# Likelihood-based deep generative models

*beyond VAEs*

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# Recap from 2020…

- We saw together **how to use deep learning as a building block within generative modelling**
- In particular, we studied **deep latent variable models (DLVMs)** and **variational autoencoders (VAEs)** in depth
- You studied with Pr. Precioso many deep architectures, including **convolutional neural nets (CNNs)** and **recurrent neural nets (RNNs)**
- Today, **we will see how these architectures can be used to create deep generative models**

# What's a generative model?

- We have some data $x_1, \ldots, x_n \in \mathcal{X}$ from an unknown distribution $p_{\text{true}}$
- We want to learn a probability distribution $p_\theta$ such that $p_\theta \approx p_{\text{true}}$
- Why is this interesting to have access to $p_\theta(x)$?

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  - **We can generate new data points! …like images…**

**Images generated by a VAE**
Vahdat and Kautz (NeurIPS 2020)

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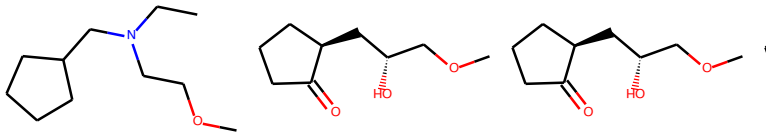
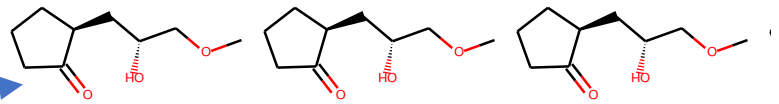
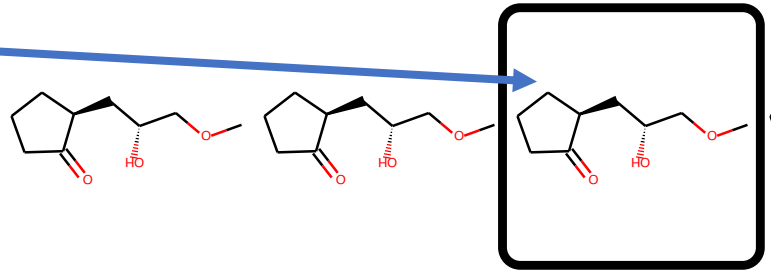
- Why is this interesting to have access to $p_\theta(x)$?
  - **We can generate new data points! …or molecules!**





molecules generated by a VAE

real molecule



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

# What's a generative model?

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- We want to learn a probability distribution $p_\theta$ such that $p_\theta \approx p_{\text{true}}$
- Why is this interesting to have access to $p_\theta(x)$?
  - It can allow to **assess uncertainty!**

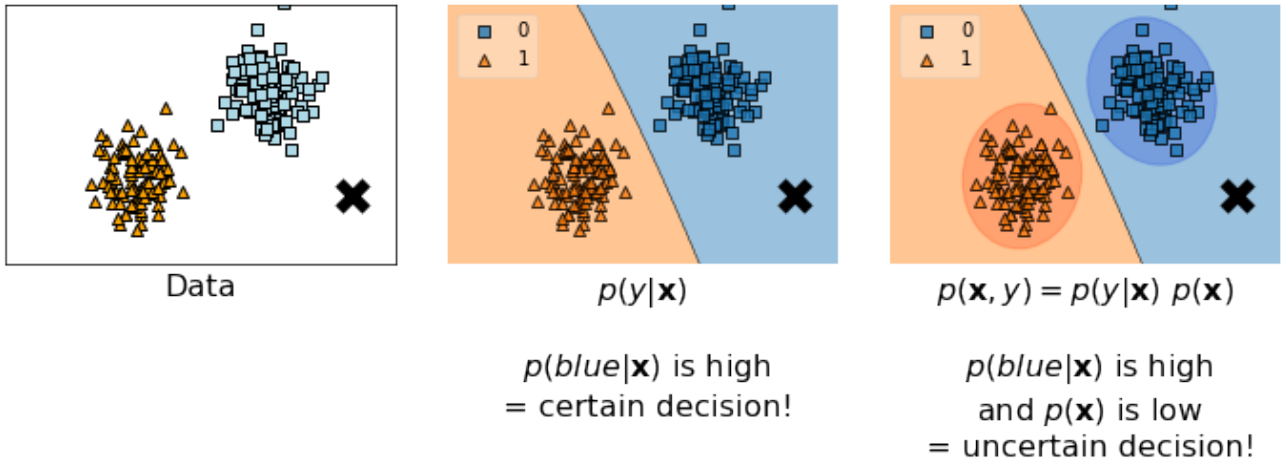


Fig. from Jakub Tomczak's blog

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- We want to learn a probability distribution $p_\theta$ such that $p_\theta \approx p_{\text{true}}$
- Why is this interesting to have access to $p_\theta(x)$?
  - **It can be used to handle missing data!**

Single imputation with a VAE

Multiple imputation with a VAE

Mattei and Frellsen (ICML 2019)

# How to train generative models?

- We have a family of probability distributions $\left(p_\theta(x)\right)_{\theta \in \Theta}$
- We want to find the **right** $\theta$ in order to have $p_\theta \approx p_{\text{true}}$

- What techniques do you know to do this?

# How to train generative models?

- We have a family of probability distributions $(p_\theta(x))_{\theta \in \Theta}$
- We want to find the **right** $\theta$ in order to have $p_\theta \approx p_{\text{true}}$

- What techniques do you know to do this?
- **Maximum likelihood** chooses

$$\hat{\theta} = \text{argmax}_\theta \log p_\theta(x_1, ..., x_n)$$

- We'll focus today on maximum likelihood techniques, but there are alternatives, for example **adversarial training (cf GANs)** or **score matching**

# Recap: Information-theoretic foundations of maximum likelihood

- Why is maximum likelihood a decent idea?

- We want to have $p_\theta \approx p_{\text{true}}$

- We can measure the distance between these two distributions using the **Kullback-Leibler divergence**.

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

# Recap: Information-theoretic foundations of maximum likelihood

- In the case of iid data, maximum likelihood becomes

$$\hat{\theta} = \text{argmax}_\theta \sum_{i=1}^{n} \log p_\theta(x_i)$$

- We saw in a previous lecture that, when *n* goes to infinity

$$\text{argmax}_\theta \sum_{i=1}^{n} \log p_\theta(x_i) \approx \text{argmin}_\theta \text{KL}(p_{\text{true}} || p_\theta)$$

- This means that **max. likelihood will asymptotically find the closest model to the truth** (in terms of KL divergence).

# Recap: maximum likelihood in practice

- In the case of iid data, maximum likelihood becomes

$$\hat{\theta} = \text{argmax}_\theta \sum_{i=1}^{n} \log p_\theta(x_i)$$

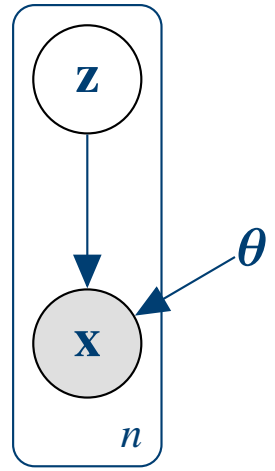
- Maximising a sum of many differentiable functions can be done efficiently via **stochastic gradient techniques** (e.g. Adam).

- We therefore mainly need to be able to compute efficiently $\nabla_\theta \log p_\theta(x_i)$
- Problem: when the model is complex, computing this is difficult!

# Recap: deep latent variable models and VAEs

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)

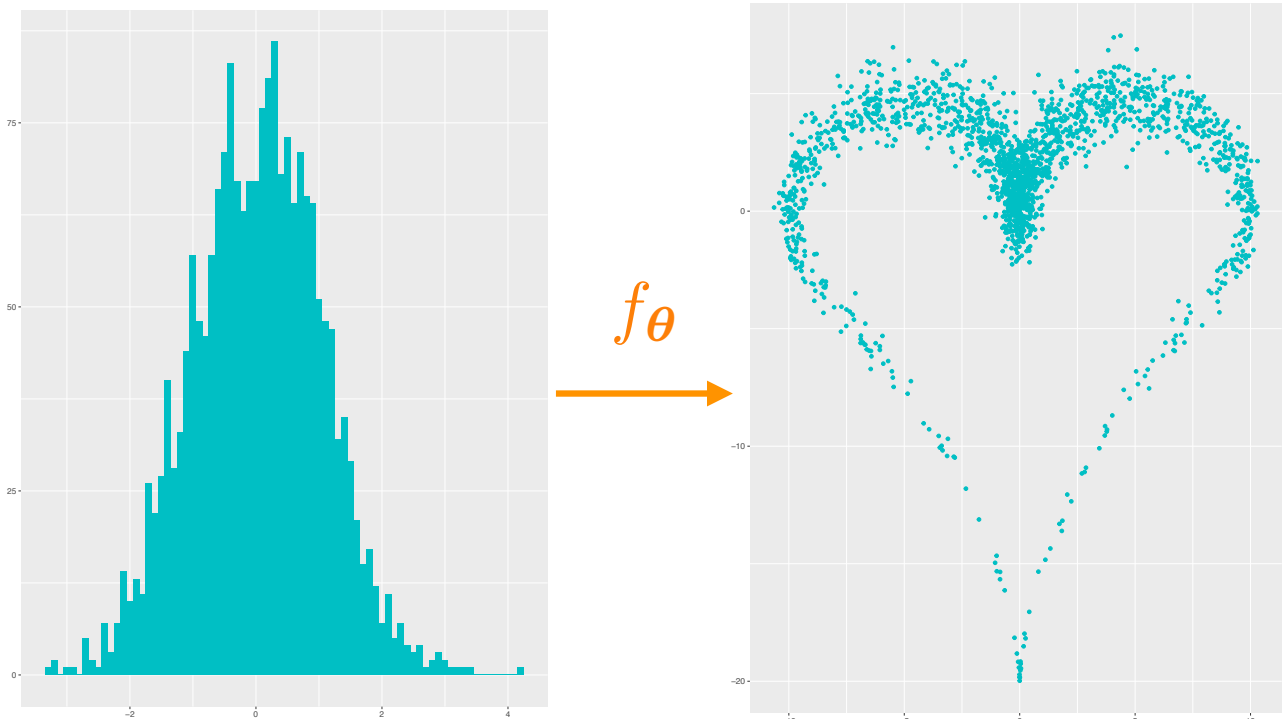
# Recap: deep latent variable models and VAEs

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

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

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

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



# Recap: deep latent variable models and VAEs

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

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

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

**Decoder network**

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

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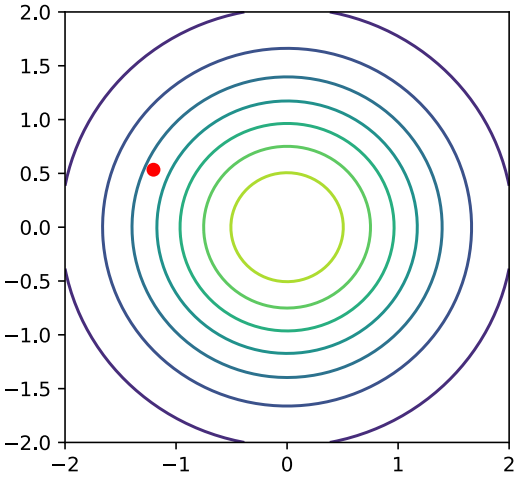
$$\mathbf{z} \sim \mathcal{N}\left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

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

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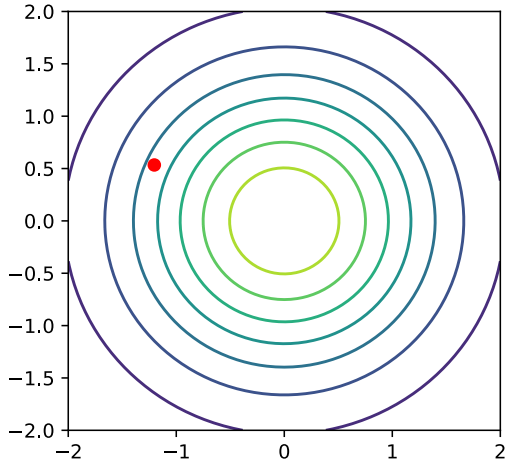


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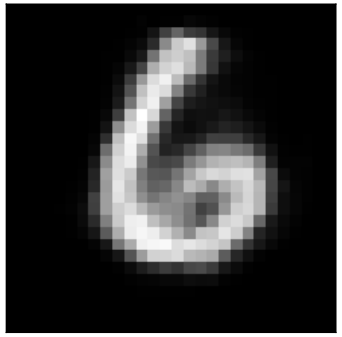

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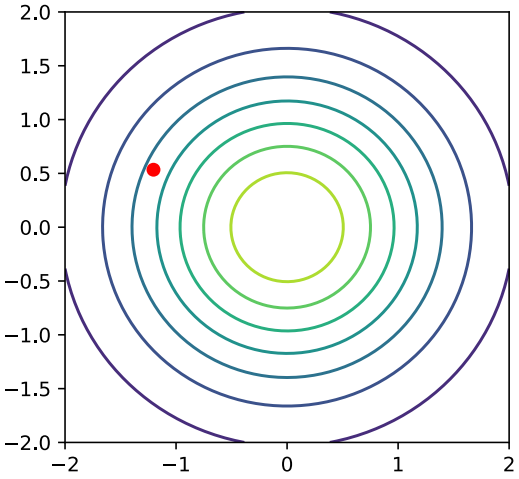


$$x^{j,k} \sim \text{Bern}(f^{j,k}(\mathbf{z}))$$

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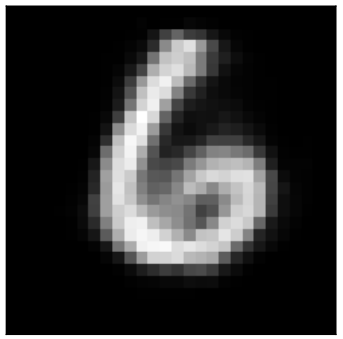

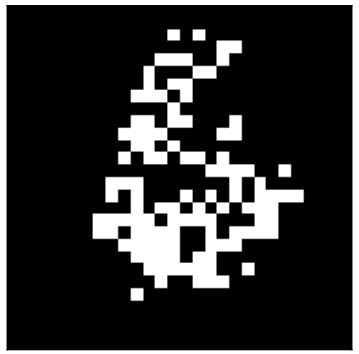

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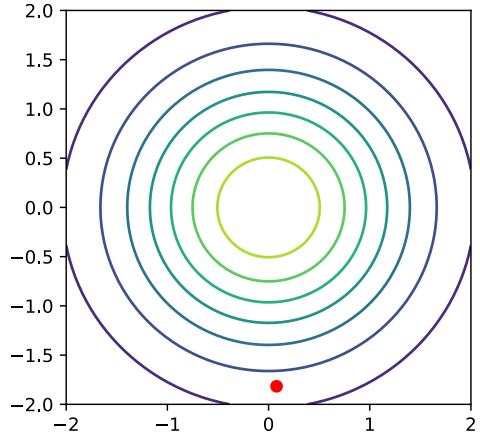


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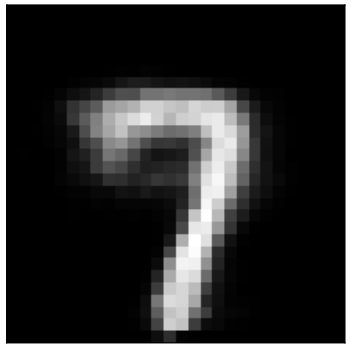
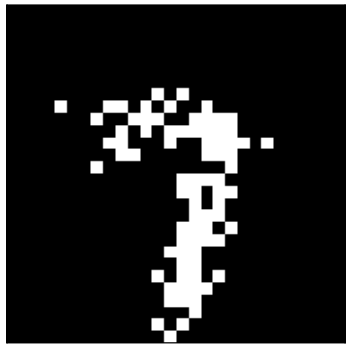


$x^{j,k} \sim \text{Bern}(f^{j,k}(z))$



# Recap: VAE training

- The likelihood is equal to $\ell(\boldsymbol{\theta}) = \log p_{\boldsymbol{\theta}}(\mathbf{X}) = \sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\mathbf{x}_i),$

which is full of the nasty intractable integrals

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

- How did we manage to train the model?

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- **How did we manage to train the model?**

# Recap: IWAE training of DLVMs

- We maximised an **approximation of the likelihood**, computed using an **encoder**

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

- This approximation also happens to be a **lower bound** of the likelihood that becomes tighter and tighter

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

- The case *K=1* corresponds to the original VAE bound.

# Going beyond VAEs

- One issue with VAEs is that we can't compute the likelihood exactly, but have to rely on approximations

- We will see other families of models where **we can compute the likelihood exactly**

- The two families we'll focus on will be **autoregressive models** and **normalising flows**

# Autoregressive models

- We want to find a way to design a flexible $p(\mathbf{x}) = p(x_1, ..., x_d)$ that we can still compute exactly.

- The main idea is to use probability chain rule

$$p(\mathbf{x}) = p(x_1, ..., x_d) = p(x_1)p(x_2|x_1)...p(x_d|x_1, ..., x_{d-1})$$

which may be rewritten

$$p(\mathbf{x}) = \prod_{j=1}^{d} p(x_j|x_1, ..., x_{j-1})$$

# Autoregressive models

- We will use neural nets to model the predictive distribution

$$p_\theta(x_j|x_1, \ldots, x_{j-1})$$

- For example, this could be modelled using a recurrent network (like a LSTM) or even a CNN with some masking

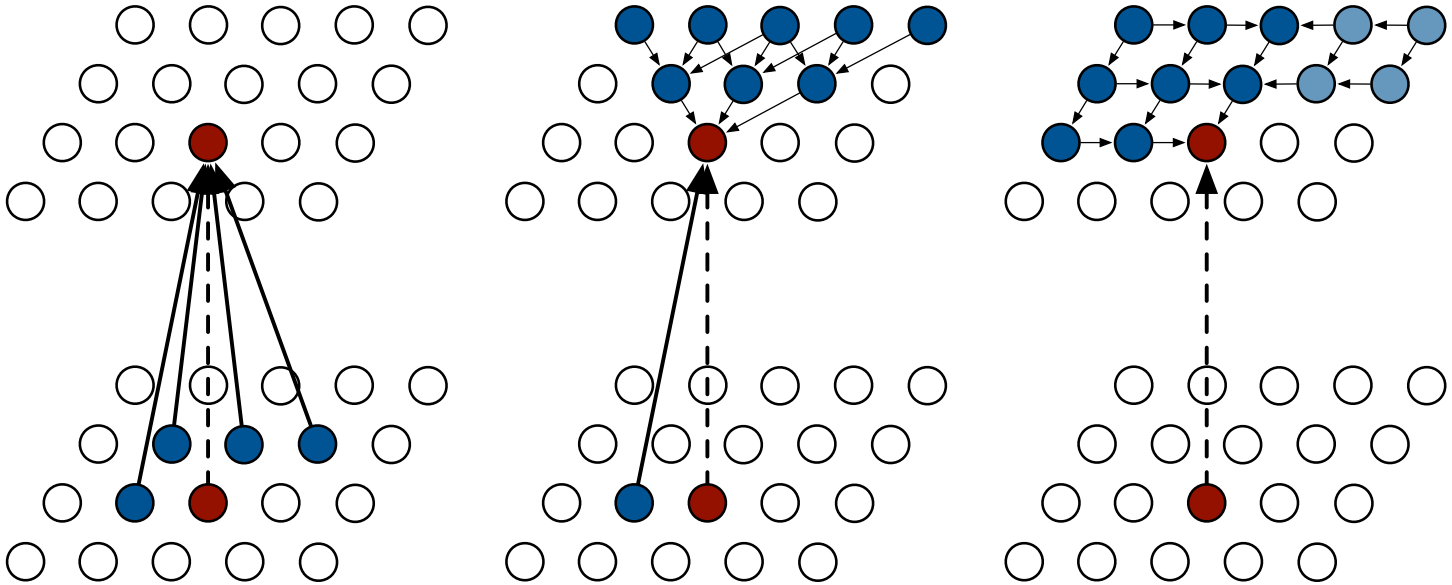
- At the end, **we can compute the likelihood of a single x exactly**

$$p_\theta(\mathbf{x}) = \prod_{j=1}^{d} p_\theta(x_j|x_1, \ldots, x_{j-1})$$

# Autoregressive models: examples

- We have a lot of freedom to choose the neural net that parametrises

$$p_\theta(x_j | x_1, \ldots, x_{j-1})$$



PixelCNN Row LSTM Diagonal BiLSTM

(van den Oord et al., ICML 2016)

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*Figure 1.* Image completions sampled from a PixelRNN.

(van den Oord et al., ICML 2016)

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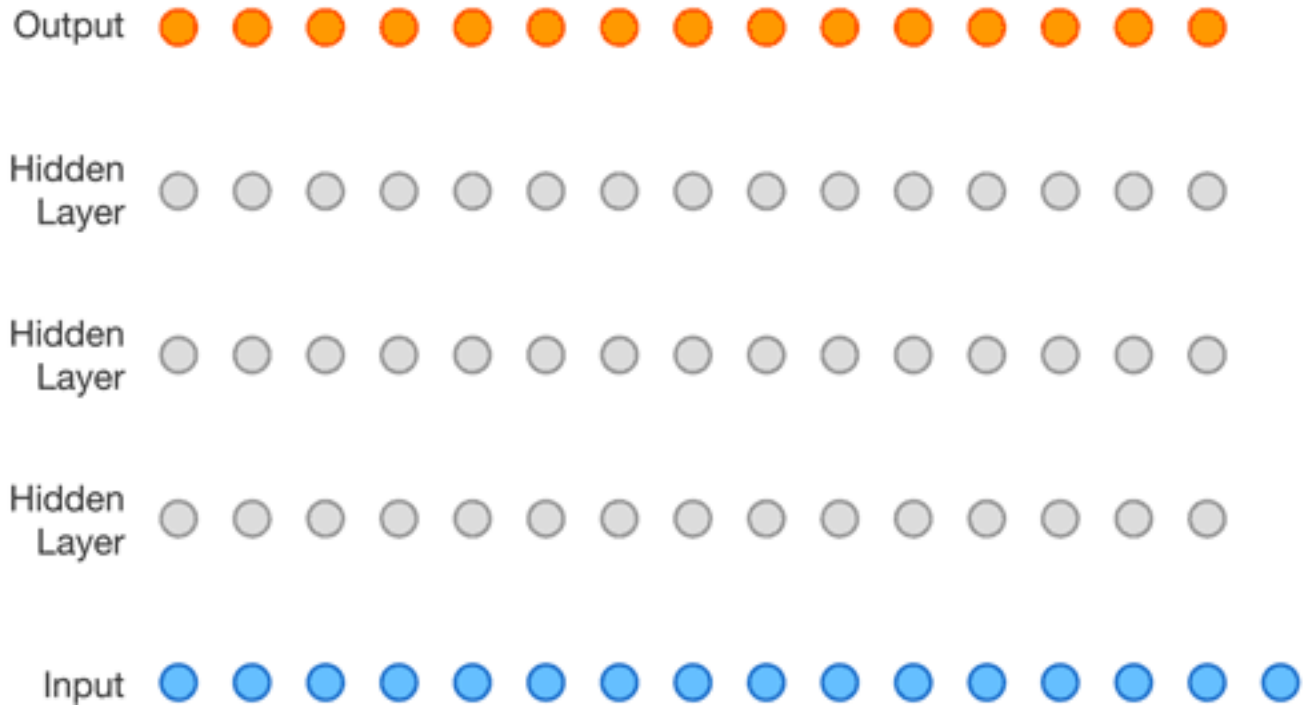


CNN architecture from van den Oord et al. (WaveNet: A Generative Model for Raw Audio, 2016)

# Normalising flows

- Key idea: sample from a simple distribution, and then pass the samples through an **invertible neural net** $f_\theta(z)$

$$z \sim p(z),\ x = f_\theta(z)$$

- It looks a lot like VAEs except that
  - **The "code" has same dimension as the data (to ensure invertibility)**
  - **The likelihood can be computed exactly** using the change of variable formula

$$p_X(\mathbf{x}) = p_Z(z) \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right|^{-1}$$

# Normalising flows

- The fact that the network is invertible allows us to use the change of variable formula

$$p_X(\mathbf{x}) = p_Z(z) \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right|^{-1}$$

- **We need to design a decoder $f_\theta(z)$ such that all terms are easy to compute.**

- There are many architures for that purpose, we will see one called **RealNVP** (Dinh et al., ICLR 2017)

# Normalising flows: RealNVP

Partition the variables $\mathbf{z}$ into two disjoint subsets, say $\mathbf{z}_{1:d}$ and $\mathbf{z}_{d+1:n}$ for any $1 \leq d < n$

- Forward mapping $\mathbf{z} \mapsto \mathbf{x}$:
  - $\mathbf{x}_{1:d} = \mathbf{z}_{1:d}$ (identity transformation)
  - $\mathbf{x}_{d+1:n} = \mathbf{z}_{d+1:n} + m_\theta(\mathbf{z}_{1:d})$ ($m_\theta(\cdot)$ is a neural network with parameters $\theta$, $d$ input units, and $n - d$ output units)
- Inverse mapping $\mathbf{x} \mapsto \mathbf{z}$:
  - $\mathbf{z}_{1:d} = \mathbf{x}_{1:d}$ (identity transformation)
  - $\mathbf{z}_{d+1:n} = \mathbf{x}_{d+1:n} - m_\theta(\mathbf{x}_{1:d})$
- Jacobian of forward mapping:

$$J = \frac{\partial \mathbf{x}}{\partial \mathbf{z}} = \begin{pmatrix} I_d & 0 \\ \frac{\partial \mathbf{x}_{d+1:n}}{\partial \mathbf{z}_{1:d}} & I_{n-d} \end{pmatrix}$$

$$\det(J) = 1$$

- **Volume preserving transformation** since determinant is 1.

Slide from Ermon and Grover