z)p(z)}{p(x_i)}$$

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$$q_i^\star(z) = \frac{p(x_i|z)p(z)}{p(x_i)} = p(z|x_i)$$

aka the posterior (again, not in a Bayesian sense).

Maximum likelihood for DLVM

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

Rationale: q_i needs to depends on $\mathbf{x}_i$, so we'll define it as a **conditional distribution parametrised by γ:**

$$q_i(\mathbf{z}) = q_\gamma(\mathbf{z}|\mathbf{x}_i).$$

How to parametrise this conditional distribution? The key idea is that **its parameters are the output of a neural net g_γ:**

$$q_\gamma(\mathbf{z}|\mathbf{x}_i) = \Psi(\mathbf{z}|g_\gamma(\mathbf{x}_i)).$$

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

Maximum likelihood for DLVM

All of this leads to the following approximation of the likelihood

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

Rather than maximising $\ell(\boldsymbol{\theta})$, **we'll maximise $\mathcal{L}_K(\theta, \gamma)$ using SGD** and the reparametrisation trick. But does it make sense to do that?

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Rather than maximising $\ell(\boldsymbol{\theta})$, **we'll maximise $\mathcal{L}_K(\theta,\gamma)$ using SGD** and the reparametrisation trick. But does it make sense to do that?

It does make sense! For several reasons:

- $\mathcal{L}_K(\boldsymbol{\theta},\gamma)$ is a **lower bound of $\ell(\theta)$** (exercise !)
- The bounds get **tighter and tighter!**

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

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

2

Properties of the bound

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Theorem. $\mathcal{L}_K(\theta, \gamma) \leq \ell(\theta)$.

$\mathbb{P}(\theta \mid X)$

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Proof. Without loss of generality, we assume that there is a single point x in our dataset. Let $z_1, \ldots, z_K \sim q_i$, and let

$$w_k = \frac{p(x|z_k)p(z_k)}{q_i(z_k)}, \text{ and } \bar{w}_K = (w_1 + \ldots + w_K)/K.$$

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With these notations, $\mathcal{L}_K = \mathbb{E}[\log \bar{w}_K]$. Because IS is unbiased, $\mathbb{E}[\bar{w}_K] = p(x)$. Now, since the log is concave, we can use Jensen's inequatity to get

$$\mathcal{L}_K \leq \mathbb{E}[\log \bar{w}_K] \leq \log \mathbb{E}[\bar{w}_K] = \log p(x)$$

$\square$

Properties of the bound

Theorem. $\mathcal{L}_1(\theta, \gamma) \leq \ldots \leq \mathcal{L}_K(\theta, \gamma) \leq \ell(\theta).$

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Then, using Jensen's leads to

$$\log\left(\frac{1}{K}\sum_{k=1}^{K} w_k\right) \geq \frac{1}{K}\sum_{j=1}^{K}\log\left(\frac{1}{K-1}\sum_{k\neq j} w_k\right)$$

and to the desired result. $\square$

What about VAEs?

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

The VAE bound can be interestingly rewritten

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

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

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

What about VAEs?

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.

$\mathbb{P}(\theta \mid X)$

What about VAEs?

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

The VAE bound can be interestingly rewritten

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

which means that, for a given $\boldsymbol{\theta}$, **the optimal $q_\gamma(\mathbf{z}_i|\mathbf{x}_i)$ 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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makes sure the encodings are not too far away from the prior.
At the end of the day, a scatter plot of the encodings will kinda look like the prior.

What about VAEs?

This motivates the name variational auto-encoder, as we can see the loss as a KL-regularised auto-encoder loss!

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Why is this a reconstruction error?

- In the particular case of a Gaussian observation model $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \sigma^2\mathbf{I}_D)$ with a constant and isotropic covariance, we can use the formula of the Gaussian density to get

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- The other terms do not depend on θ, so it makes sense to see $\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ as a reconstruction error.
- Note that the autoencoding process is stochastic, as it involves sampling $\mathbf{z} \sim q_{\gamma}(\mathbf{z}|\mathbf{x})$

Why is this a reconstruction error?

- If we have a Bernoulli observation model $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \prod_{j=1}^{d} \mathcal{B}(x_j|\boldsymbol{\pi}_{\boldsymbol{\theta}}(\mathbf{z})_j)$, we get

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = -\sum_{j=1}^{d} \mathrm{XEnt}(\mathbf{x}, \boldsymbol{\pi}_{\boldsymbol{\theta}}(\mathbf{z}))$$

Cross-entropy loss
between $\mathbf{x}_i$ and its reconstruction (obtained by auto-encoding it)

Why is the KL term a regulariser?

- The KL part of the VAE bound is equal to $\mathrm{KL}\left(\prod_{i=1}^{n} q_{\boldsymbol{\gamma}}(\mathbf{z}_i|\mathbf{x}_i) \middle\| \prod_{i=1}^{n} p_{\boldsymbol{\theta}}(\mathbf{z}_i)\right)$, which is the

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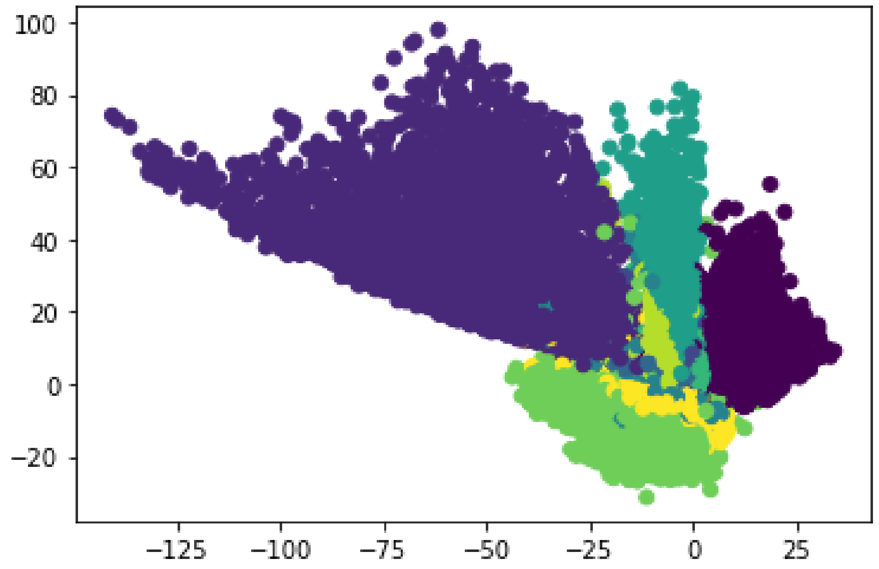

2D code space of a standard AE on MNIST

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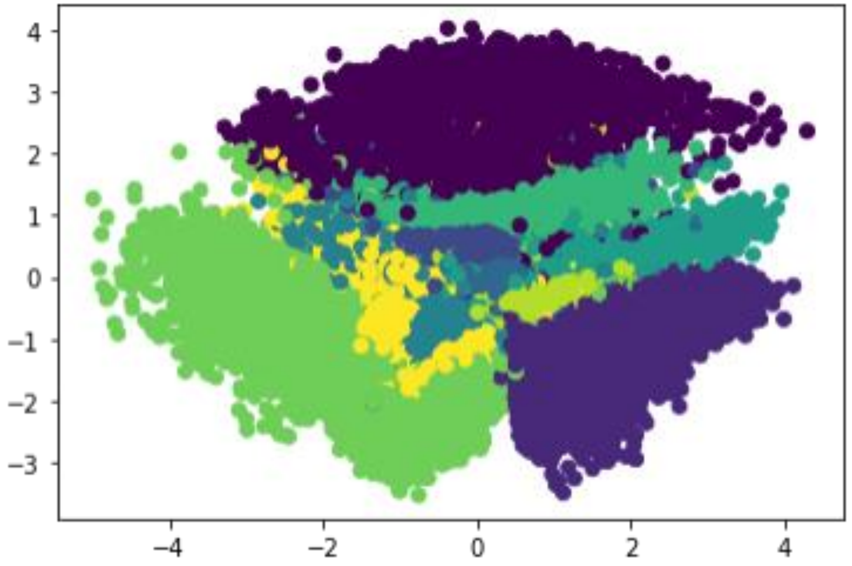

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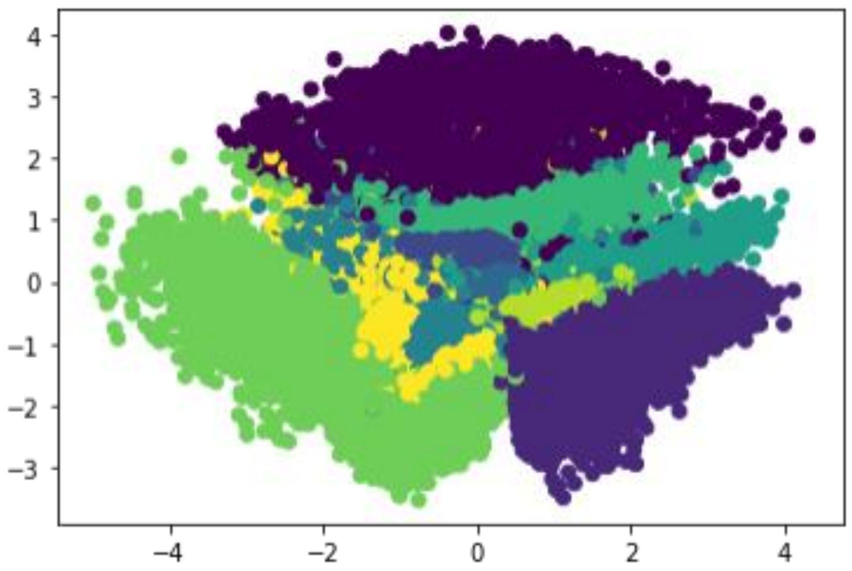

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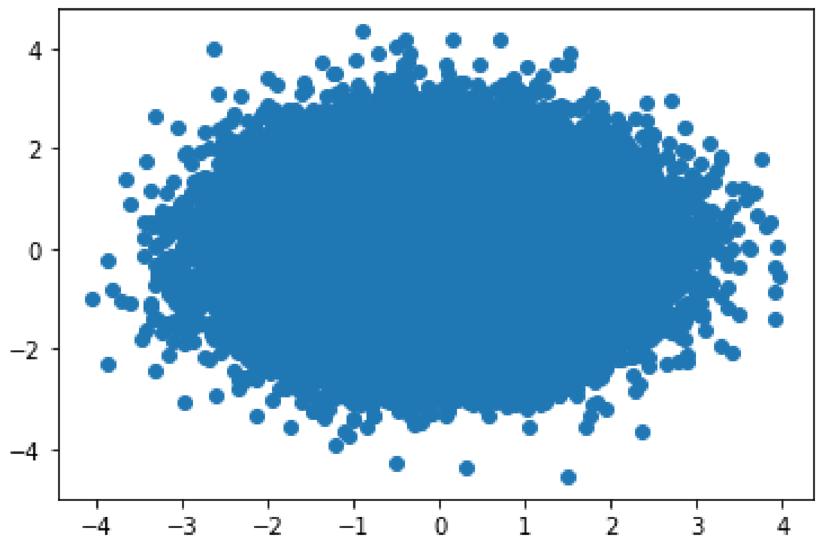

Standard Gaussian samples

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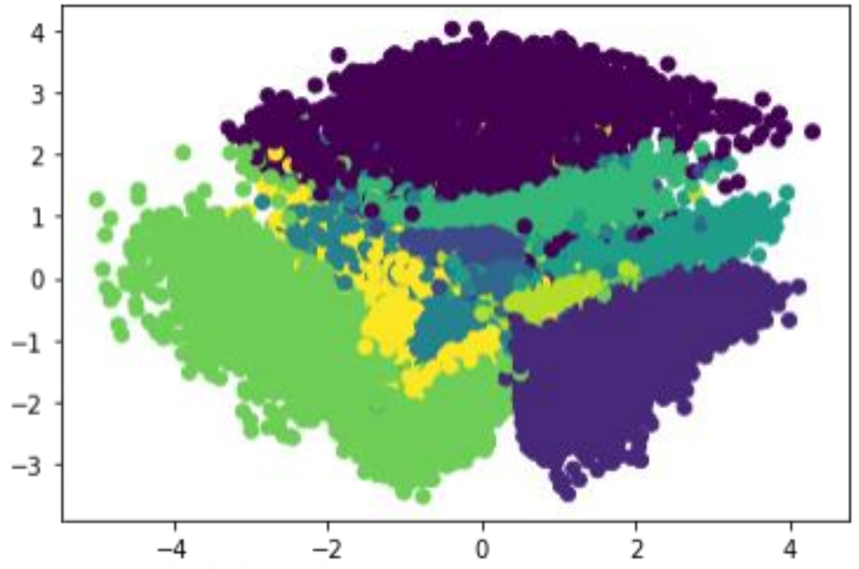

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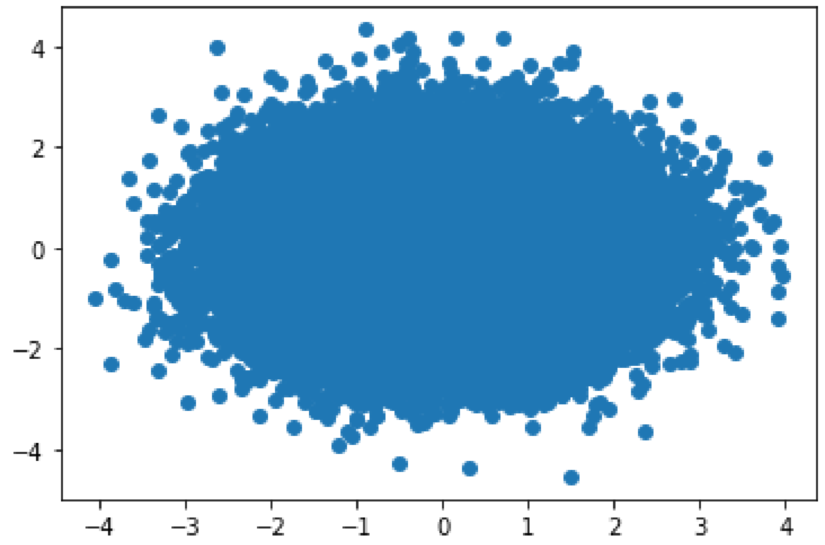

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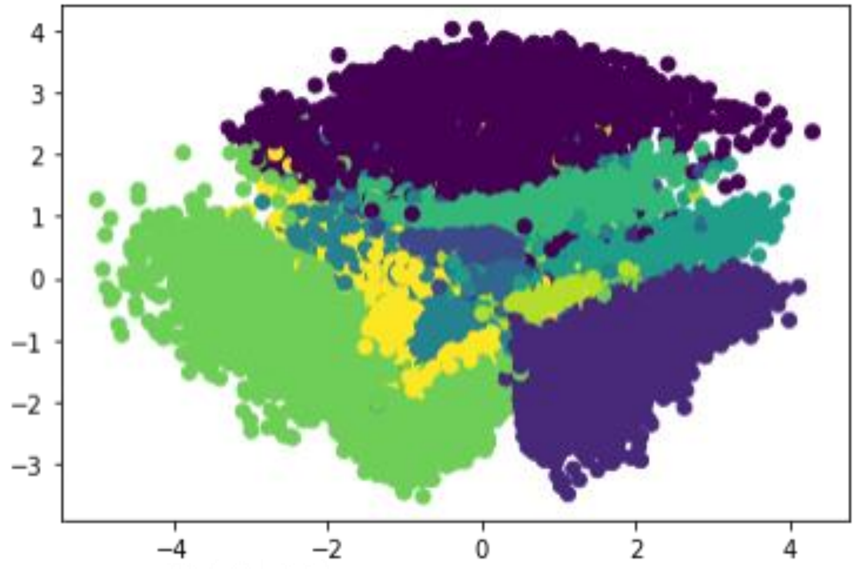

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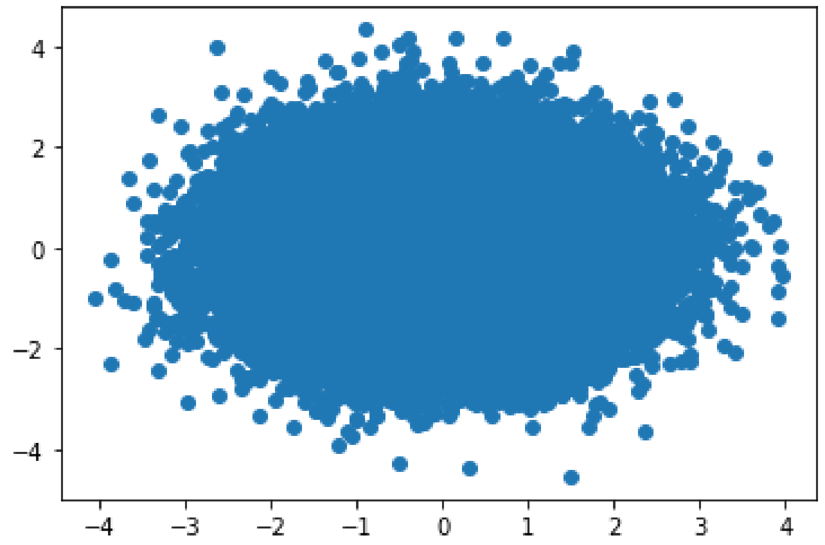

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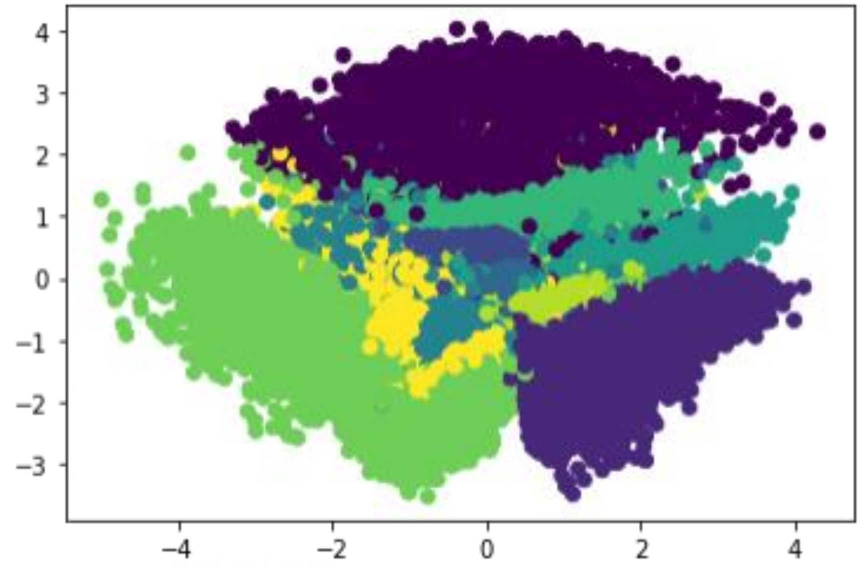

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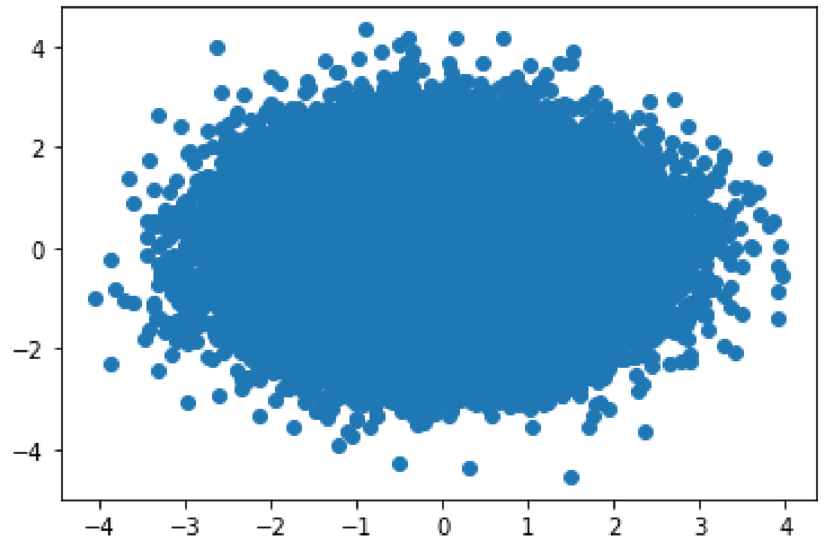

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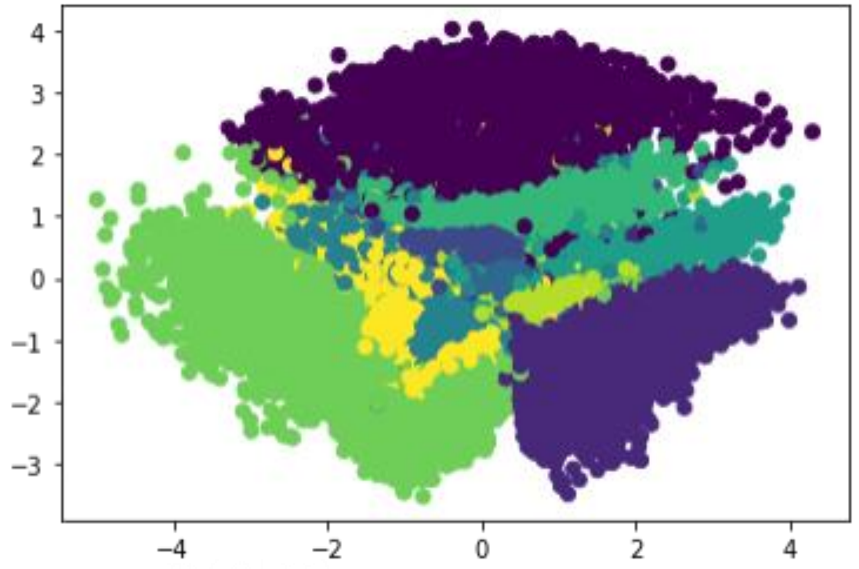

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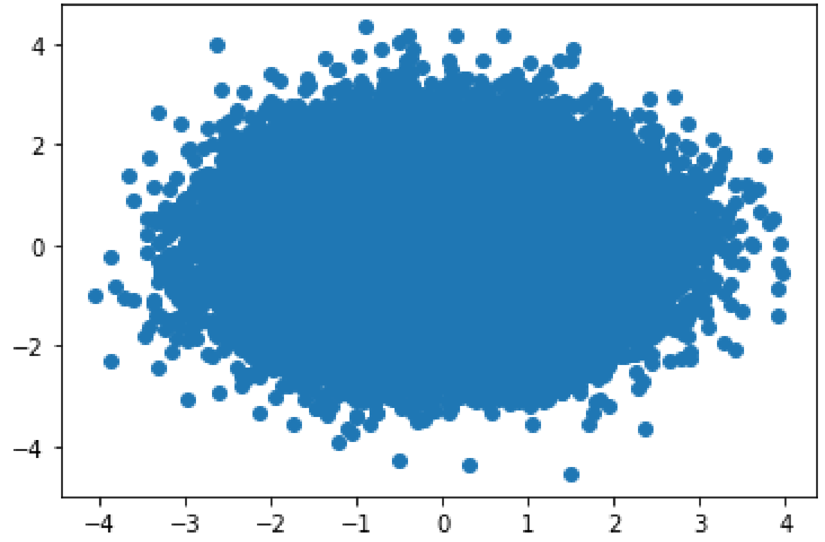

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  - **Bad:** The latent space is not discriminative! **Any idea how to simply solve this? One solution is to use a GMM prior.**

More on this KL regulariser

- In the common case where both prior and approximate posterior are Gaussian, this KL regulariser is just a KL between Gaussians, which has a closed-form expression. Here is the general formula for *p*-variate Gaussians with full covariance

$$\textbf{KL}(\mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0) || \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)) =$$

$$\frac{1}{2}\left(\textbf{tr}(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_0) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) + \log\frac{\det \boldsymbol{\Sigma}_1}{\det \boldsymbol{\Sigma}_0} - p\right)$$

$$\mathbb{P}(\theta | X)$$

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- It’s easy to backprop through this, ans this was used in the seminal VAE papers!

- Not easy to generalise beyond Gaussians…

3

How to train VAEs?

How do we actually train VAEs?

- What have we done so far? We have created a family of **lower bounds of the log-likelihood**, but how do optimise them?

- Remember that the IWAE bounds are defined as

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

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- **How do we maximise this? We can’t even compute this exactly?**

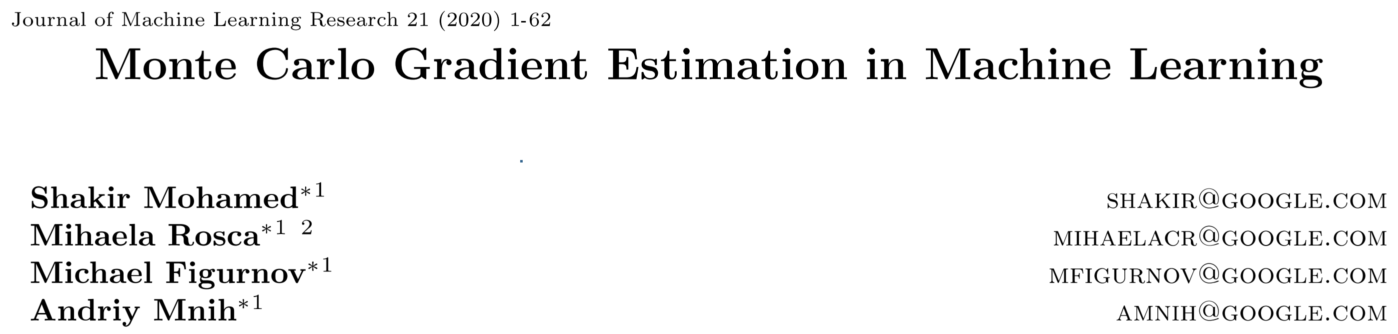
- The idea is to use stochastic gradient descent (SGD, or one of its variants). What do we need to compute to perform SGD on an objective? **Unbiased estimates of the gradients!**
- As we’ll see, it is doable to compute unbiased estimates of $\nabla_{\theta,\gamma} \mathcal{L}_K(\boldsymbol{\theta}, \gamma)$

Unbiased IWAE gradients: looking at a more general problem

- Let’s look at the problem in a more general form, we want unbiased estimates of the gradients of a function of the form

$$f(\boldsymbol{\theta}, \gamma) = \mathbb{E}_{\mathbf{w} \sim \pi_{\boldsymbol{\gamma}}(\mathbf{w})} \left[g(\boldsymbol{\theta}, \gamma, \mathbf{w}) \right]$$

- In the next few slides, we will describe a few recipes to compute such estimates. **This is a task that is useful in a lot of ML contexts**, e.g. reinforcement learning, explainability… For more details, and more recipe, you may look at the following nice review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Monte Carlo Gradient Estimation in Machine Learning

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Mihaela Rosca*[1 2] MIHAELACR@GOOGLE.COM
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Andriy Mnih*[1] AMNIH@GOOGLE.COM

Let's start with the easy part: ∇_θ

- Note that the first parameter only appears **inside** the expectation

$$f(\boldsymbol{\theta}, \boldsymbol{\gamma}) = \mathbb{E}_{\mathbf{w} \sim \pi_{\boldsymbol{\gamma}}(\mathbf{w})} \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \right]$$

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- Therefore, if g and π are nice enough (e.g. when $\nabla_\theta g$ can be dominated), we can use Leibniz's integral rule to get

$$\nabla_\theta f(\boldsymbol{\theta}, \boldsymbol{\gamma}) = \mathbb{E}_{\mathbf{w} \sim \pi_{\boldsymbol{\gamma}}(\mathbf{w})} \left[\nabla_\theta g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \right]$$

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which means that we can get an unbiased estimate of $\nabla_\theta f(\boldsymbol{\theta}, \gamma)$ by simply sampling $\mathbf{w}_1, ..., \mathbf{w}_K \sim \pi_\gamma(\mathbf{w})$ and then computing

$$\nabla_\theta f(\boldsymbol{\theta}, \gamma) \approx \frac{1}{K} \sum_{k=1}^{K} \nabla_\theta g(\boldsymbol{\theta}, \gamma, \mathbf{w}_k)$$

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Often *K*=1 will be enough!

Now the tricky part: ∇_γ

- This parameter appears both **inside** and **outside** the expectation:

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- So it’s not that simple… Let us write the expectation:

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- **It makes sense to use Leibniz’s rule again:**

$$\nabla_{\gamma} f(\boldsymbol{\theta}, \gamma) = \int \nabla_{\gamma} \left[g(\boldsymbol{\theta}, \gamma, \mathbf{w}) \pi_{\gamma}(\mathbf{w}) \right] d\mathbf{w}$$

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And now we can use the usual rule to **differentiate a product**:

$$\nabla_\gamma f(\boldsymbol{\theta}, \boldsymbol{\gamma}) = \int \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \right] \pi_{\boldsymbol{\gamma}}(\mathbf{w}) d\mathbf{w} + \int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \nabla_\gamma \left[\pi_{\boldsymbol{\gamma}}(\mathbf{w}) \right] d\mathbf{w}$$

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- **Which one of these two terms is easy to unbiasedly estimate?**

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And now we can use the usual rule to **differentiate a product**:

$$\nabla_\gamma f(\boldsymbol{\theta}, \boldsymbol{\gamma}) = \int \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \right] \pi_{\boldsymbol{\gamma}}(\mathbf{w}) d\mathbf{w} + \int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \nabla_\gamma \left[\pi_{\boldsymbol{\gamma}}(\mathbf{w}) \right] d\mathbf{w}$$

- **Which one of these two terms is easy to unbiasedly estimate? The first one because it is an expectation!**

$$\int \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \right] \pi_{\boldsymbol{\gamma}}(\mathbf{w}) d\mathbf{w} \approx \frac{1}{K} \sum_{k=1}^{K} \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}_k) \right]$$

Now the tricky part: ∇_{γ}

- The real tricky part is what's left: the second term $\int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \nabla_{\gamma} \left[\pi_{\boldsymbol{\gamma}}(\mathbf{w}) \right] d\mathbf{w}$

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$\mathbb{P}(\theta \mid X)$

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$$\int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \nabla_\gamma \left[\pi_{\boldsymbol{\gamma}}(\mathbf{w})\right] d\mathbf{w} = \mathbb{E}_{\mathbf{w} \sim \pi_{\boldsymbol{\gamma}}} \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \nabla_\gamma \log \pi_{\boldsymbol{\gamma}}(\mathbf{w})\right]$$

$$\approx \frac{1}{K} \sum_{k=1}^{K} g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}_k) \nabla_\gamma \log \pi_{\boldsymbol{\gamma}}(\mathbf{w}_k)$$

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- In the next slide, we'll see one of such cases: **the Gaussian reparametrisation trick.**

Reparametrisation trick for ∇_γ

- Our goal is still to estimate our tricky term $\nabla_\gamma \int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \pi_{\boldsymbol{\gamma}}(\mathbf{w}) d\mathbf{w}$

- Again, the main issue is that the density depends on the parameter of interest. Can we destroy this dependence? Can we **push γ away from the density** we're integrating against?

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- In some important cases, **yes!** The main example is the **Gaussian case** $\pi_\gamma = \mathcal{N}(\mu_\gamma, \Sigma_\gamma)$

- In this setting, it is clear that sampling $\mathbf{w} \sim \pi_\gamma$ can be done by computing

$$\mathbf{w} = \mu_\gamma + \underbrace{C_\gamma \varepsilon}_{\sim \mathcal{N}(0, \Sigma)}$$

where C_γ is the Cholesky decomposition of the covariance, and $\varepsilon \sim \mathcal{N}(0, \mathbf{I})$

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- But now, the only random thing is ε. This means we can rewrite our expectation as an expectation over ε

$$\nabla_\gamma \int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \pi_{\boldsymbol{\gamma}}(\mathbf{w}) d\mathbf{w} = \nabla_\gamma \int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mu_{\boldsymbol{\gamma}} + C_{\boldsymbol{\gamma}} \boldsymbol{\varepsilon}) p(\boldsymbol{\varepsilon}) d\boldsymbol{\varepsilon}$$

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…and finally use Leibniz's rule

$$\nabla_\gamma \int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w}) \pi_{\boldsymbol{\gamma}}(\mathbf{w}) d\mathbf{w} = \int \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mu_{\boldsymbol{\gamma}} + C_{\boldsymbol{\gamma}} \boldsymbol{\varepsilon}) \right] p(\boldsymbol{\varepsilon}) d\boldsymbol{\varepsilon}$$

$$\approx \frac{1}{K} \sum_{k=1}^{K} \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mu_{\boldsymbol{\gamma}} + C_{\boldsymbol{\gamma}} \boldsymbol{\varepsilon}_k) \right]$$

Reparametrisation trick for ∇_γ

- The estimate

$$\nabla_\gamma \int g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mathbf{w})\pi_{\boldsymbol{\gamma}}(\mathbf{w})d\mathbf{w} = \int \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mu_{\boldsymbol{\gamma}} + C_{\boldsymbol{\gamma}}\boldsymbol{\varepsilon})\right] p(\boldsymbol{\varepsilon})d\boldsymbol{\varepsilon}$$
$$\approx \frac{1}{K}\sum_{k=1}^{K} \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mu_{\boldsymbol{\gamma}} + C_{\boldsymbol{\gamma}}\boldsymbol{\varepsilon}_k)\right]$$

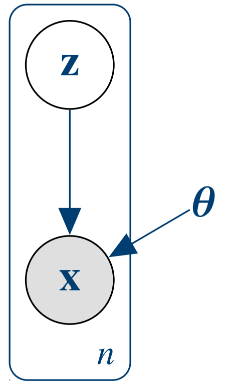
is often called the **reparametrisation trick** estimate. It has considerably less variance in practice than the score gradient, but can be less generally applied.

- Beyond Gaussians, this can be done for more complex distributions (Dirichlet, Student’s t, GMMs), but this is not easy, in particular for **discrete distributions.**

- It is automatically implemented in many libraries, for instance **Tensorflow Probability**, or **Pytorch distributions**

A quick summary of VAEs/IWAEs so far

- We have defined a graphical model called a **deep latent variable model**



- We have seen how to train this model by doing **approximate maximum likelihood via amortised variational inference**

- We saw that there was an **important interplay between this inference technique, and various sampling techniques** (importance sampling to define the bounds, various methods to estimate its gradients without bias).

4

On d-separation and latent variable models

D-separation

- D-separation means **directed separation.**

- It’s a general framework for answering questions à la «$X_A \perp\!\!\!\perp X_B | X_C?$» where A, B, C are three subsets of the set of nodes.

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- **D-separation recipe:** we consider all chains between any node in A and any node in B. Any of these chains is said to be **blocked by C** if it includes a node such that either
  - the chain is a v-structure at the node, and neither the node, nor its descendants, are in C
  - the arrows on the chain meet either head-to-tail or tail-to-tail at the node, and the node belongs to C

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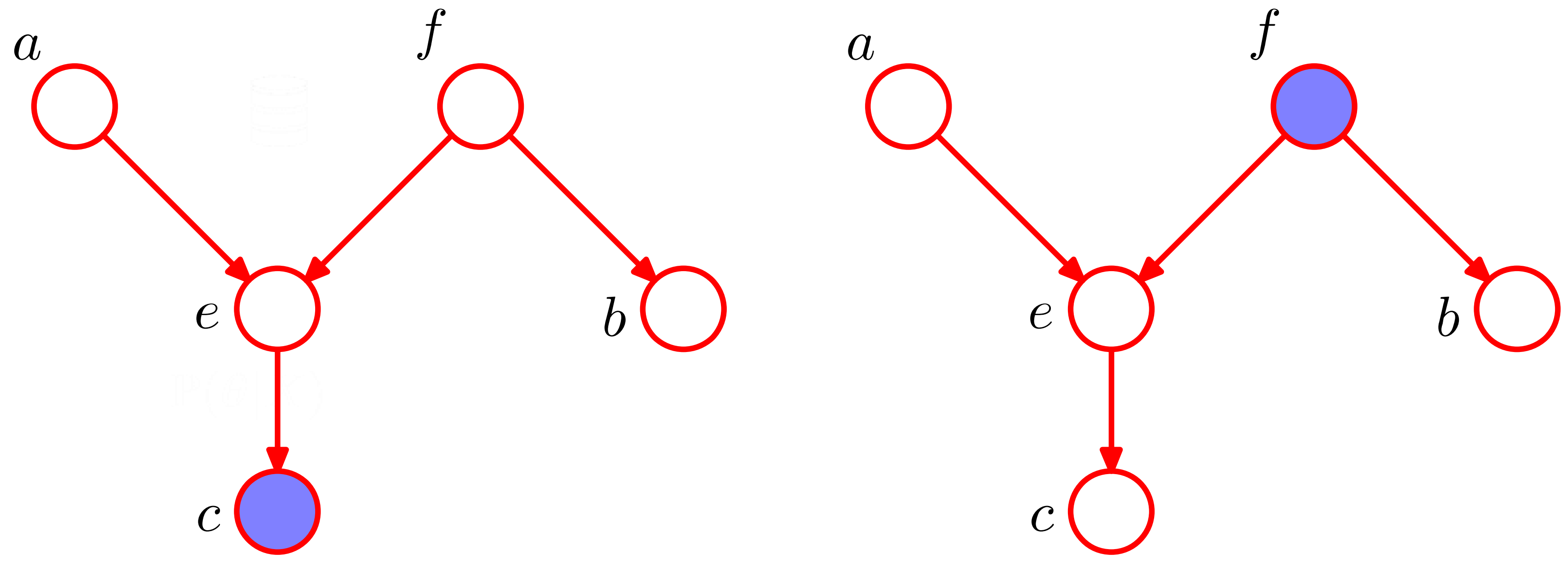
Definition. *We say that A* ***and*** *B* ***are d-separated by*** *C if all chains between A and B are blocked by C.*

Examples of d-separation

- I took this figure from [Bishop, Fig. 8.22]. Does the blue node d-separate a and b?



(a) (b)

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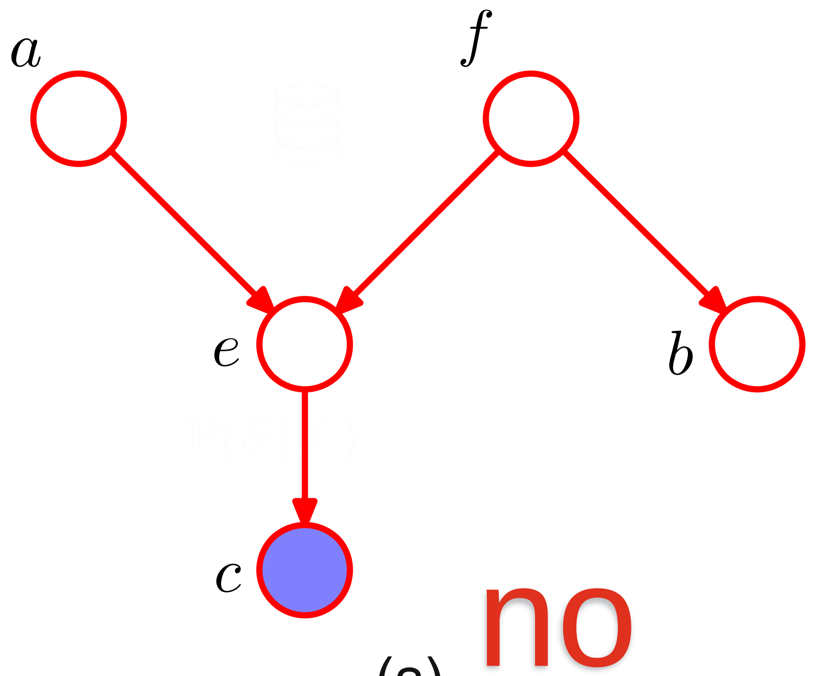
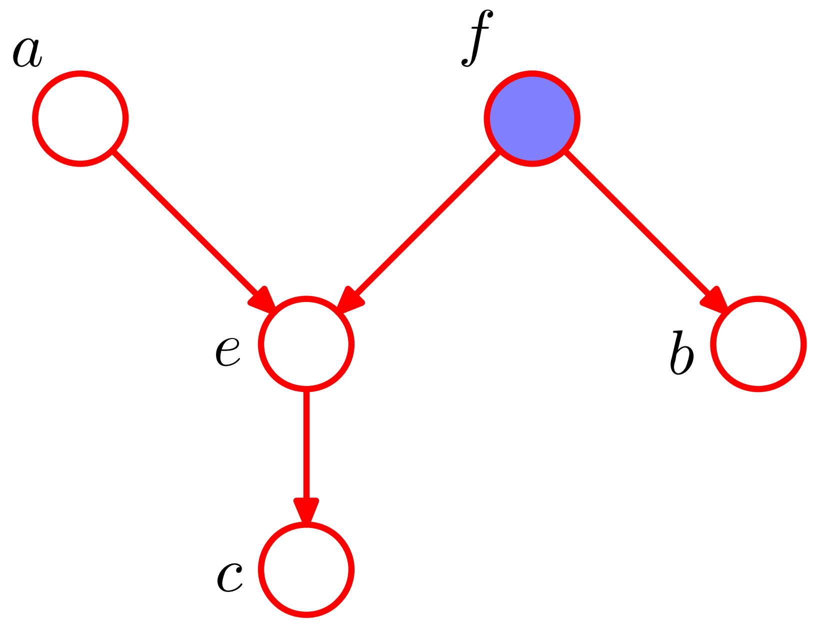


(a)

no



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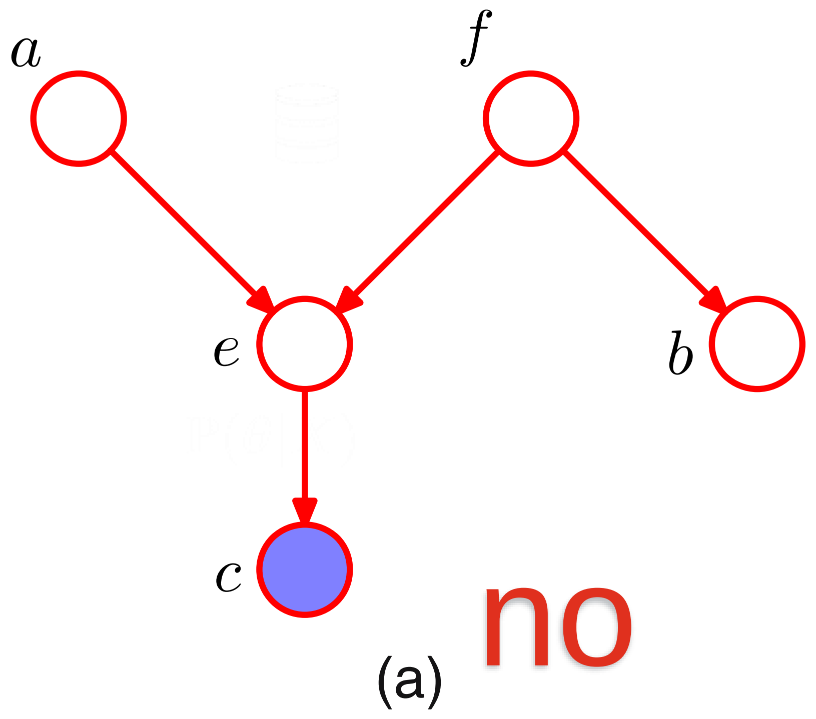

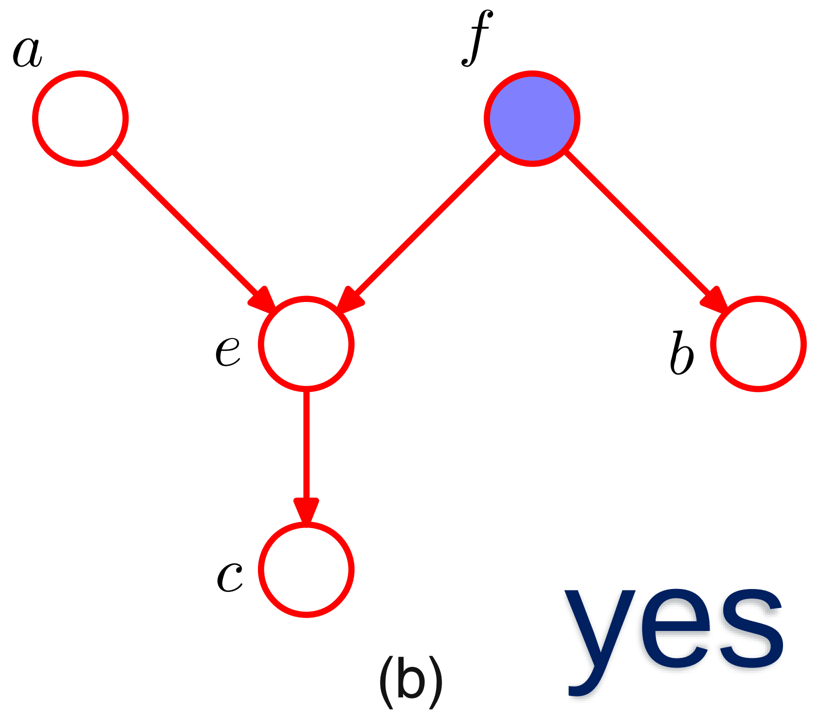

Properties of d-separation

Theorem (soundness of d-separation). *If A and B are d-separated by C and $p \in \mathcal{L}(G)$, then $X_A \perp\!\!\!\perp X_B | X_C$.*

Theorem (completeness of d-separation). *If A and B are not d-separated by C, then there exist $p \in \mathcal{L}(G)$ such that $X_A \not\perp\!\!\!\perp X_B | X_C$.*

For more details, including proofs, see [PGM, Sec. 3.3.2].

Applications of d-separation

- We previously mentioned conditional independence properties. Try to prove them using d-separation:

$$\begin{tikzcd} x_1 \arrow[r] & x_2 \arrow[r] & x_3 \end{tikzcd}$$

$$x_3 \perp\!\!\!\perp x_1 | x_2$$

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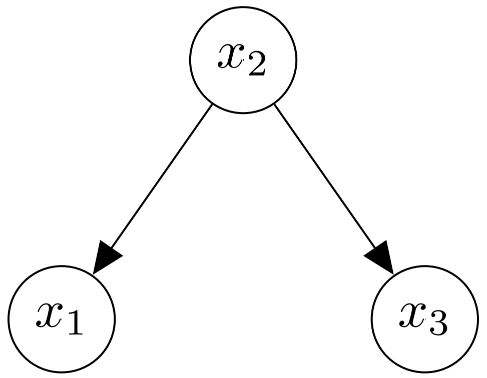

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