Linear and deep latent variable models

from PPCA to VAEs

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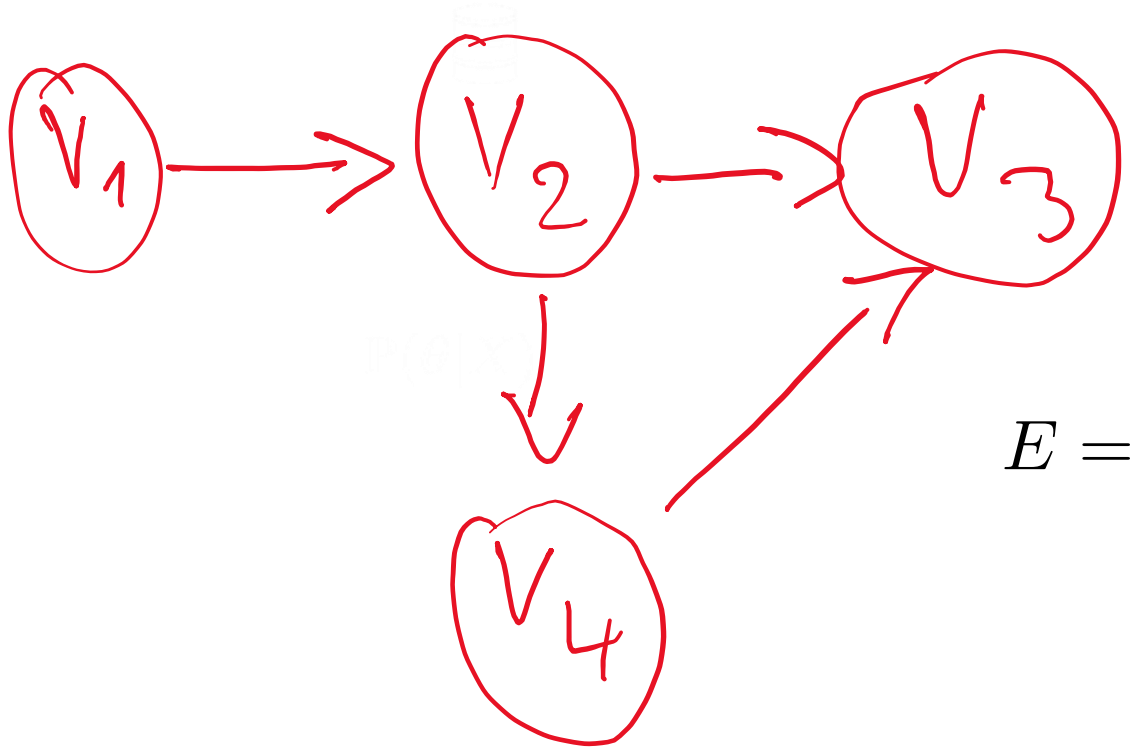
Recap on directed graphical models

What's a graph, mathematically?

Definition (directed graph)**.** *A* graph *is a pair* $G = (V, E)$ *comprising a set* V *of* ***vertices or nodes*** *together with a set* $E \subset V \times V$ *of* ***edges or arcs****.*



$$V = \{v_1, v_2, v_3, v_4\}$$

$$E = \{(v_1, v_2), (v_2, v_3), (v_2, v_4), (v_3, v_4)\}$$

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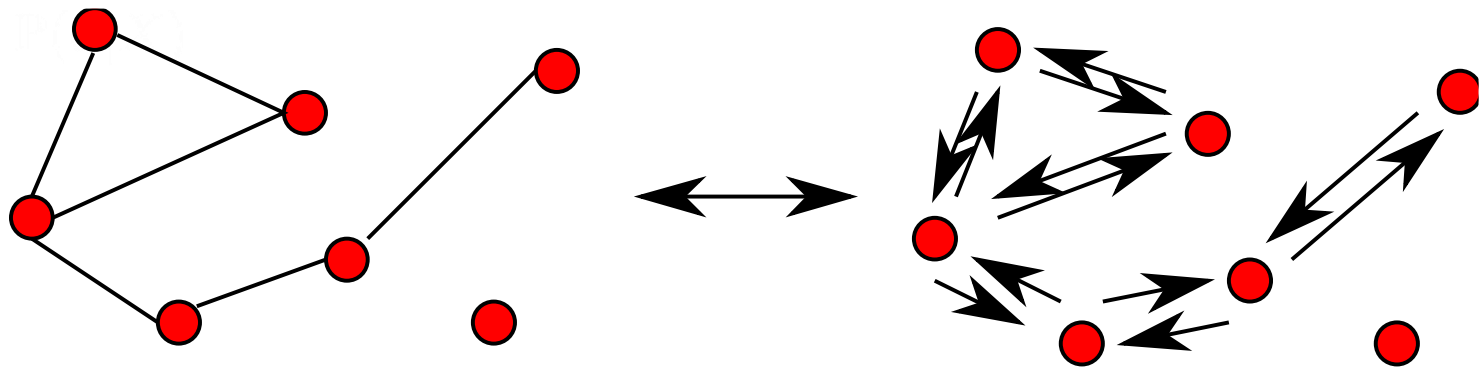
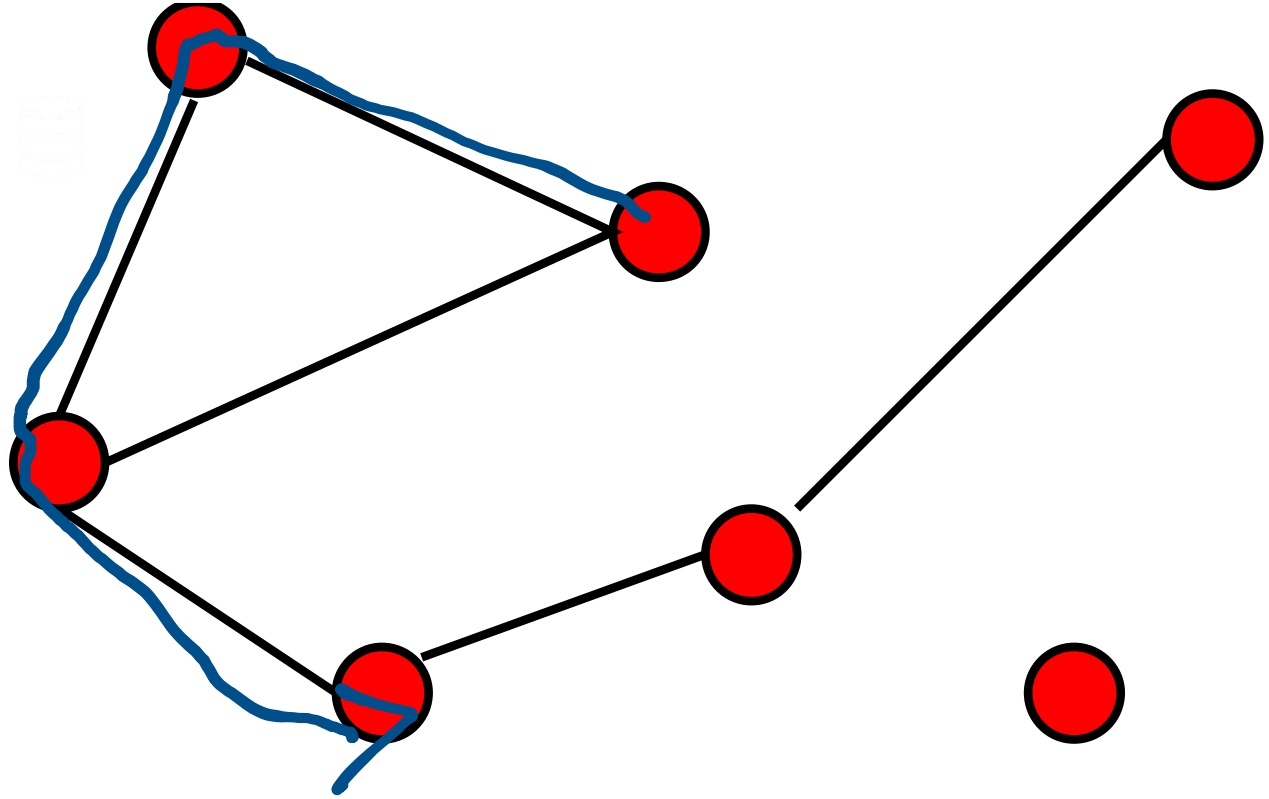
Definition (undirected graph)**.** $G = (V, E)$ *is* ***undirected*** *if all edges go in both directions: for all* $(u, v) \in V \times V$ *such that* $u \neq v$*, we have:*

$$(u, v) \in E \iff (v, u) \in E.$$



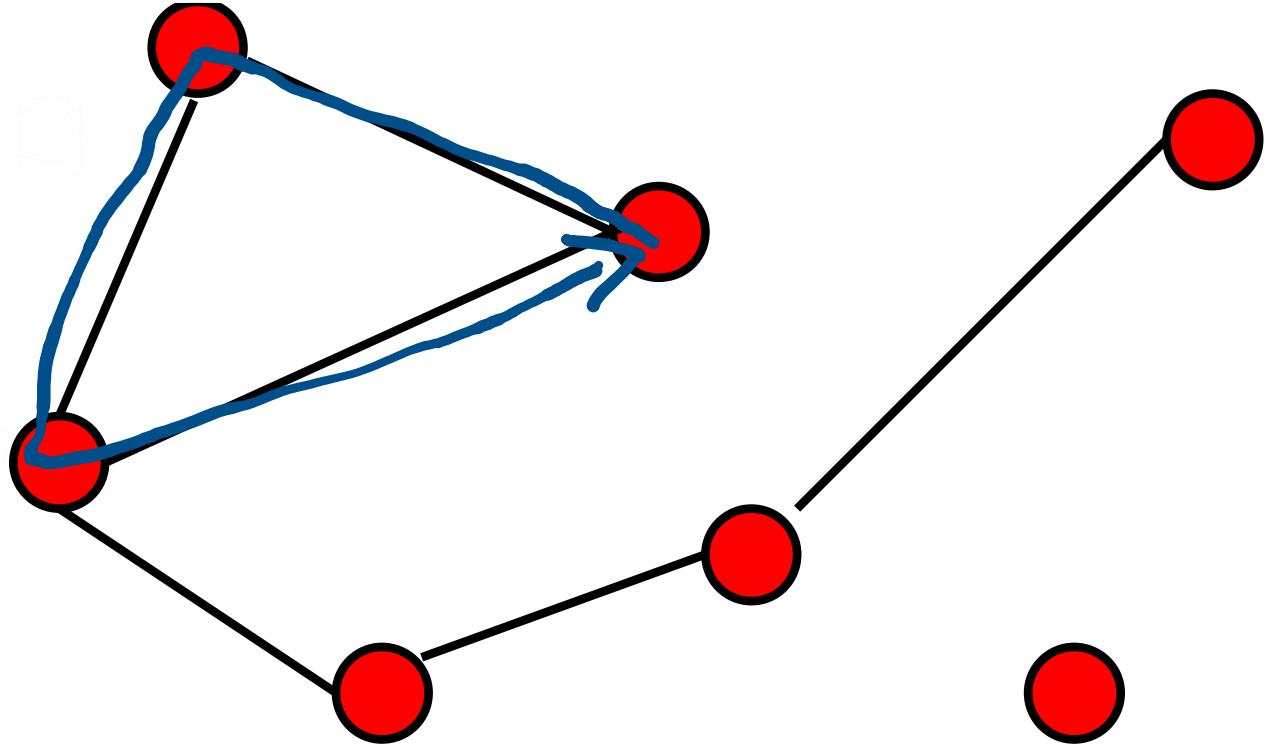
What's a path?

Definition. *A* ***path*** *is a sequence of connected vertices that are globally distinct.*



What's a cycle?

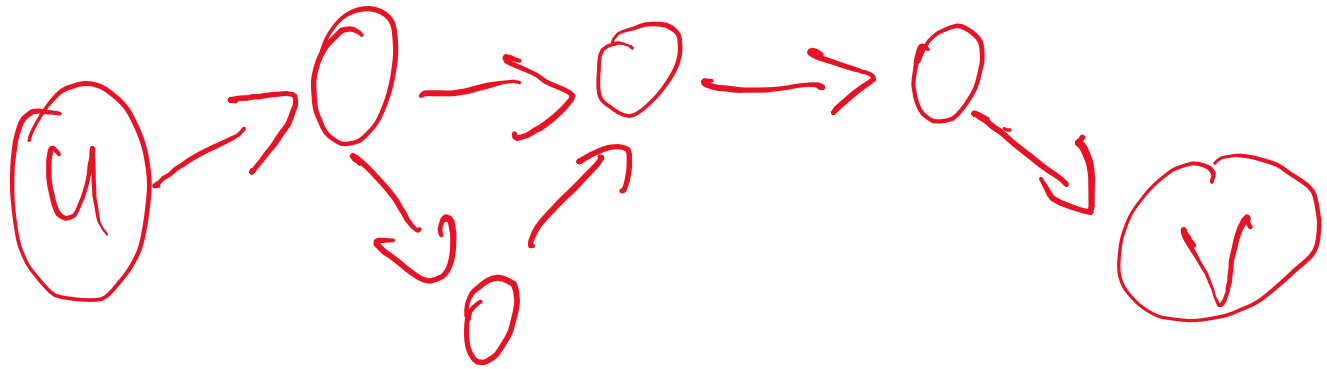
Definition. *A path that begins and end at the same point is called a* ***cycle****.*



Some definitions specific to directed graphs

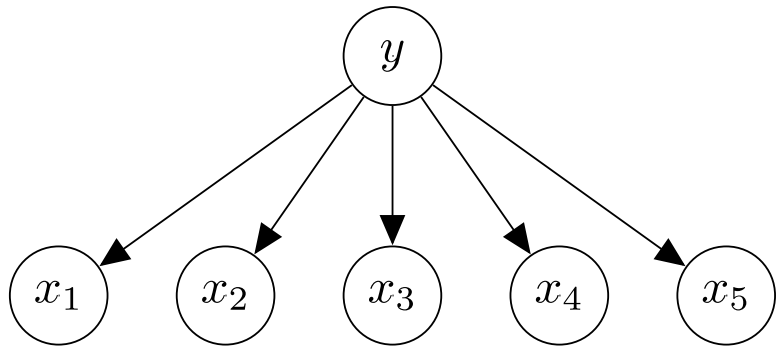
Definition. *u is a **parent** of v if $(u, v) \in E$. We also say that v is a **children** of u.*

Definition. *u is an **ancestor** of v if there exists a path from u to v. We also say that v is a **descendant** of u.*

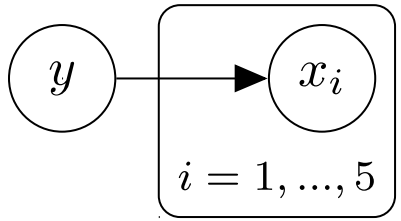


The useful plate notation

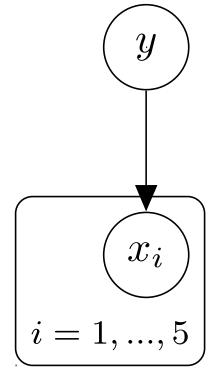
- Often we deal with graphs with recurring stucture, for instance



- The **plate notation** is a more compact way of drawing the same graph:



or



A key concept: DAGs

Definition (DAG). *A* ***directed acyclic graph*** *(DAG) is a directed graph without any cycle.*

What are directed graphical models?

- Let $G = (V, E)$ be a DAG whose nodes are denoted $V = \{1, ..., d\}$
- Let $X = (X_1, ..., X_d)$ be a random variable with density $p(x) = p(x_1, ..., x_d)$.
- Every node of the graph corresponds to a random variable (one vertex for each feature)

Definition (Directed graphical model)**.** *We say that p* ***factorises in*** *G (denoted $p \in \mathcal{L}(G)$) when, for all x,*

$$p(x) = \prod_{i=1}^{d} p(x_i | x_{\mathrm{pa}_i}),$$

where, for all node i, pa_i denotes the set of parents of node i.

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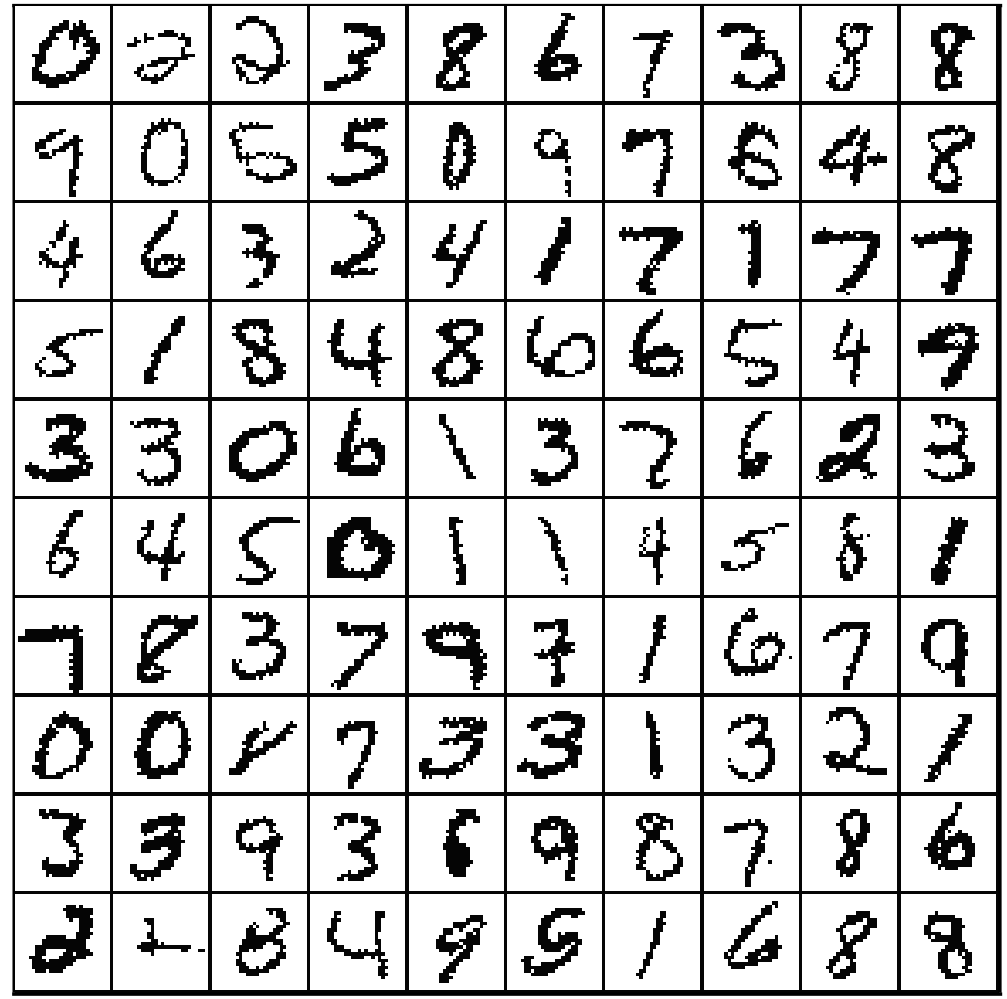
More examples of directed models and notations

Recurring « fil rouge » example

- We will often consider as a working example a **binary version of MNIST**

- $x_1, ..., x_n \in \mathcal{X} \quad \mathcal{X} = \{0,1\}^{28\times 28}$

- $y_1, ..., y_n \in \{0, \ldots, 9\}$



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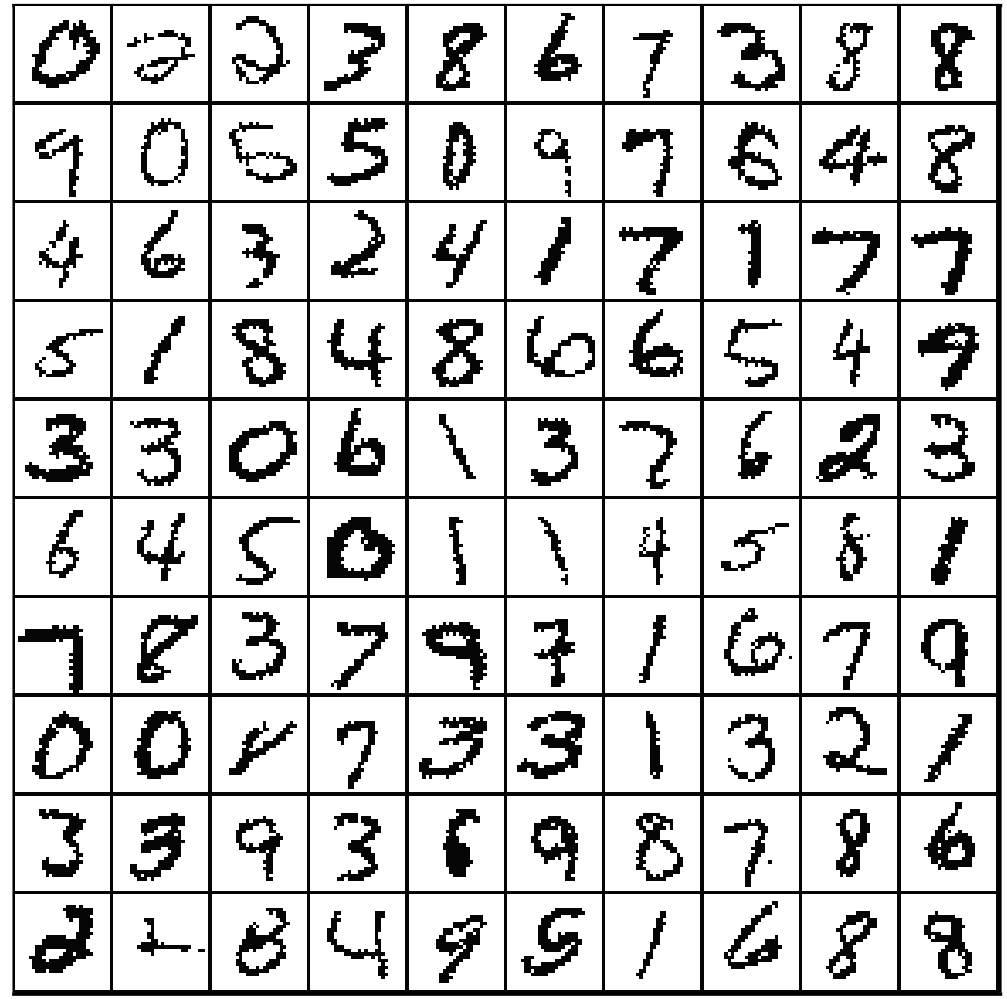
- Binarised by Hugo Larochelle
- Sometimes called « statical binary MNIST » in VAE papers



A basic example of parametrised distribution for binary MNIST

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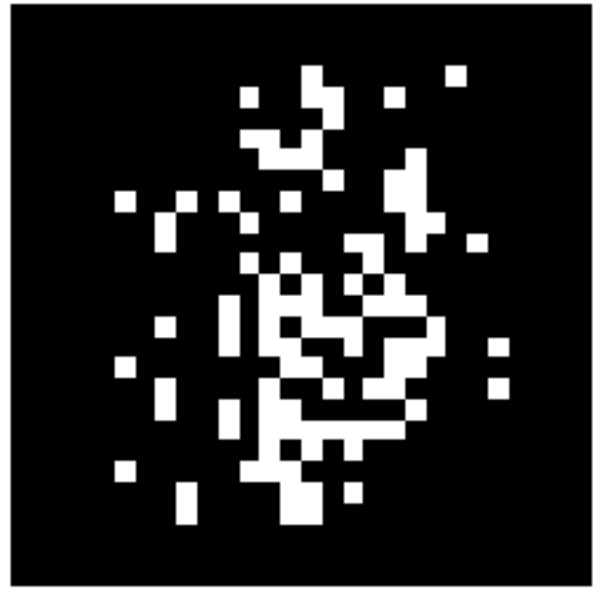
- This may be rewritten

$$p_\theta(x_1, \ldots, x_n) = \prod_{i=1}^{n} p_\theta(x_i) = \prod_{i=1}^{n} \prod_{j=1}^{28\times 28} \mathcal{B}(x_{ij}|\theta_j)$$

Why is this model not great?

The MLE is just $\hat{\theta}_j = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$

Here is a sample from the model…



Real pixels are not independent!

The graphical model for this weak baseline

The factorisation is

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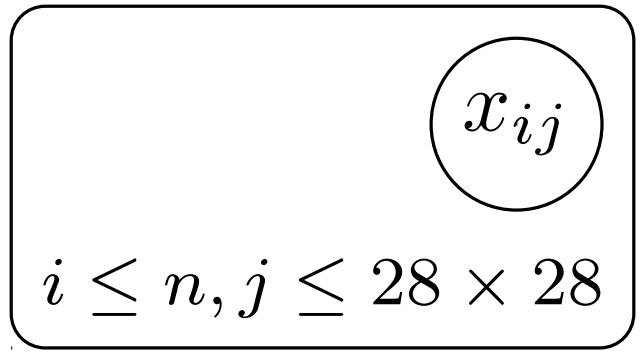

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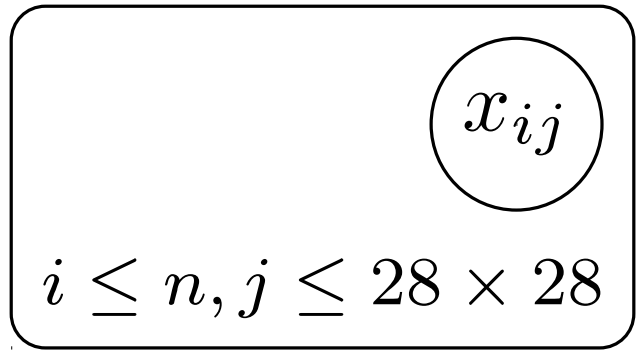

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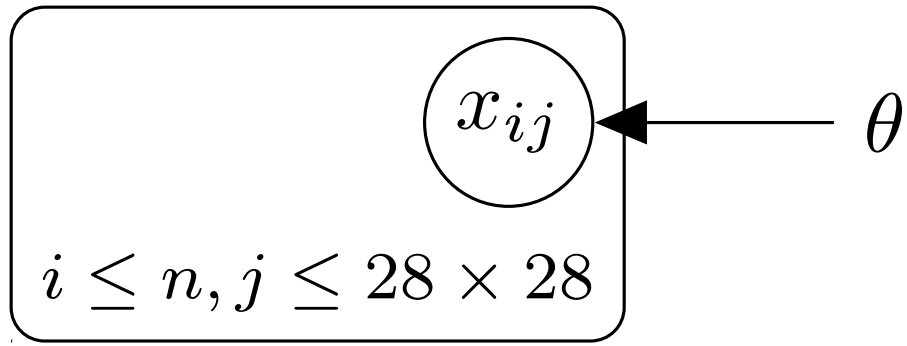

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How do we improve this weak model?

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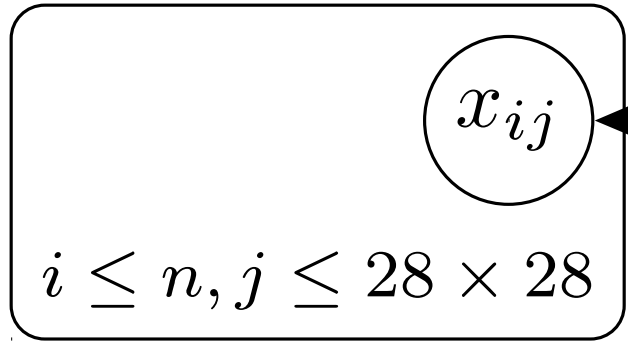

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How do we improve this weak model?

Hint: think of GMMs!

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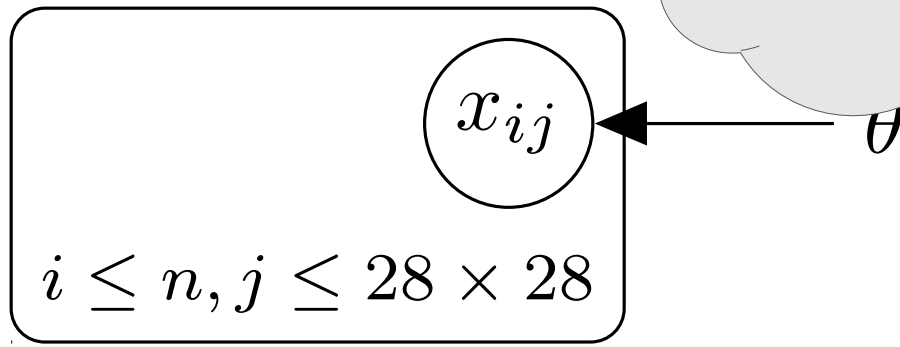

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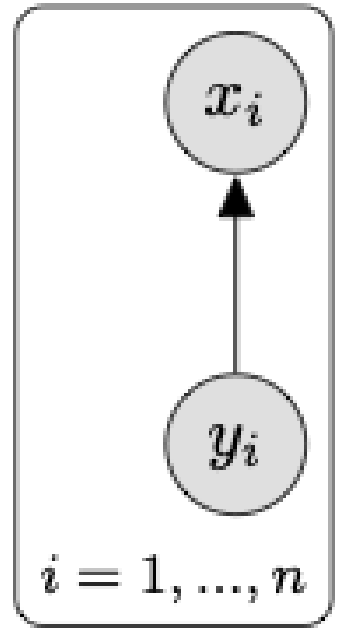
Adding a node that represents the class improves the model!

$$p_\theta(x_1, \ldots, x_n, y_1, \ldots, y_n) = \prod_{i=1}^{n} p_\theta(y_i) p_\theta(x_i|y_i) \text{ with } p_\theta(y) = \mathcal{M}(y|1, \pi) \text{ and } p_\theta(x|y) = \mathcal{B}(x|\mu_{yj})$$



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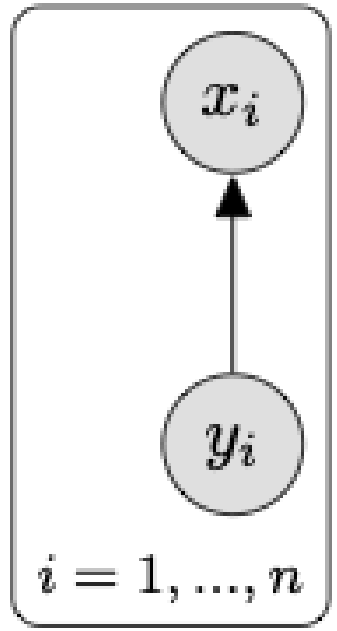

But this is a supervised model… How to make it unsupervised?

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Latent class analysis (aka mixtures of products of Bernoullis)

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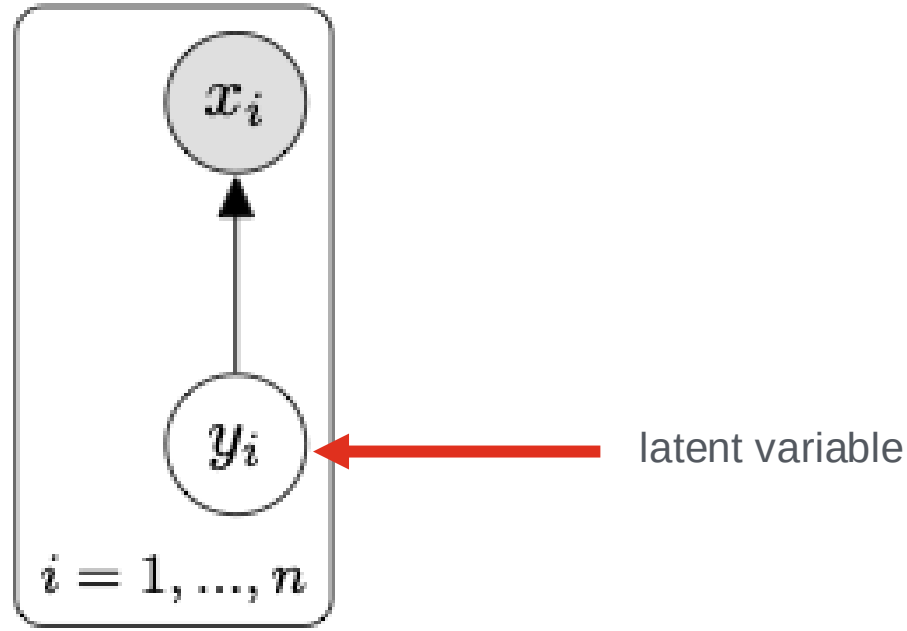

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Two very similar models, two very different likelihoods…

The likelihood of the supervised model is just a sum of log-densities of simple distributions:

$$\log p_\theta(x_1, \ldots, x_n, y_1, \ldots, y_n) = \sum_{i=1}^{n} (\log p_\theta(y_i) + \log p_\theta(x_i | y_i))$$

This is very easy to maximise, it has a simple closed-form solution.

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What would be ways to maximise it? EM, gradient descent, etc.

3

Technical aparté 1

Sampling with graphical models: ancestral sampling

Why sampling from a graphical model

1. The samples are useful by themselves

Images generated by a GAN

Brock, Donahue, and Simonyan (ICLR 2019)

2. Samples allow us to appximate integrals using Monte Carlo

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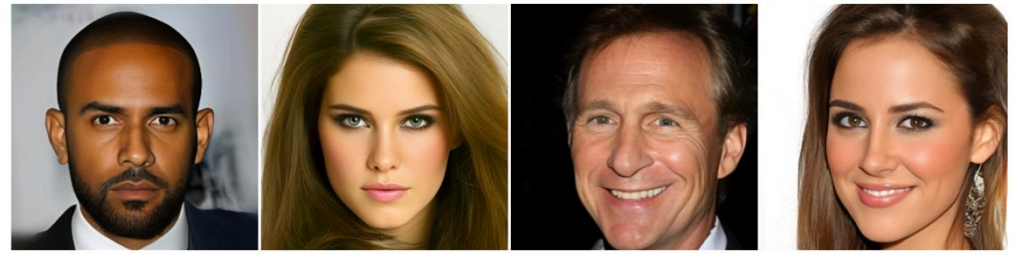

Images generated by a VAE

Vahdat and Kautz (NeurIPS 2020)

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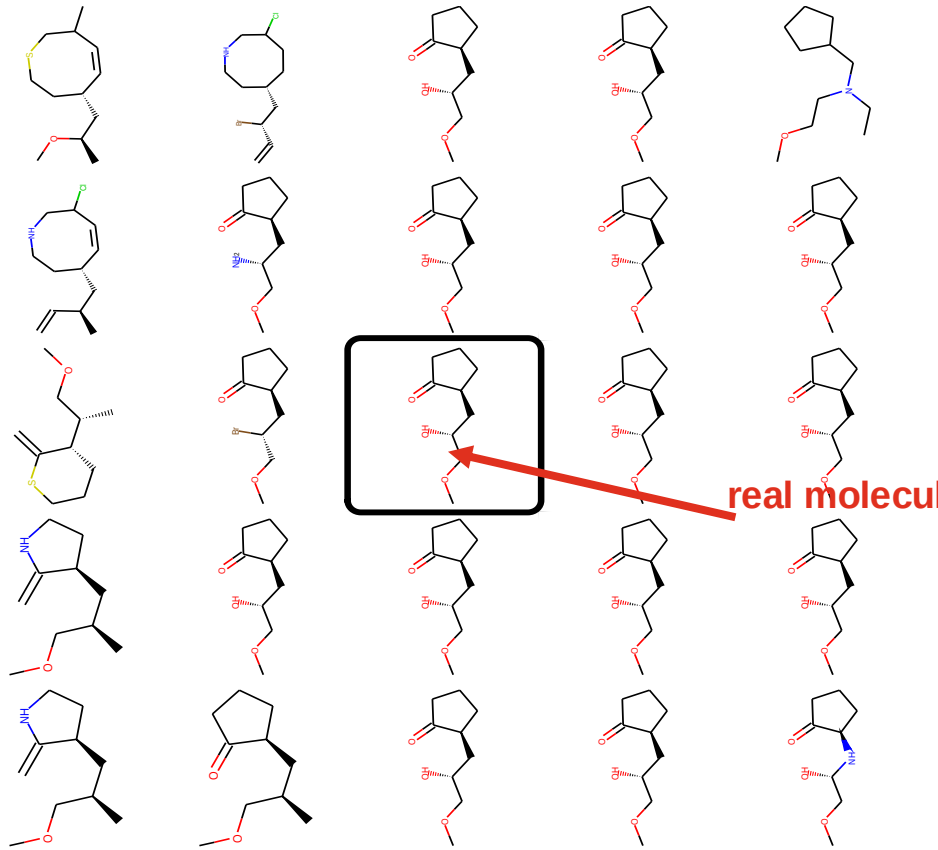

Kusner, Paige, and Hernández-Lobato (ICML 2017)

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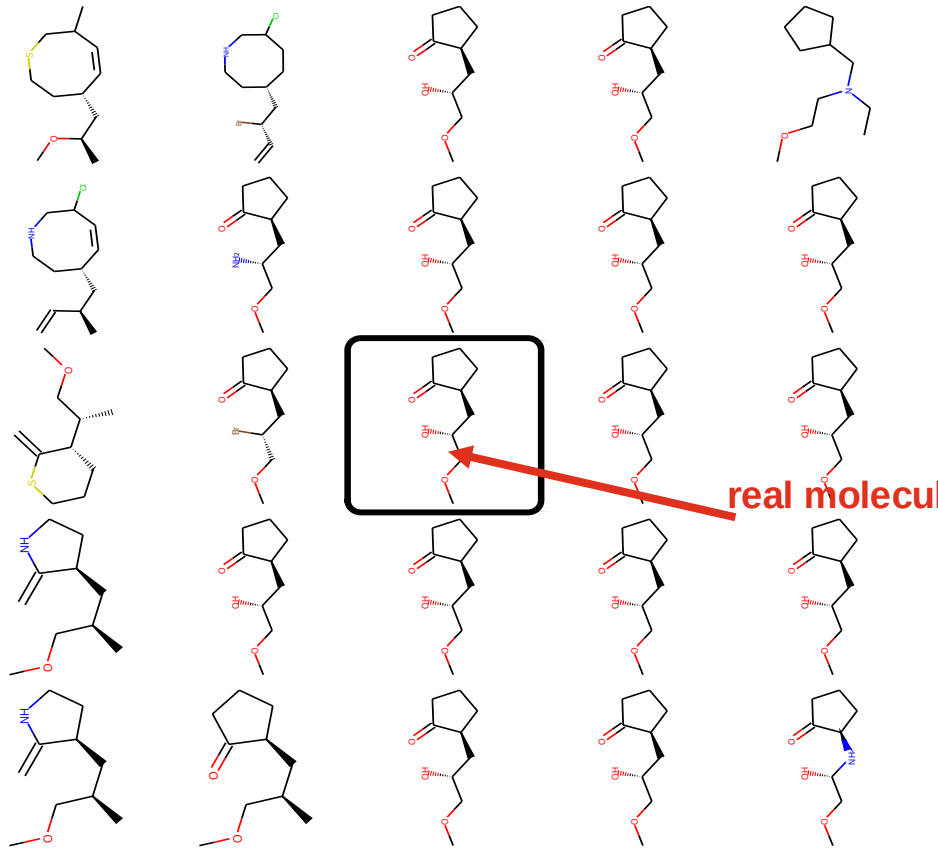

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2. Samples allow us to appximate integrals using Monte Carlo

$$\int f(x)p(x)dx \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

Monte Carlo basics

- Until now, we have written integrals as sums that we can compute exhaustively, but this is quite rarely the case.

- When this integral is an expected value over something we know how to sample from, we can use **simple Monte Carlo**

Algorithm 1 Simple Monte Carlo

1: Draw $X^{(1)}, ..., X^{(n)} \overset{i.i.d.}{\sim} p$
2: $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} f(X^{(i)})$

- Why are we expecting this to work?

Monte Carlo basics

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Proposition (Law of Large Numbers)**.**

$$\hat{\mu} \xrightarrow{a.s.} \mu \quad \textit{iff} \quad \mu \textit{ is finite}$$

Proposition (Central Limit Theorem)**.** *If* $\mathbb{V}ar(f(X)) = \sigma^2 < \infty$*, then*

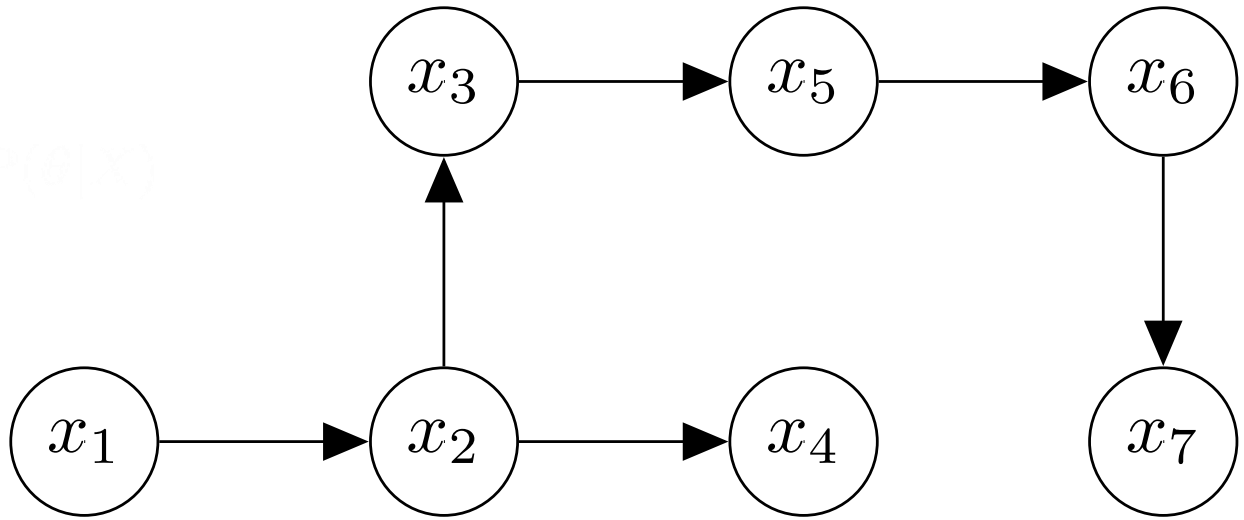
$$\sqrt{n}(\hat{\mu} - \mu) \xrightarrow{\mathcal{D}} \mathcal{N}(0, \sigma^2)$$

How to sample from a directed graph?

Algorithm 1 Ancestral sampling with topological ordering

for $i = 1$ to d **do**
  Draw z_i from $p(X_i = .|X_{\mathrm{pa}_i} = z_{\mathrm{pa}_i})$
end for
  return $(z_1, \ldots, z_d)$

We follow the ordering, sampling one descendant after the other…



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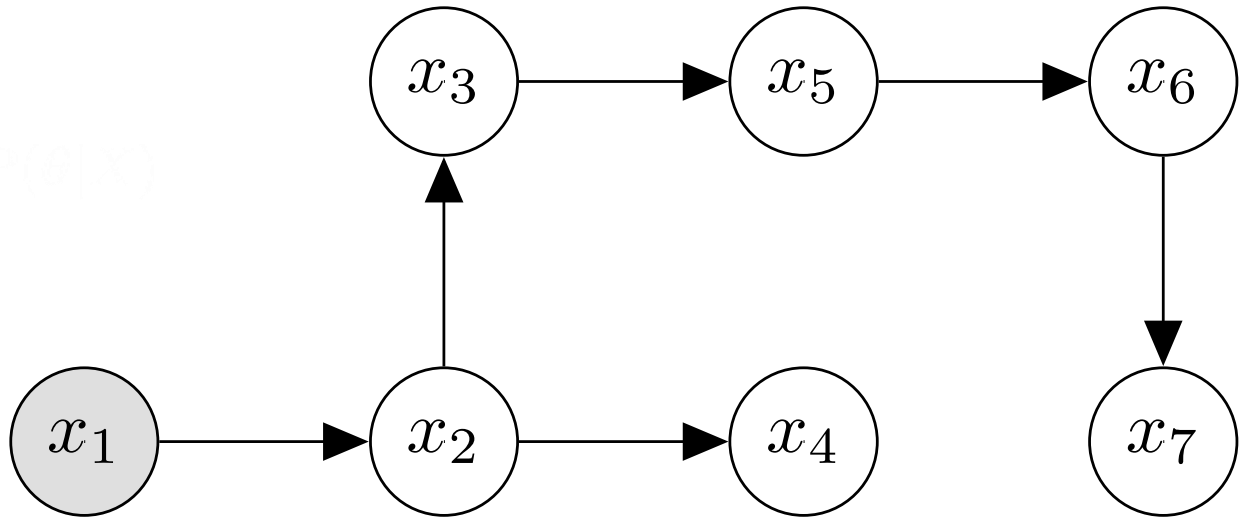

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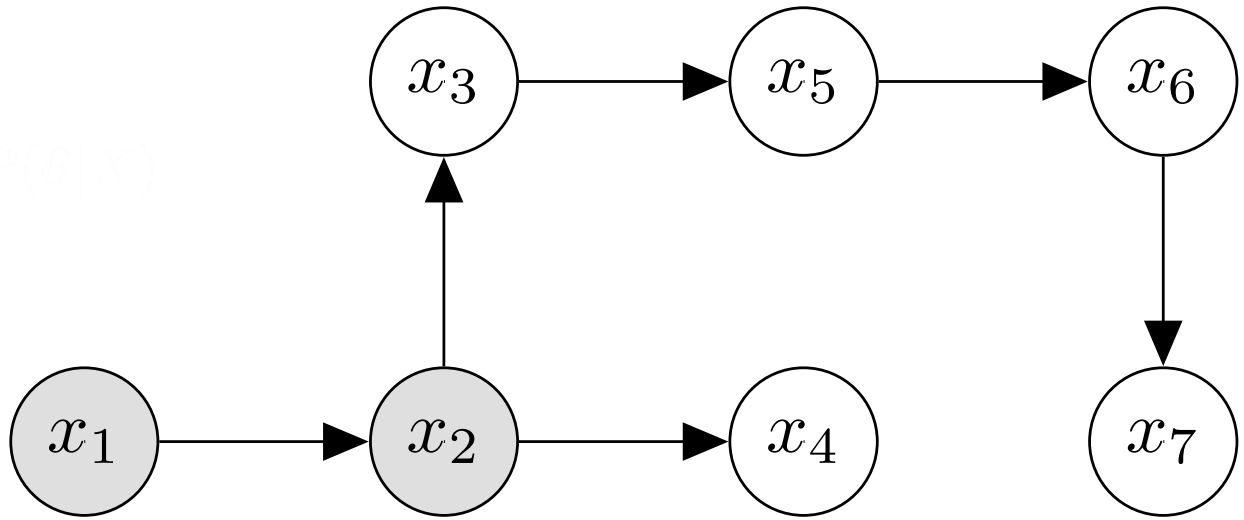

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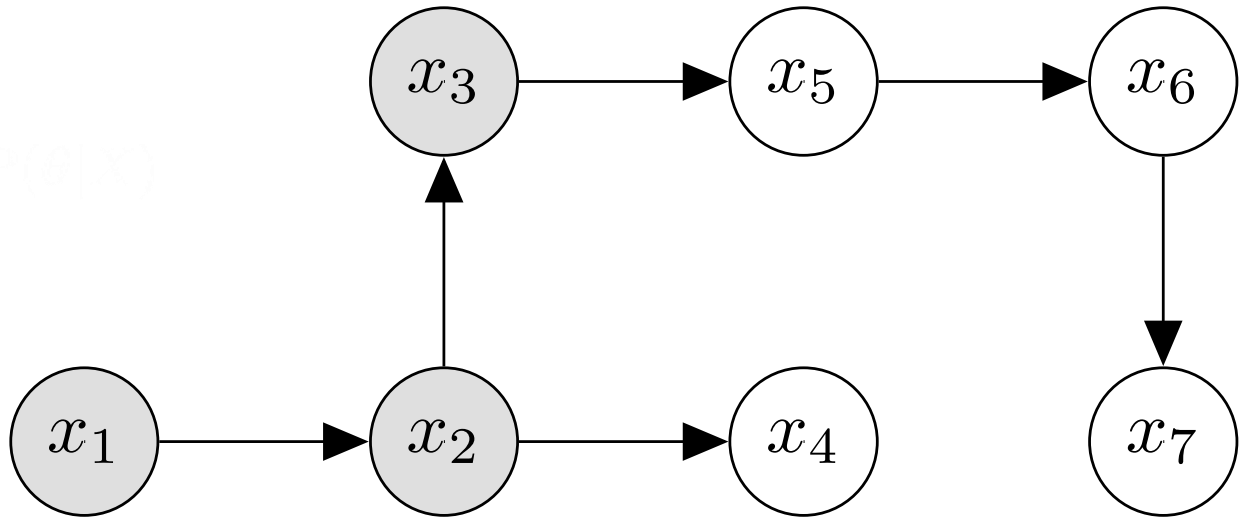

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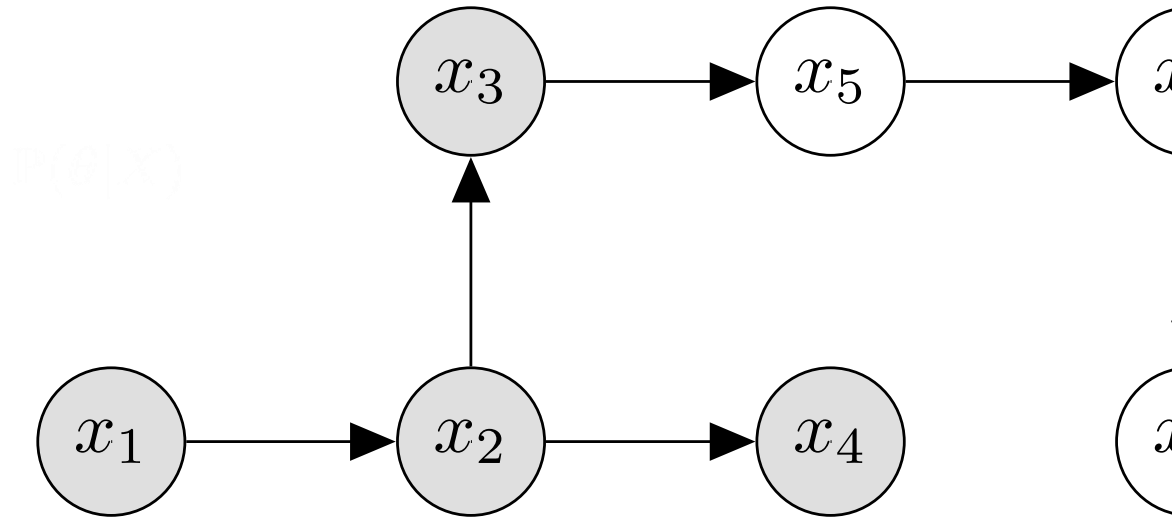

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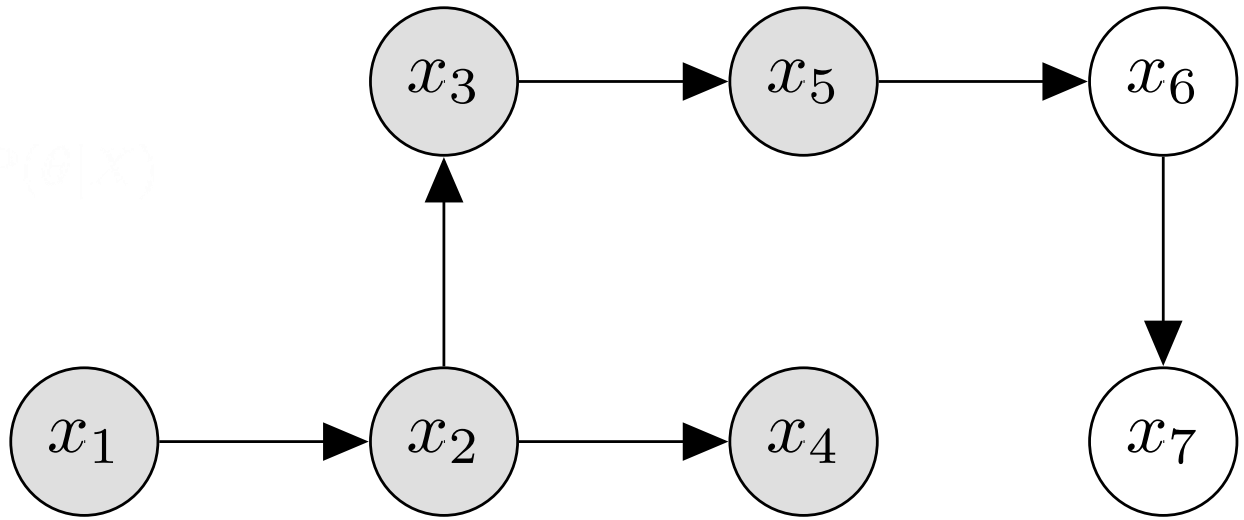

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  return $(z_1, \ldots, z_d)$

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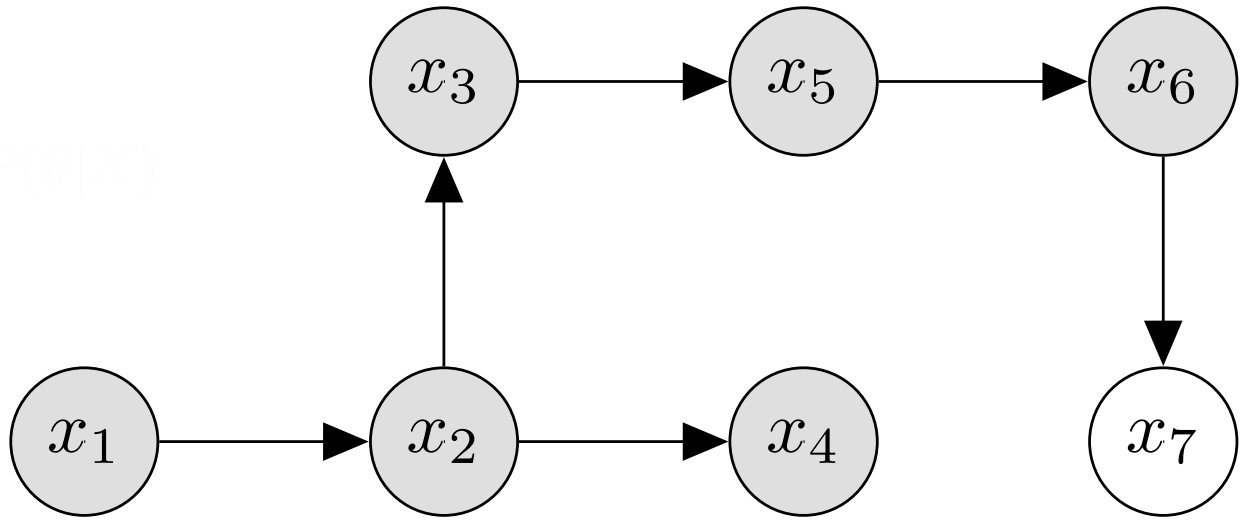

How to sample from a directed graph?

Algorithm 1 Ancestral sampling with topological ordering

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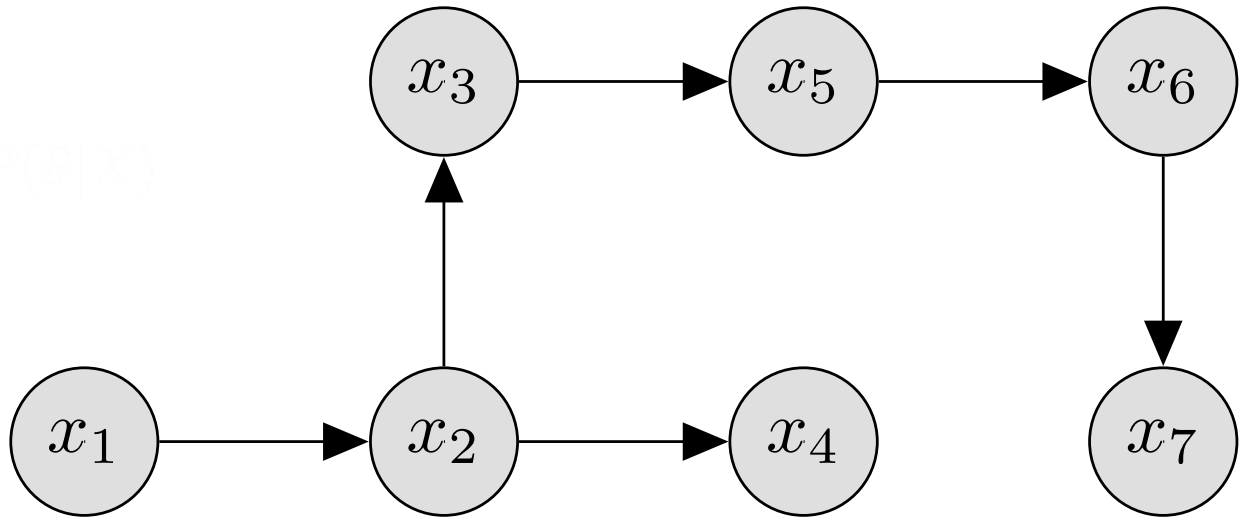

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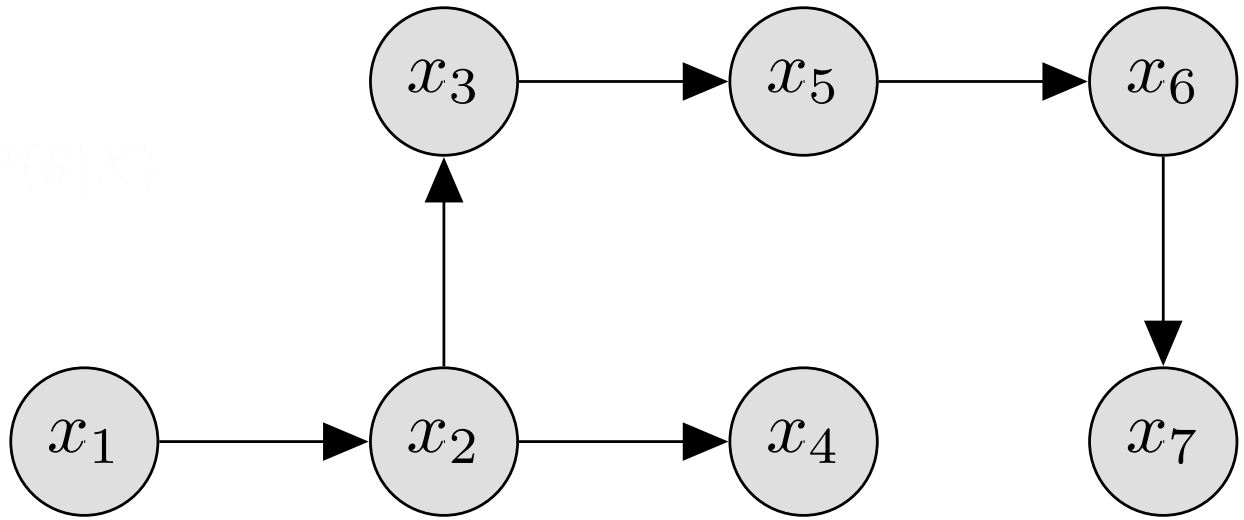

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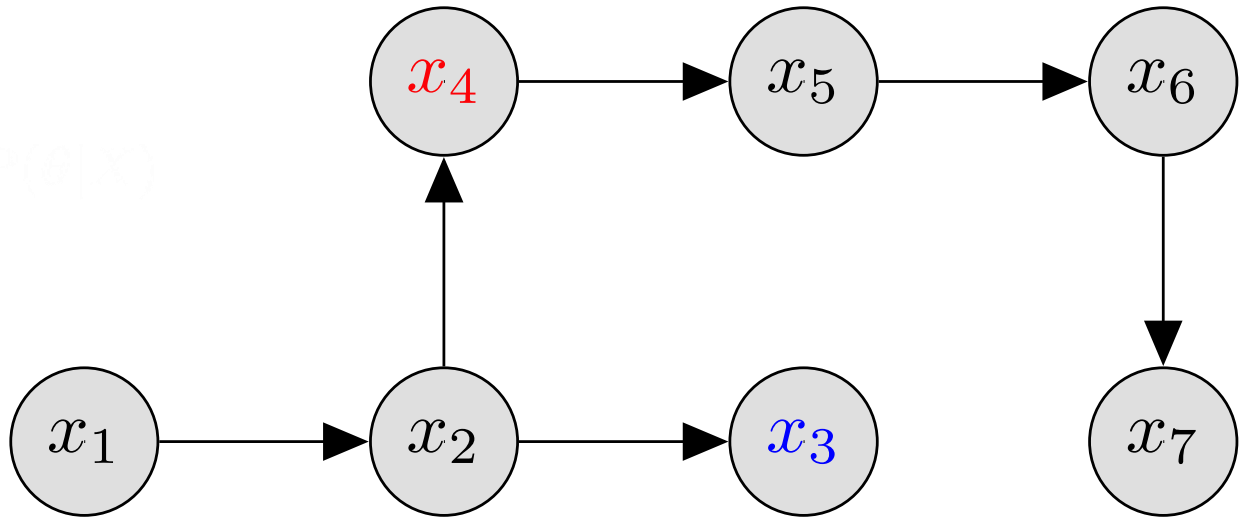

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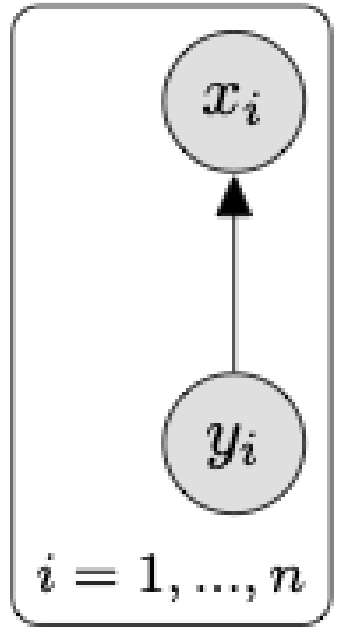
Proposition (ancestral sampling)**.** *Algorithm 1 provides samples from the joint distribution* $p(x_1, ..., x_d)$*.*

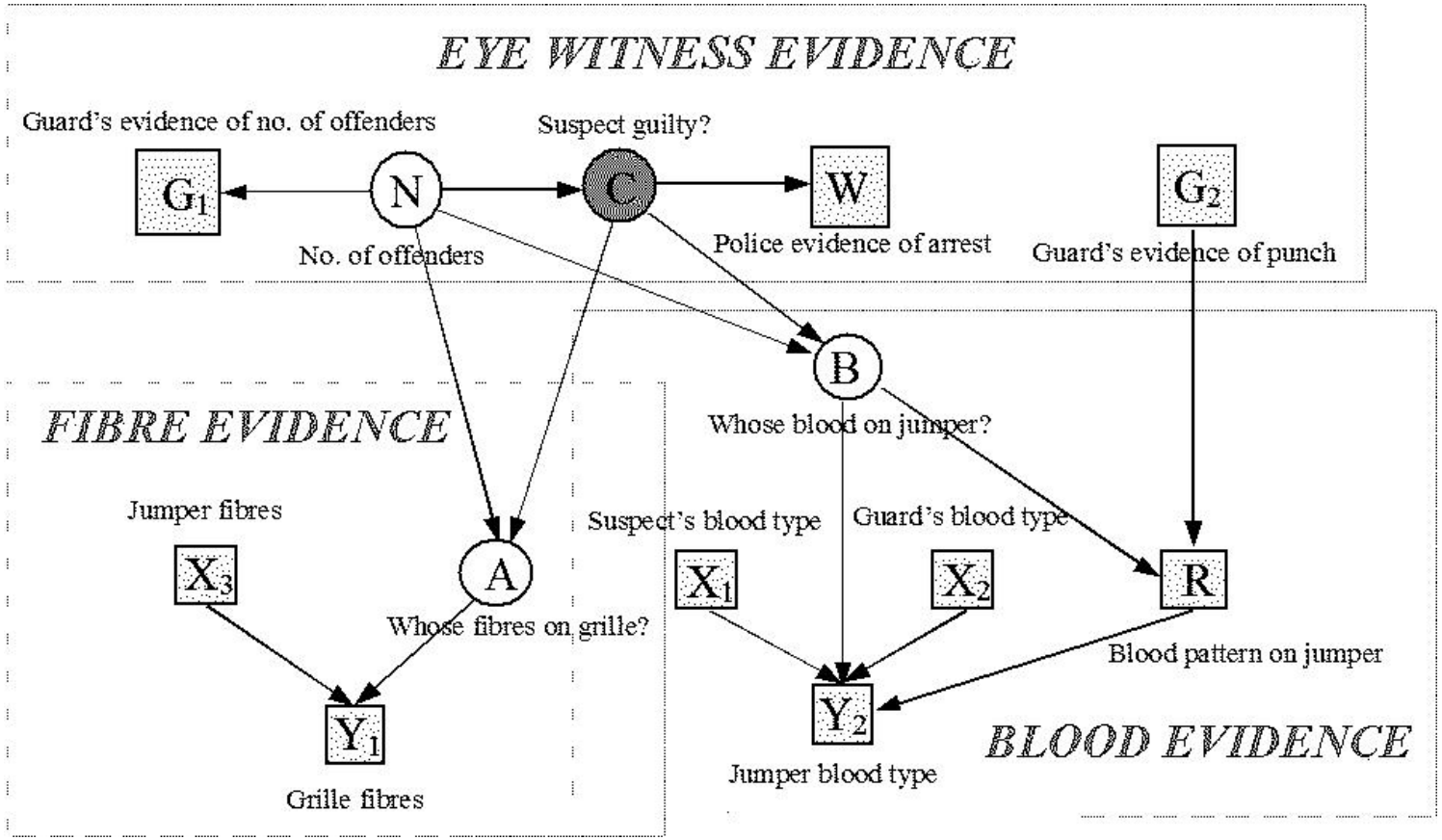
Proof. By induction on the topological ordering. □

Think of ways to implement this for some of the graphs we saw



Think of ways to implement this for some of the graphs we saw

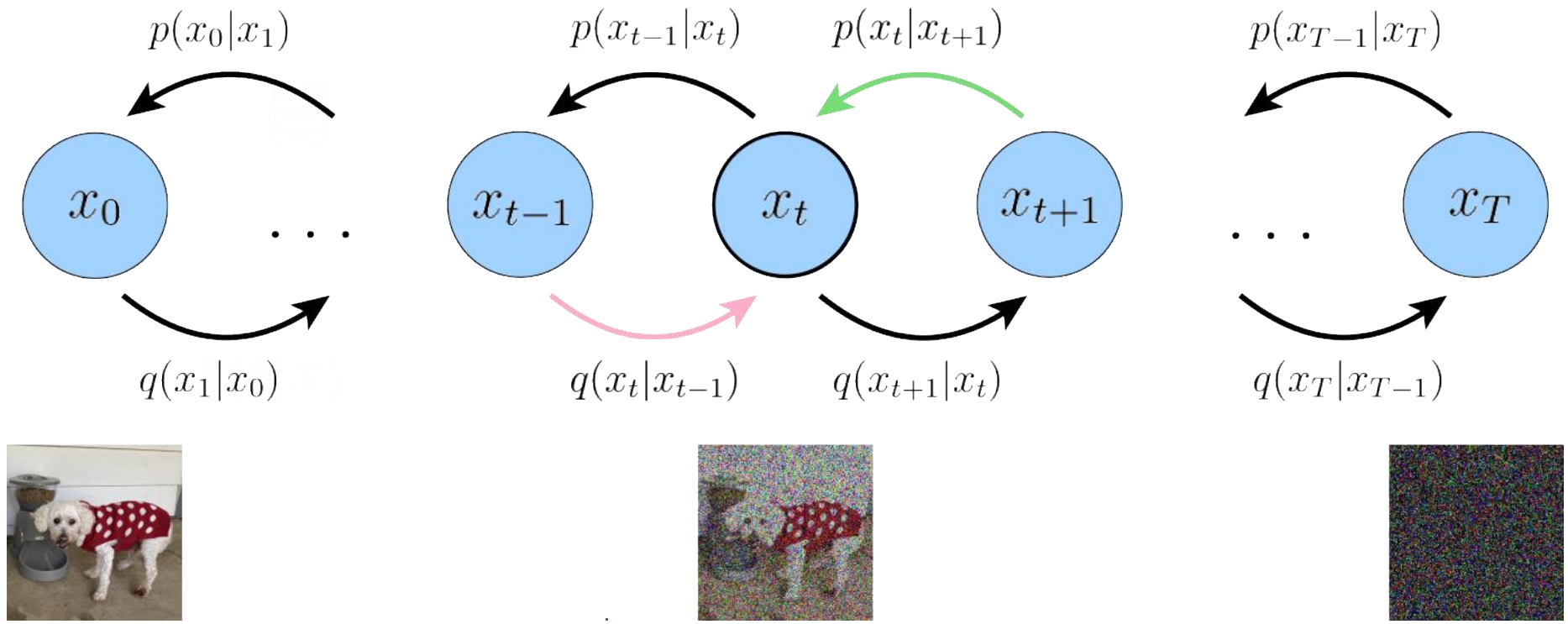
- The big graph from the forensic science example… Here the topological ordering is related to the time of the events…



Dawid and Evett, Using a graphical method to assist the evaluation of complicated patterns of evidence. Journal of Forensic Sciences, 1997

Think of ways to implement this for some of the graphs we saw

- Diffusion model (again, two DAGs!)



Luo, Understanding Diffusion Models: A Unified Perspective, arXiv preprint, 2022

4

Linear latent variable models
PPCA and friends

Why latent-variable models?

Let's assume that we have i.i.d. data $\mathbf{x}_1, \ldots, \mathbf{x}_n$ that live in a **high-dimensional space** $\mathcal{X}$ (for example images of newspaper articles).

Often, it is reasonable to assume that **these data essentially depend on a few important factors of variation:**

- if we have images of faces: size of nose, color of hair, glasses or not...
- if we have newspaper articles: topics of the paper, style...
- if we have molecules: physical properties, geometrical shape...

This assumption is the cornerstone of **latent variable models**, that assume that the data are governed by **unobserved random variables** $\mathbf{z}_1, \ldots, \mathbf{z}_n$ **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 $\mathbf{x}_i$.

Linear latent-variable models

In this slide, we assume that the data are continuous (i.e. $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^p$).

Factor analysis is probably one of the oldest latent variable models (studied since at least the 1940s). The generative process is:

- $\mathbf{z}_i \sim \mathcal{N}(0, \mathbf{I}_d)$,
- $\mathbf{x}_i | \mathbf{z}_i \sim \mathcal{N}(\mathbf{W}\mathbf{z}_i + \boldsymbol{\mu}, \boldsymbol{\Psi})$.

Probabilistic PCA (PPCA, Tipping and Bishop, JRSSB, 1999) is a a slightly less general model

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- For such models, performing maximum likelihood is not too hard:
  - EM algorithm for FA
  - Closed-form MLE for PPCA (based on the SVD of the data matrix)

From linear (« shallow ») to deep variable models

How do we transform this kind of model

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...into "something deep"?

We can replace the affine function $\mathbf{z} \mapsto \mathbf{W}\mathbf{z} + \mu$ by a neural net!

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).

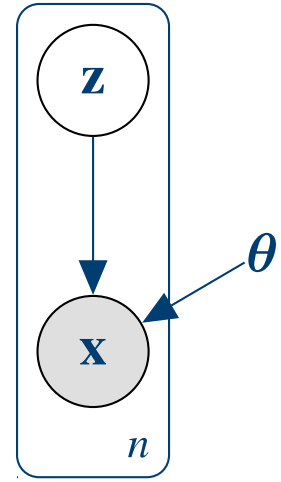
4

Deep latent variable models

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: back to PPCA

$$p(z) = \mathcal{N}(z|0, I_Q)$$

$$p_\theta(x|z) = \mathcal{N}(x|Wz + \mu, \sigma^2 I_D)$$

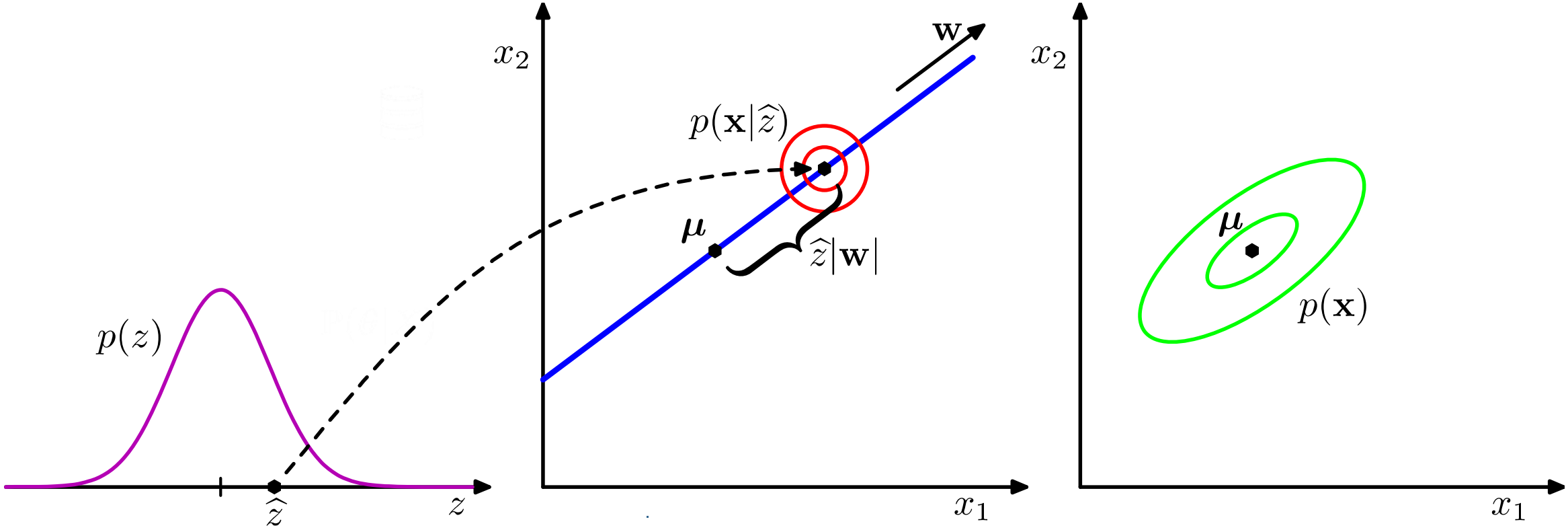


Fig. 12.9 in Bishop's Pattern Recognition and Machine Learning

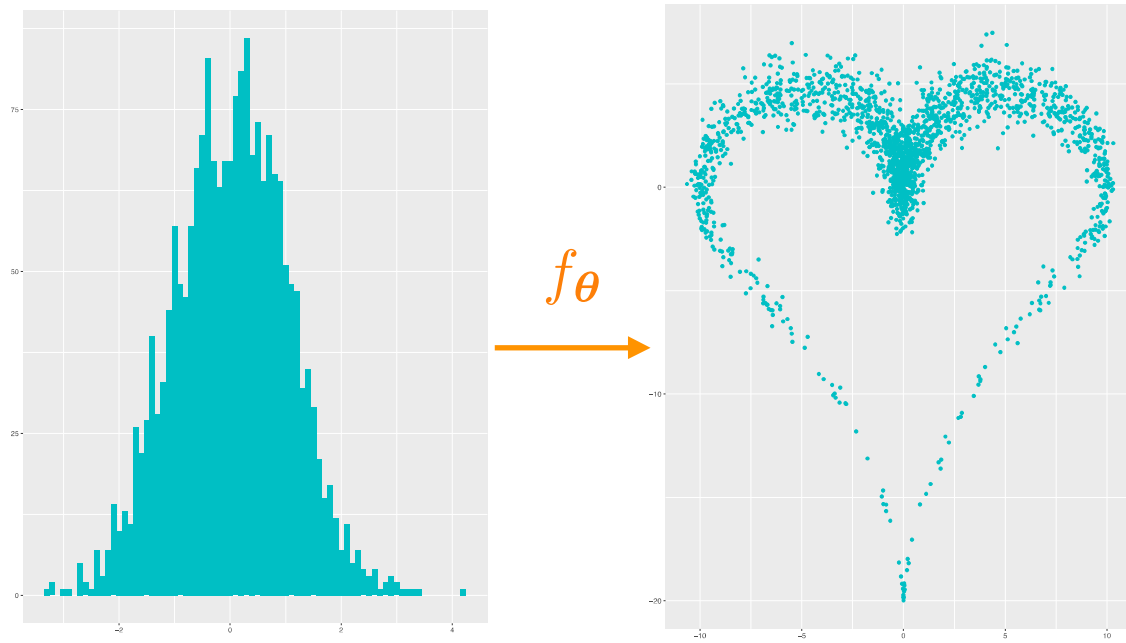
Deep latent variable models: the role of the decoder

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.

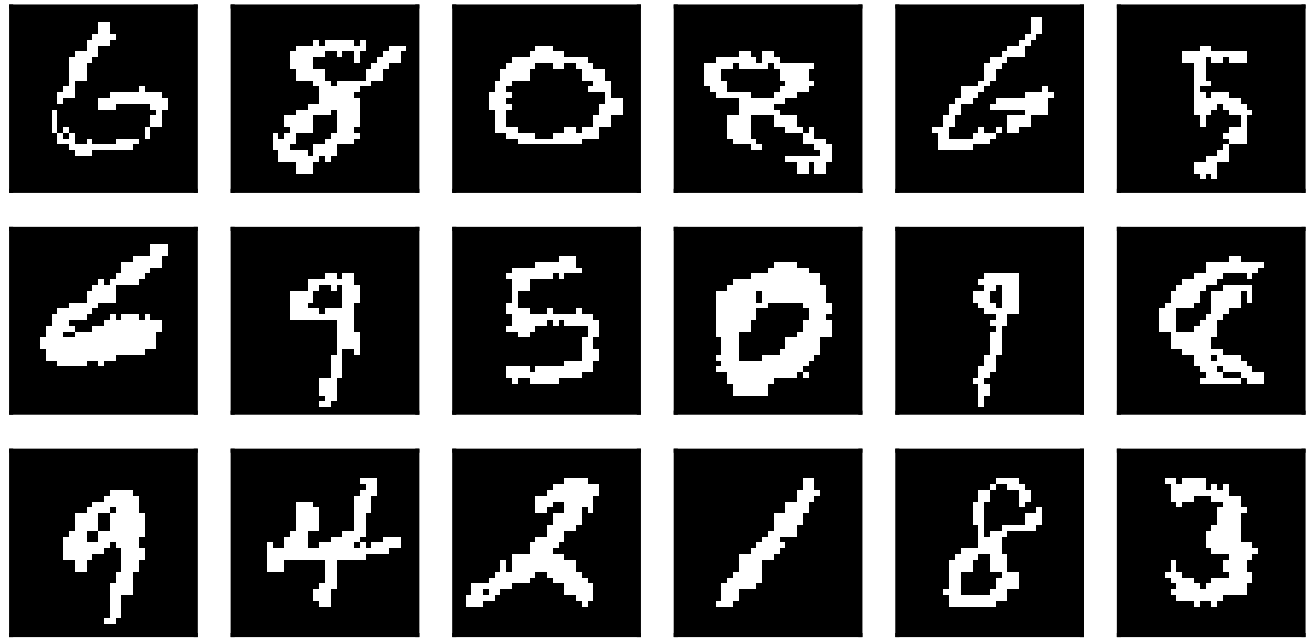
Simple non-linear decoder **($d = 1$, $p = 2$)**: $f_{\boldsymbol{\theta}}(z) = \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\Sigma}_{\boldsymbol{\theta}}(\mathbf{z})$ with, for all $z \in \mathbb{R}$,

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



Illustrative example of a DLVM for binary images

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



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

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

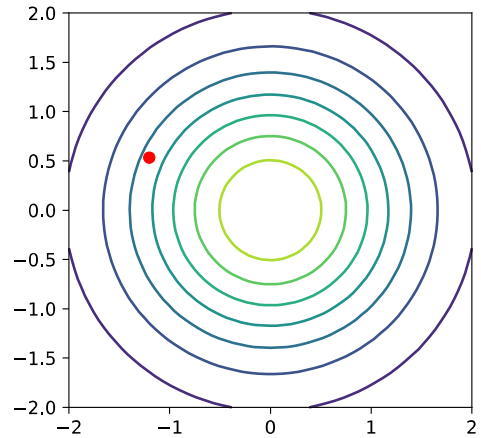
Decoder network

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

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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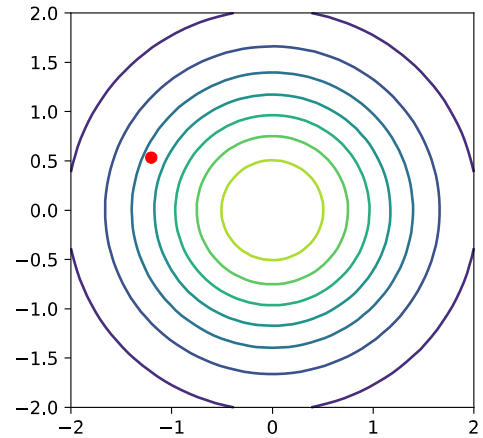
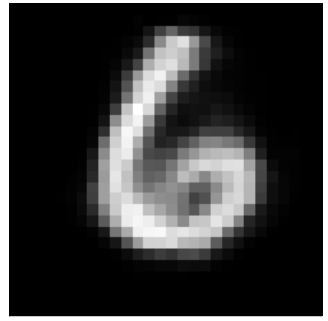


$f(\mathbf{z})$



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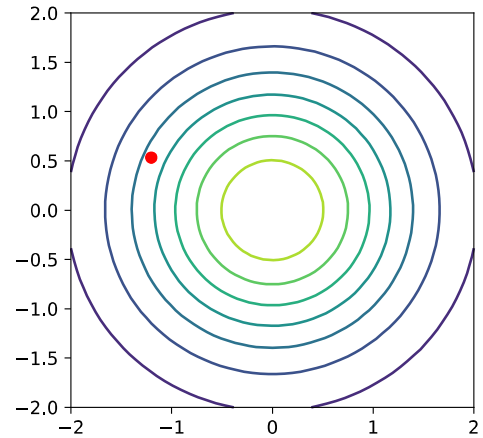

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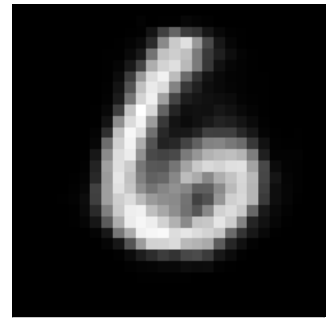

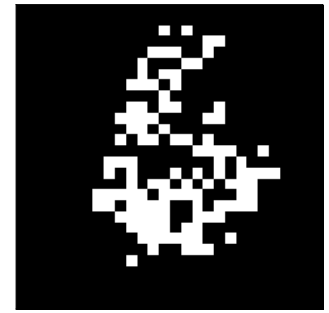

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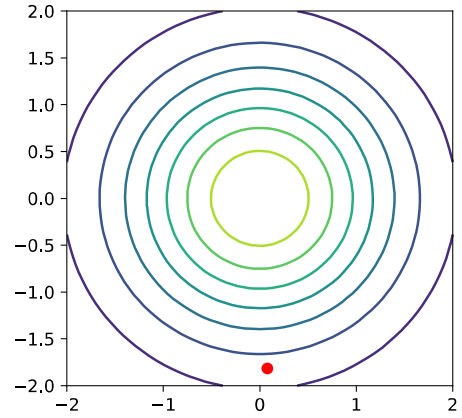
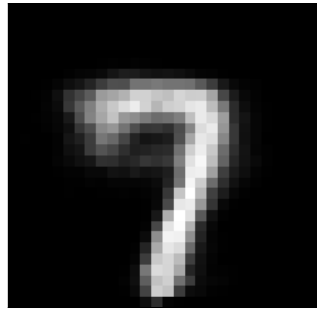


$f(z)$



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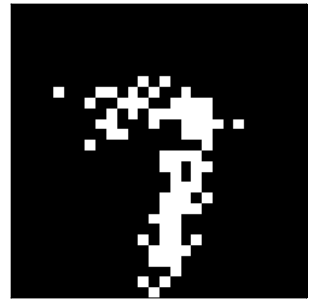

Maximum likelihood for DLVM

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

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

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

Maximum likelihood for DLVMs via importance sampling

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).**

Here, **I am going to derive this approach in a slightly different manner**, largely inspired by the following paper:

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

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: 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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- This estimate has nice properties:
  - Unbiasedness: $\mathbb{E}[\hat{I}_K] = I$
  - Consistency: $\hat{I}_K \xrightarrow{a.s.} I$
  - 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 $\mathbb{V}[\hat{I}_K] = \frac{1}{K}\mathbb{V}[f(x_1)]$

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 $\mathbb{V}[\hat{I}_K] = \frac{1}{K}\mathbb{V}[f(x_1)]$
- 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**

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

- 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*?**

Beyond simple MC: importance sampling

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

- 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*? Yes!**

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

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

Beyond simple MC: importance sampling

- This new estimate $\hat{I}_K^q$ is called an **importance sampling** estimate.
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- The variance will be $\mathbb{V}_{x\sim q}[f(x)p(x)/q(x)]/K$

Beyond simple MC: importance sampling

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- For $q^*(x) \propto f(x)p(x)$, **the variance will be exaclty zero!**
- **That seems a bit too good to be true… What's the catch?**

The optimal importance sampling proposal

- For $q^*(x) \propto f(x)p(x)$, **the variance will be exactly zero!**

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

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

… and I is precisely the thing we want to compute!

The optimal importance sampling proposal

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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

We want to approximate

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

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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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

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

$$q_i^*(\mathbf{z}) = p_\theta(\mathbf{z}|\mathbf{x}_i)$$

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

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

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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 !)
- 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 VAEs?

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!

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 $p_{\boldsymbol{\theta}}(\mathbf{z}_i|\mathbf{x}_i)$**.

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

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.

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

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

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- 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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- Note that the autoencoding process is stochastic, as it involves sampling $\mathbf{z} \sim q_{\boldsymbol{\gamma}}(\mathbf{z}|\mathbf{x})$

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

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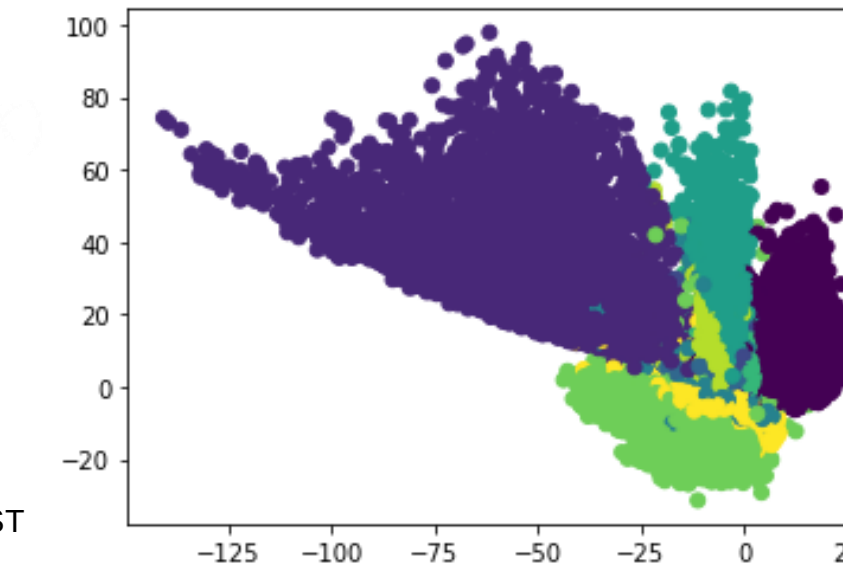

2D code space of a standard AE on MNIST

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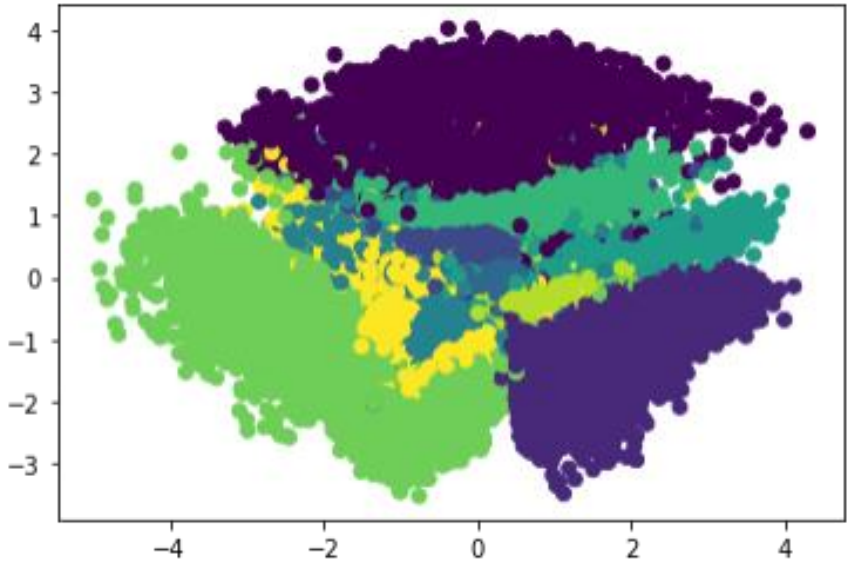

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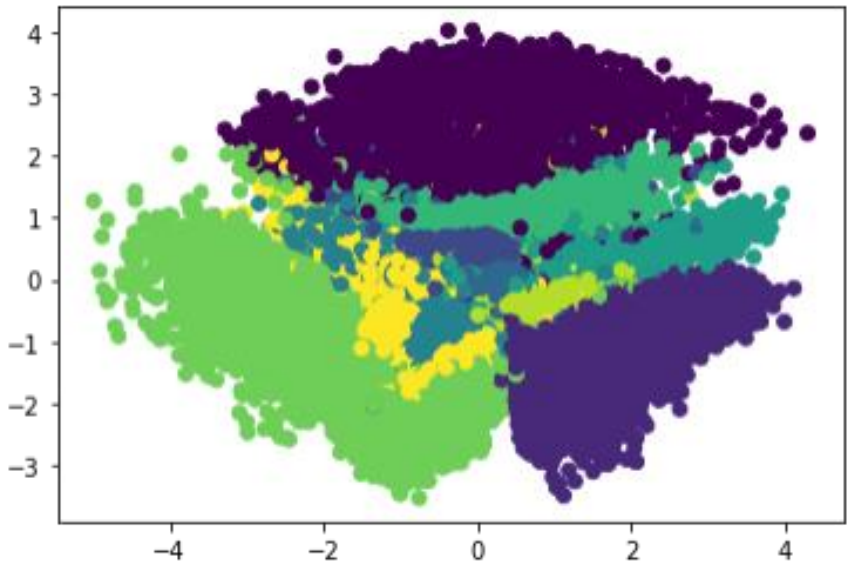

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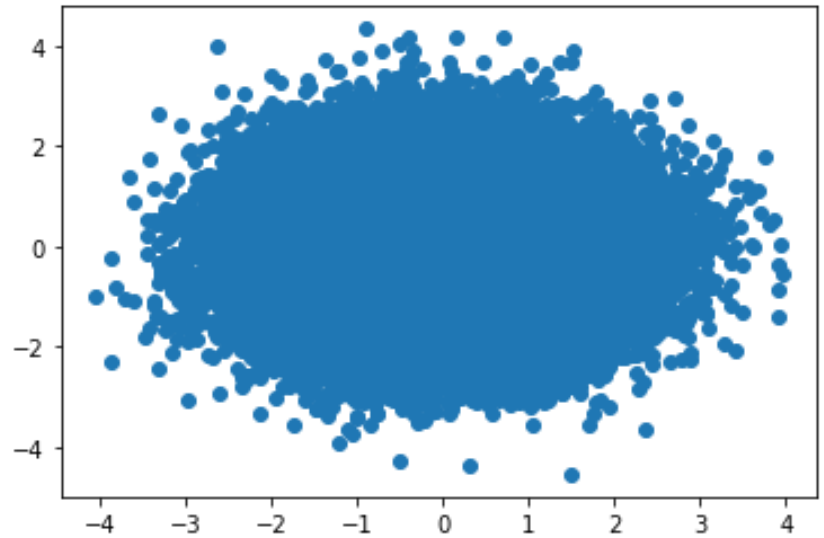

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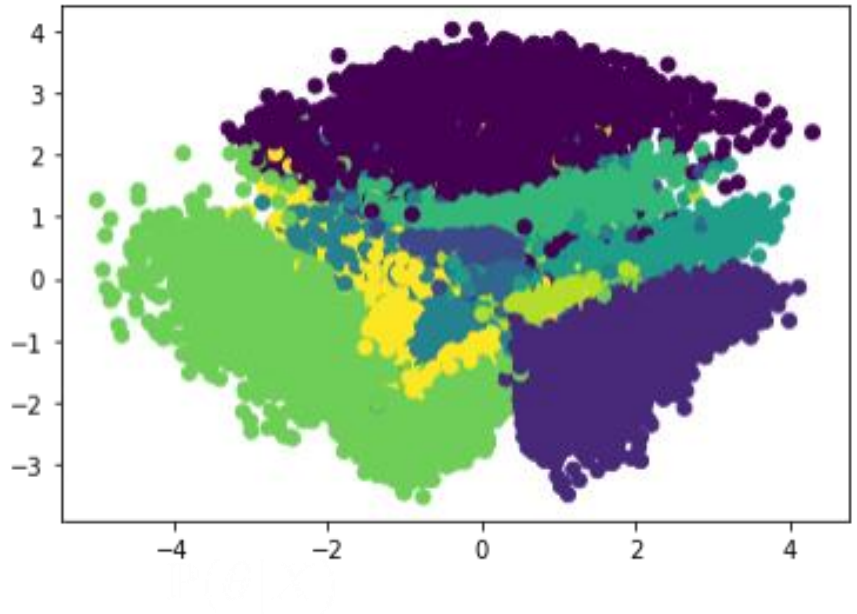

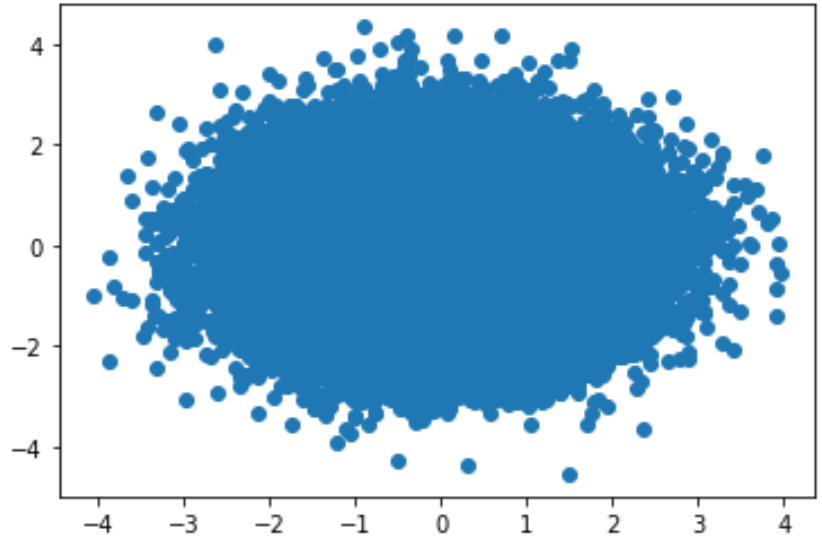

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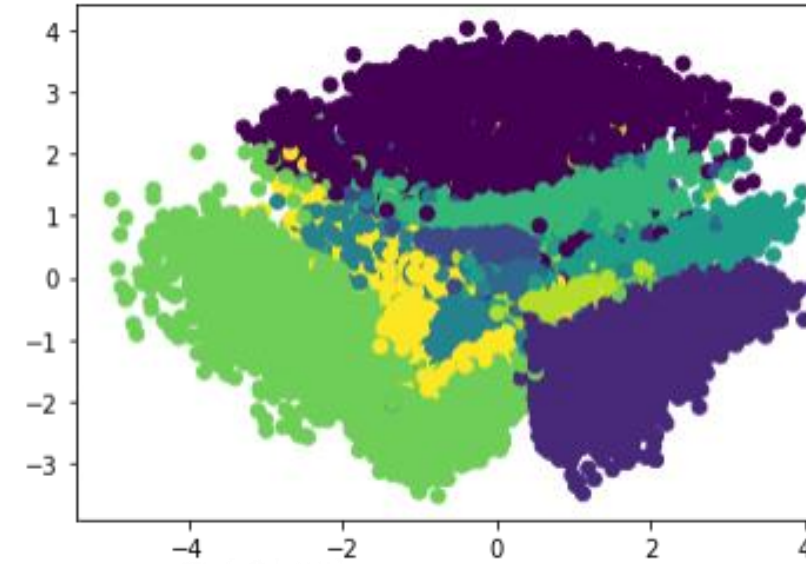

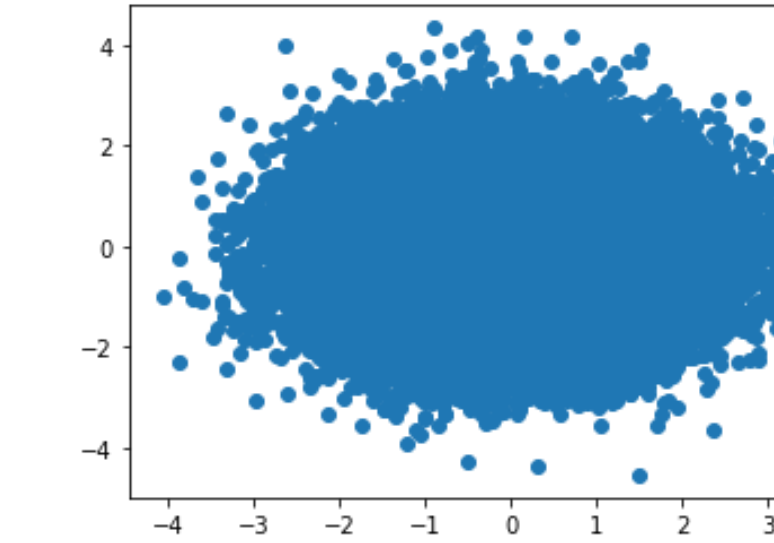

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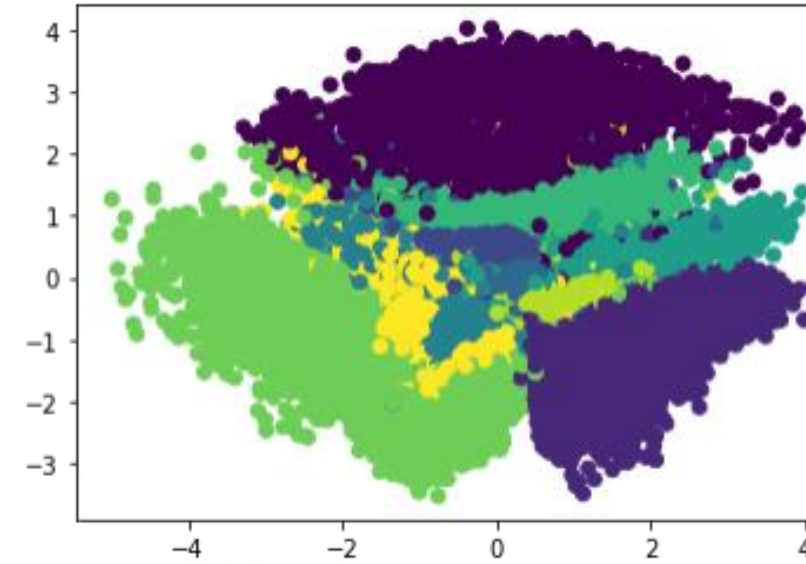

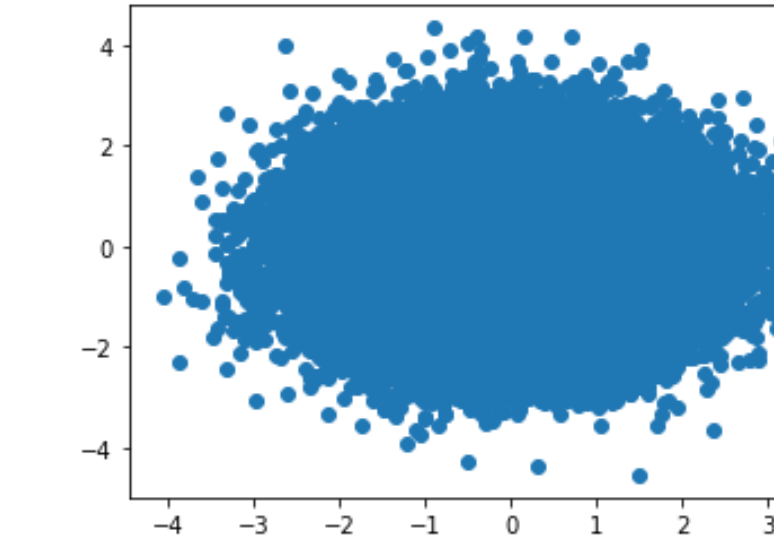

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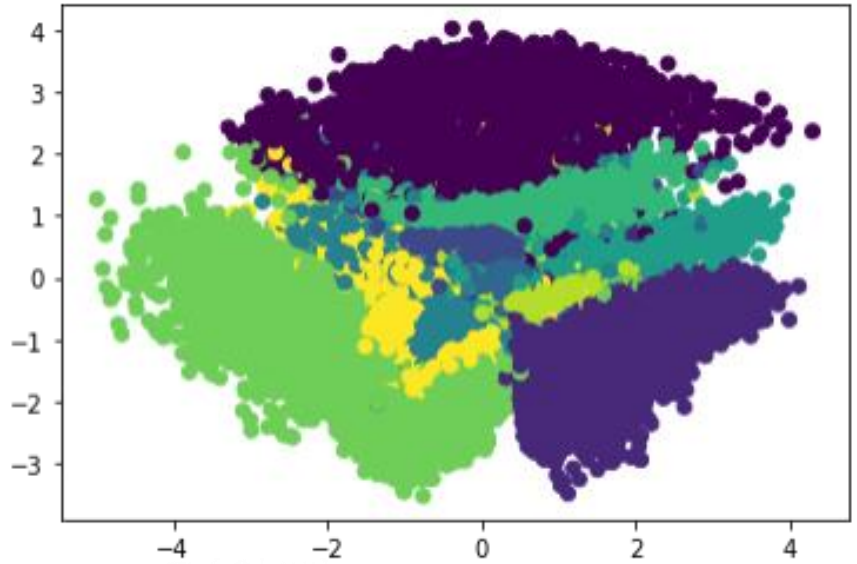

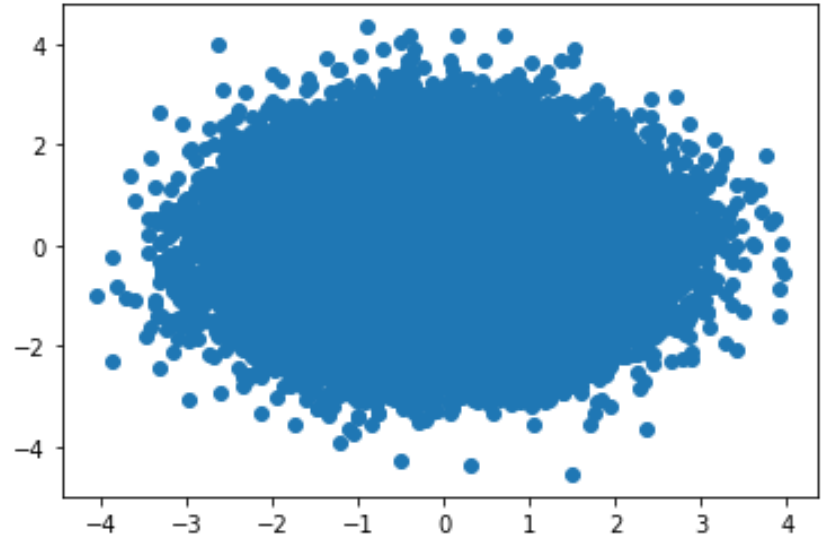

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More on this KL regulariser

- 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

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

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

- Not easy to generalise beyond Gaussians…

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

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- 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 $\nabla_{\boldsymbol{\theta},\boldsymbol{\gamma}} \mathcal{L}_K(\boldsymbol{\theta}, \boldsymbol{\gamma})$

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

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

- 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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Let's start with the easy part: ∇_θ

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

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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 $\mathbf{w}_1, \ldots, \mathbf{w}_K \sim \pi_{\boldsymbol{\gamma}}(\mathbf{w})$ 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:**

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

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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? The first one because it is an expectation!**

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

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- 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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- So, it's not an expected value, but we can turn it into one by dividing/multiplying!

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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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- Sampling $\mathbf{w} \sim \pi_{\boldsymbol{\gamma}}$ can be done by computing $$\mathbf{w} = \mu_{\boldsymbol{\gamma}} + C_{\boldsymbol{\gamma}} \boldsymbol{\varepsilon}$$

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- But now, the only random thing is $\boldsymbol{\varepsilon}$. This means we can rewrite our expectation as an expectation over $\boldsymbol{\varepsilon}$

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

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…and finally use Leibniz's rule

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

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

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- The estimate

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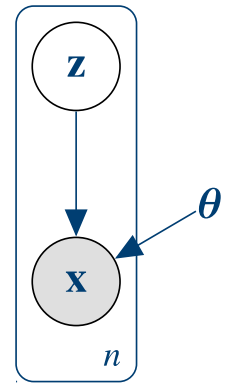
$$\approx \frac{1}{K} \sum_{k=1}^{K} \nabla_\gamma \left[g(\boldsymbol{\theta}, \boldsymbol{\gamma}, \mu_{\boldsymbol{\gamma}} + C_{\boldsymbol{\gamma}} \boldsymbol{\varepsilon}_k) \right]$$

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).