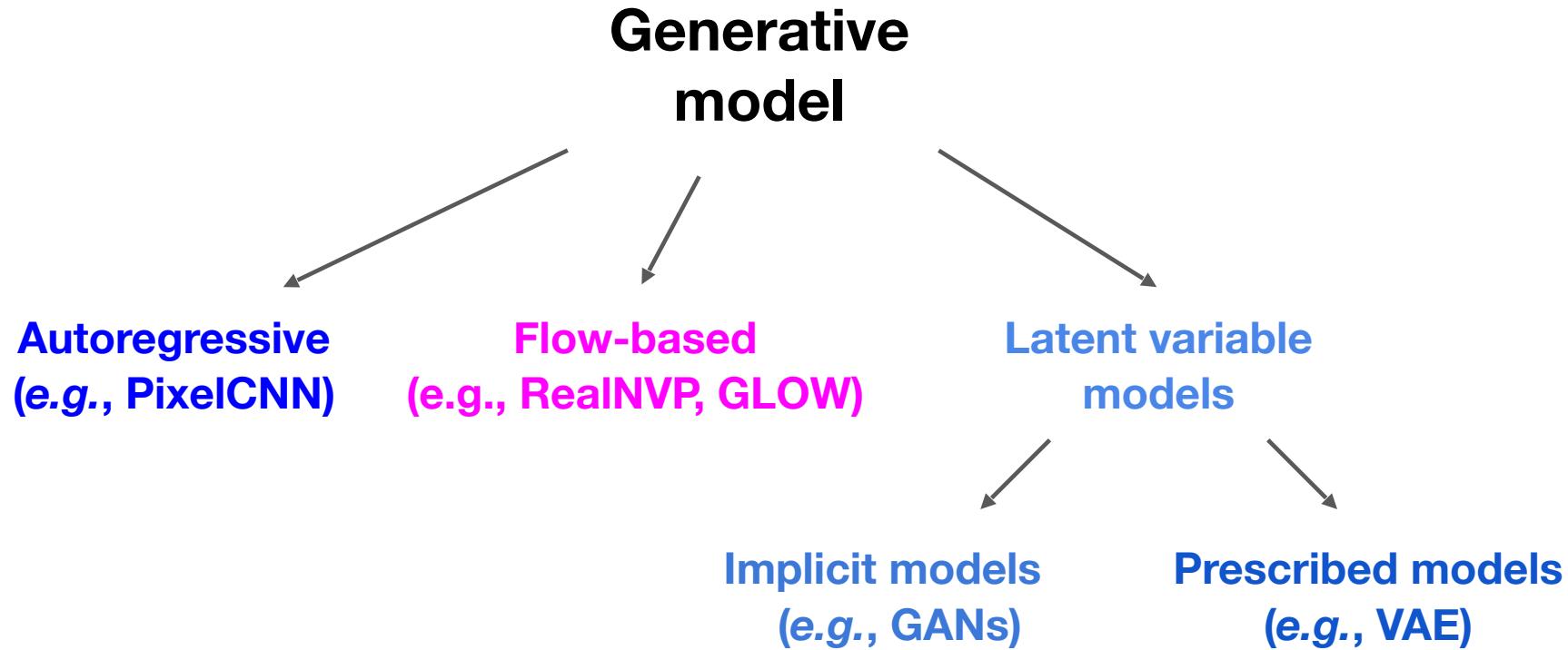


Deep generative modeling: ARM and Normalizing Flows

Jakub M. Tomczak
Deep Learning 2020

TYPES OF GENERATIVE MODELS



GENERATIVE MODELS

	Training	Likelihood	Sampling	Compression
Autoregressive models (e.g., PixelCNN)	Stable	Exact	Slow	No
Flow-based models (e.g., RealNVP)	Stable	Exact	Fast/Slow	No
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ARM: AUTOREGRESSIVE MODELS

REPRESENTING A JOINT DISTRIBUTION

There are two main rules in the probability theory:

- Sum rule: $p(x) = \sum_y p(x, y)$
- Product rule: $p(x, y) = p(y | x) p(x)$

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Before, we used these two rules for latent-variable models:

$$\begin{aligned} p(\mathbf{x}) &= \int p(\mathbf{x}, \mathbf{z}) \, d\mathbf{z} \\ &= \int p(\mathbf{x} | \mathbf{z}) p(\mathbf{z}) \, d\mathbf{z} \end{aligned}$$

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Now, we will use the product rule to express the distribution of $\mathbf{x} \in \mathbb{R}^D$:

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Can we do better that?

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However, it is still pretty **limiting**, because we need to decide on the length of the dependency.

AUTOREGRESSIVE MODELS (ARM)

Instead, we can use RNNs to model the conditionals:

$$p(x_d | \mathbf{x}_{<d}) = p(x_d | RNN(x_{d-1}, h_{d-1}))$$

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USING CONVOLUTIONAL NEURAL NETWORKS FOR MODELING SEQUENCES

Let us consider a sequence $\mathbf{x} = [x_1, x_2, \dots, x_D]^\top$.

We assume all observed data are D -dimensional.

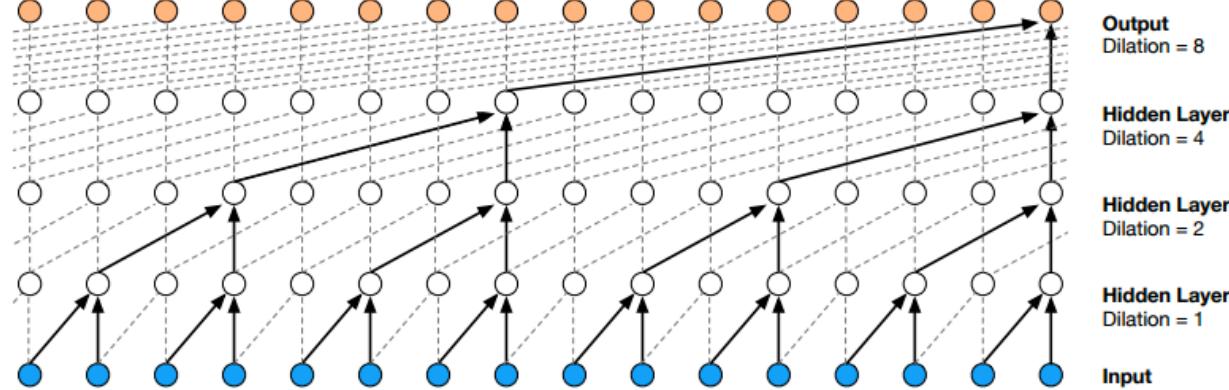
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Let us consider a sequence $\mathbf{x} = [x_1, x_2, \dots, x_D]^T$.

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We can use **1D convolutional layers** to process all signals at once.

Moreover, we can use **dilation** to learn **long-range dependencies**.

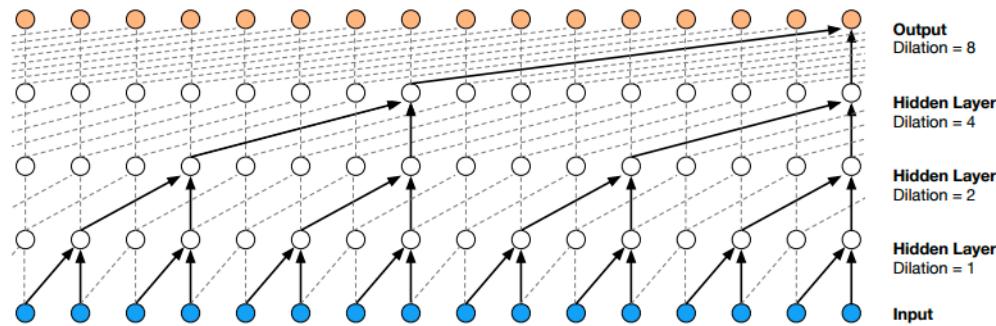


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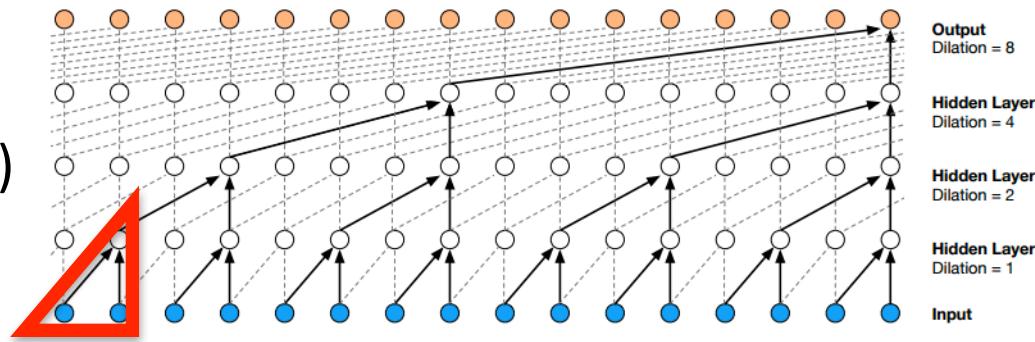


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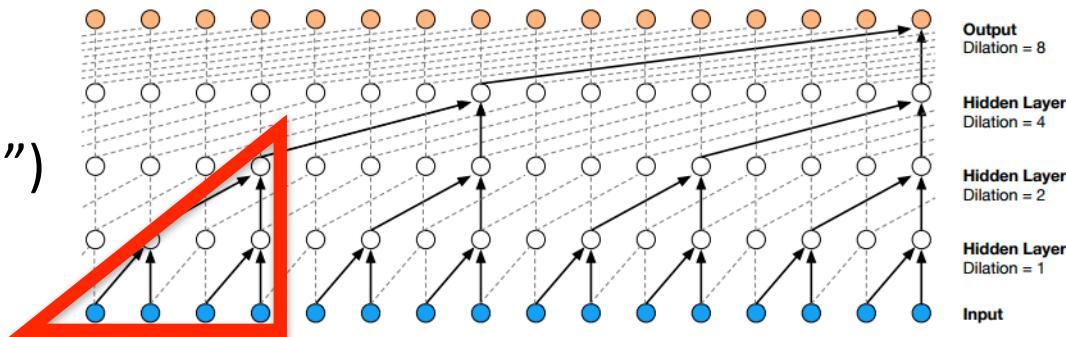


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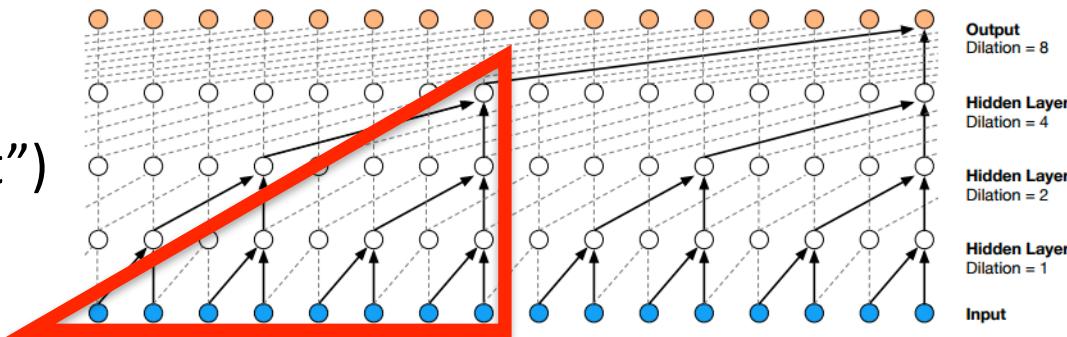


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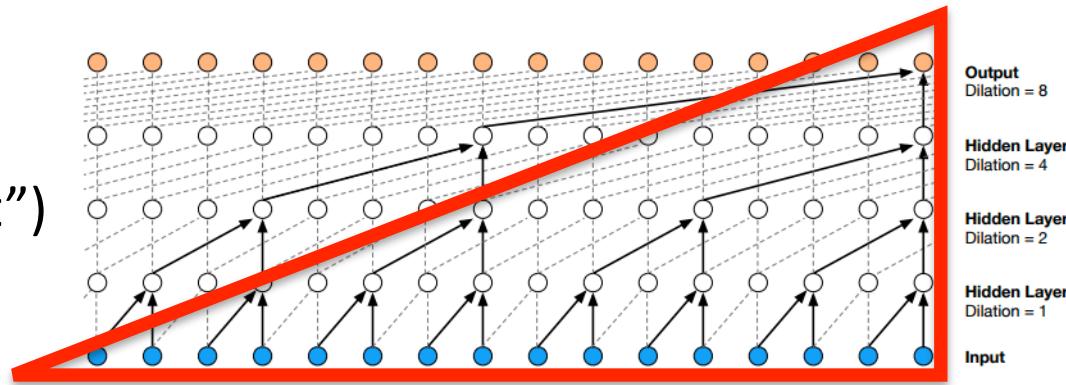


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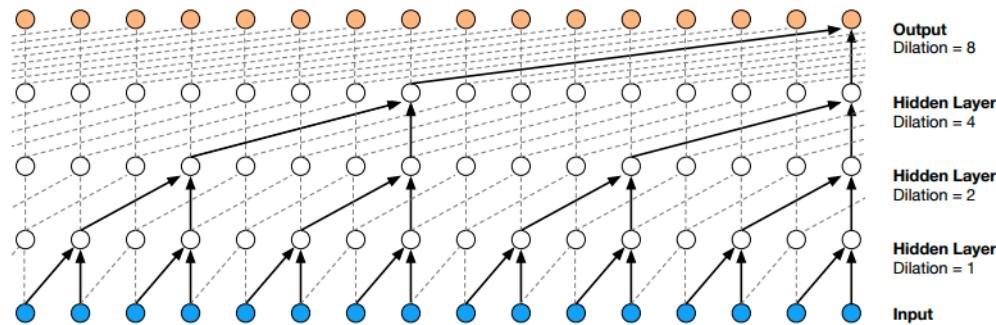


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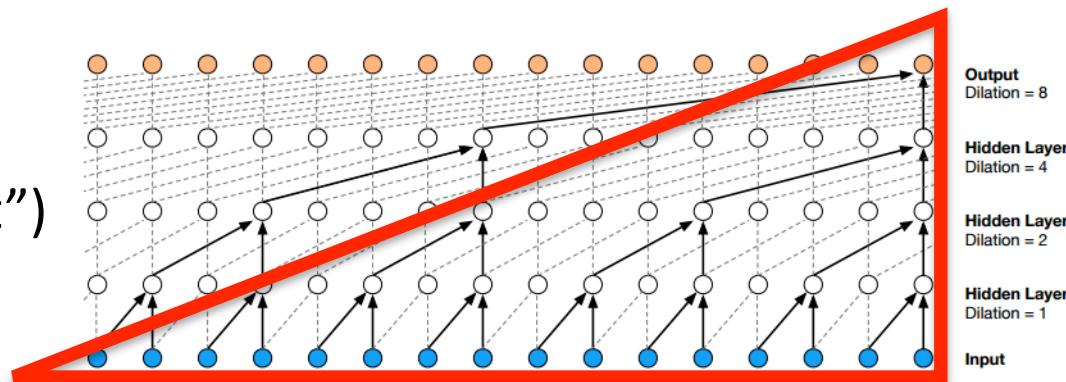


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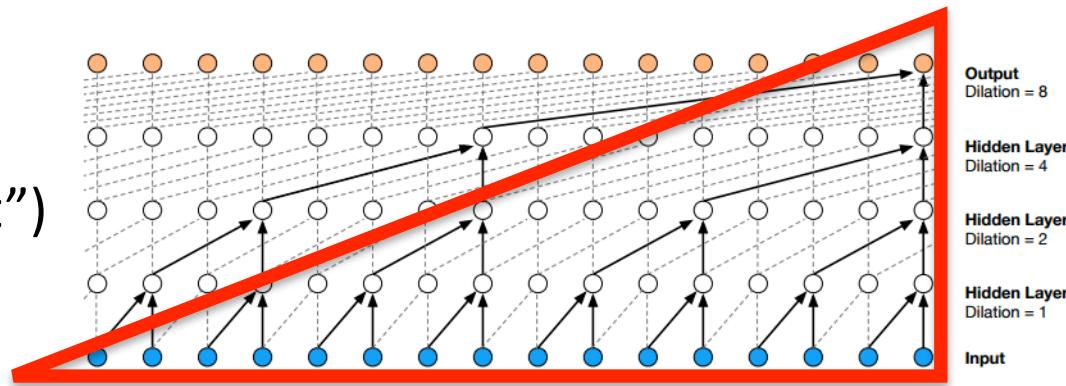


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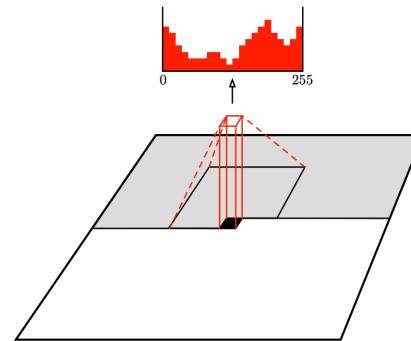
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We need to remember about **causal convolutions!**

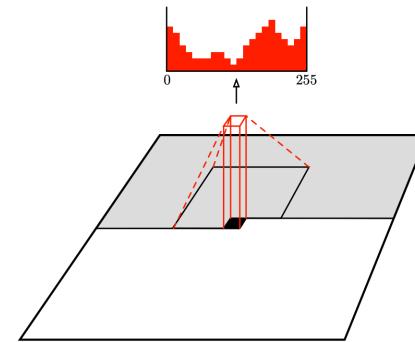


1	1	1	1	1
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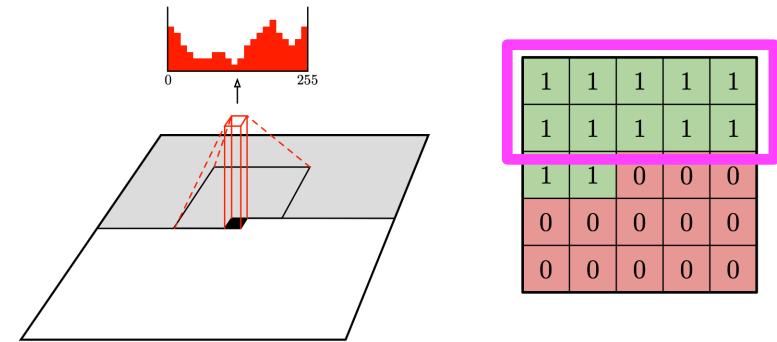
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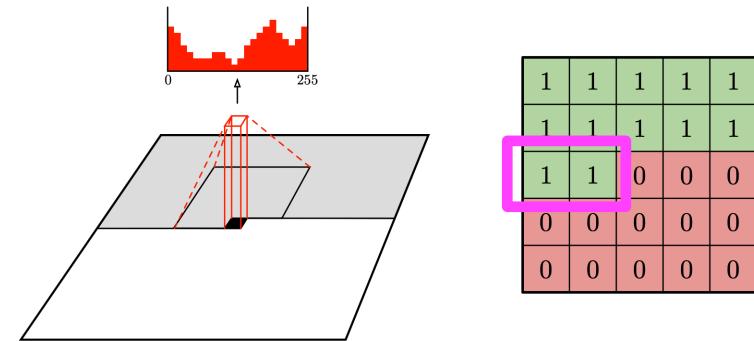
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³⁴Van den Oord, Aaron, et al. "Conditional image generation with PixelCNN decoders." NIPS. 2016.

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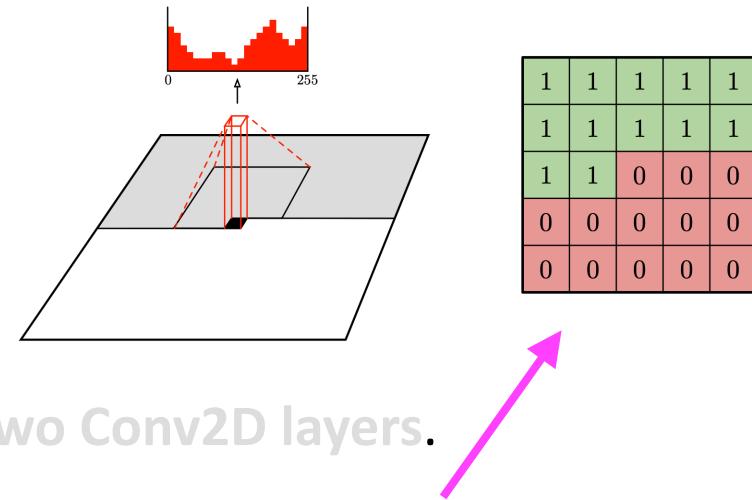
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using masking for kernel weights.

Originally, PixelCNN used the **softmax non-linearity** at the end to output integers between 0 and 255 (i.e., pixel values).

Currently, a **mixture of discretized logistic distributions** is used:

$$P(x \mid \pi, \mu, s) = \sum_{i=1}^K \pi_i \left[\sigma\left(\frac{(x + 0.5 - \mu_i)}{s_i}\right) - \sigma\left(\frac{(x - 0.5 - \mu_i)}{s_i}\right) \right]$$

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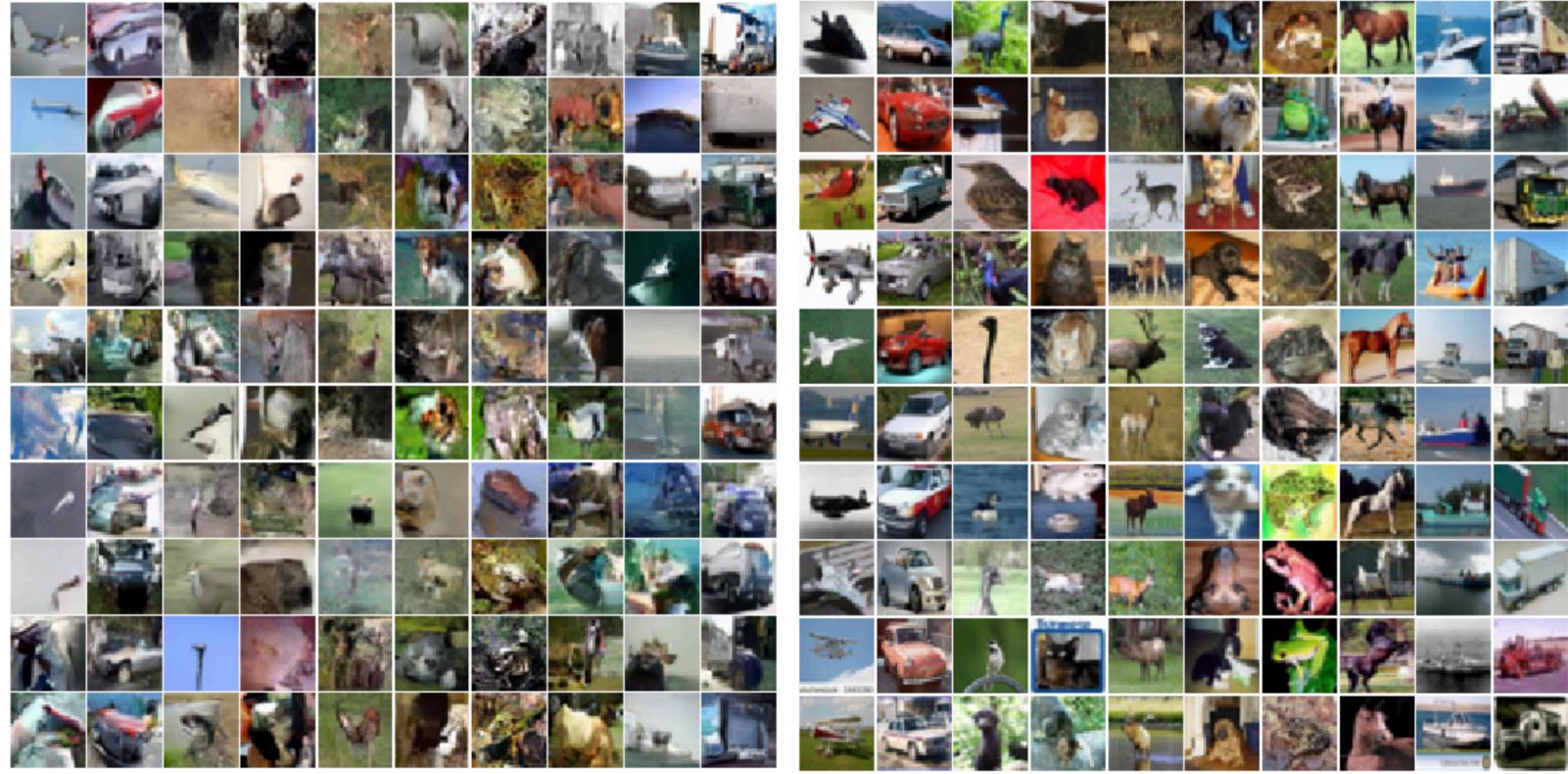
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PIXELCNN



Sampled

Real

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Advantages

- ✓ Exact likelihood.
- ✓ Stable training.

Disadvantages

- Very slow sampling.
- No compression.
- Sometimes, low visual quality.

FLOW-BASED MODELS

CHANGE OF VARIABLES

Let us consider a random variable $v \in \mathbb{R}$ with $p(v) = \mathcal{N}(v | 0, 1)$.

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Then, we take the following transformation: $u = 0.75 \cdot v + 1$.

Q: What is the pdf for u ?

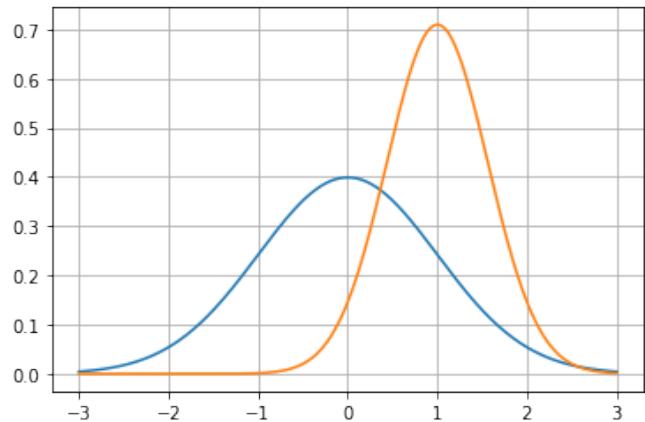
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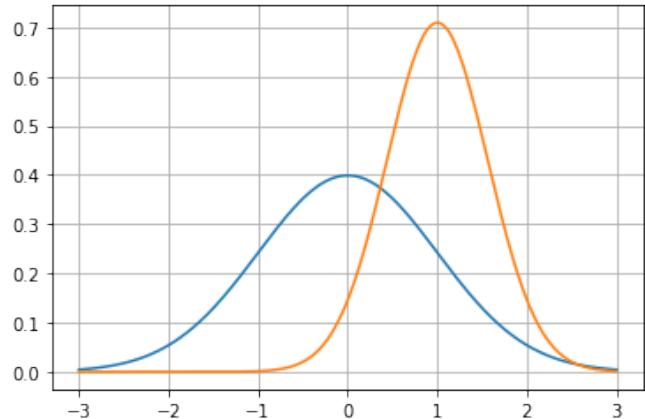
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$$f^{-1}(u) = \frac{u - 1}{0.75}$$

$$\left| \frac{\partial f^{-1}(u)}{\partial u} \right| = \frac{4}{3}$$

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$$p(u) = p\left(\frac{u-1}{0.75}\right) \frac{4}{3} = \frac{1}{\sqrt{2\pi} 0.75^2} \exp\left\{-\frac{(u-1)^2}{0.75^2}\right\}$$

Multidimensional case:

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where:

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How can we utilize this idea?

APPLYING CHANGE OF VARIABLES AND INVERTIBLE TRANSFORMATIONS

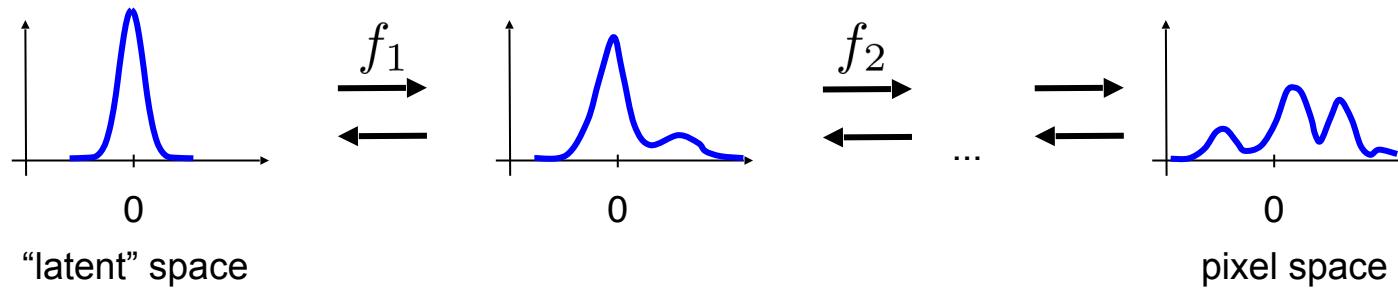
Let us consider a sequence of invertible transformations $f_k : \mathbb{R}^D \rightarrow \mathbb{R}^D$.

We can start with a *simple* distribution, e.g., $\pi(\mathbf{z}) = \mathcal{N}(\mathbf{z} | \mathbf{0}, \mathbf{I})$.

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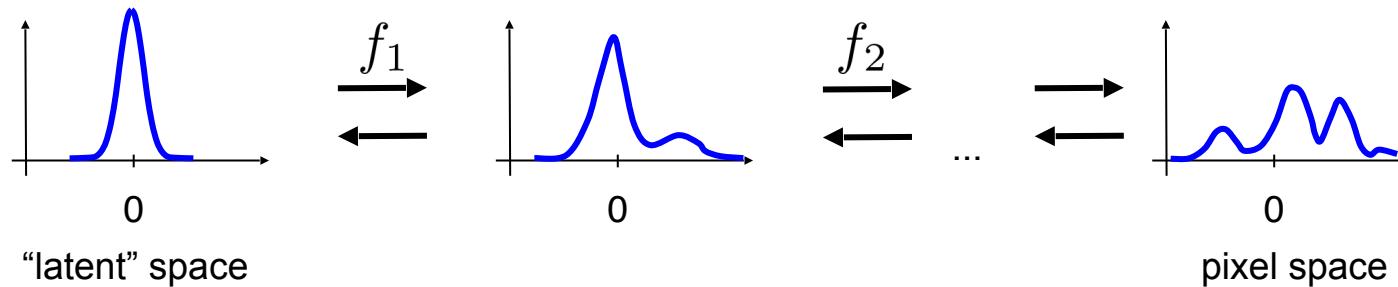
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This results in: $p(\mathbf{x}) = \pi(\mathbf{z}_0) \prod_{i=1}^K \left| \det \frac{\partial f_i(\mathbf{z}_{i-1})}{\partial \mathbf{z}_{i-1}} \right|^{-1}$

2D EXAMPLE

Inference

$$x \sim \hat{p}_X$$

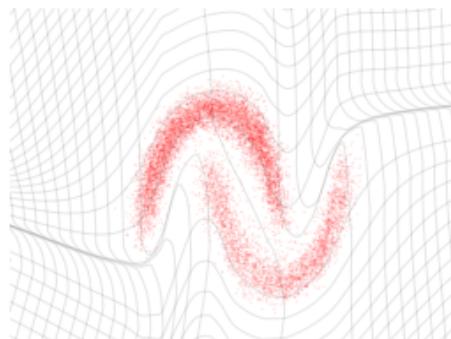
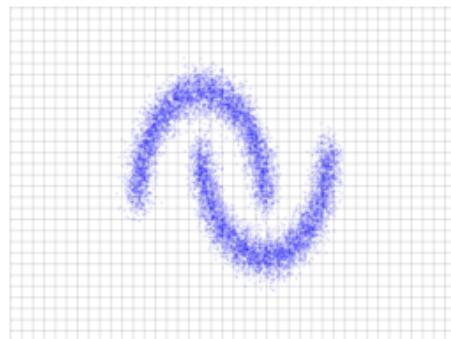
$$z = f(x)$$

Generation

$$z \sim p_Z$$

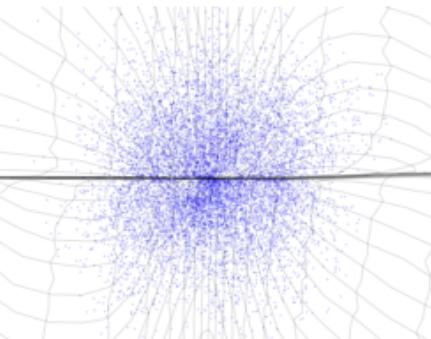
$$x = f^{-1}(z)$$

Data space \mathcal{X}



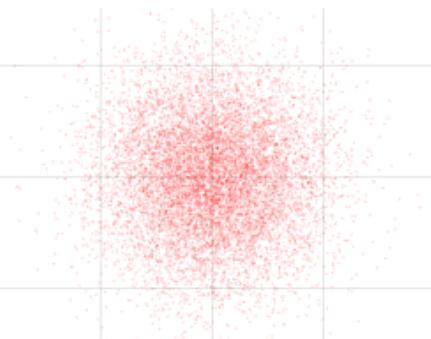
$$\{f_k\}$$

\Rightarrow



$$\{f_k^{-1}\}$$

\Leftarrow



Latent space \mathcal{Z}

DENSITY MODELING WITH INVERTIBLE NEURAL NETWORKS

The density model: $p(\mathbf{x}) = \pi(\mathbf{z}_0) \prod_{i=1}^K \left| \det \frac{\partial f_i(\mathbf{z}_{i-1})}{\partial \mathbf{z}_{i-1}} \right|^{-1}$

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In order to obtain flexible transformations f_k , we use **neural networks**.

However, we need to ensure that they are **invertible**.

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However, we need to ensure that they are **invertible**.

Moreover, we cannot use any invertible neural network, because we need to remember about the **Jacobian**!

DENSITY MODELING WITH INVERTIBLE NEURAL NETWORKS

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In order to obtain flexible transformations f_k , we use **neural networks**.

However, we need to ensure that they are **invertible**.

Moreover, we cannot use any invertible neural network, because we need to remember about the **Jacobian**!

Calculating Jacobian is the main challenge in flow-based models.

Design the invertible transformations as follows:

$$\mathbf{y}_{1:d} = \mathbf{x}_{1:d}$$

$$\mathbf{y}_{d+1:D} = \mathbf{x}_{d+1:D} \odot \exp\left(s\left(\mathbf{x}_{1:d}\right)\right) + t\left(\mathbf{x}_{1:d}\right)$$

where: $s(\cdot)$ and $t(\cdot)$ are **arbitrary** neural networks.

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where: $s(\cdot)$ and $t(\cdot)$ are **arbitrary** neural networks.

This is **invertible by design**, because:

$$\mathbf{x}_{d+1:D} = \mathbf{y}_{d+1:D} \oslash \exp\left(s(\mathbf{x}_{1:d})\right) - t(\mathbf{x}_{1:d})$$

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Known as
affine coupling layer

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What about the Jacobian?

$$\mathbf{J} = \begin{bmatrix} \mathbb{I}_d & \mathbf{0}_{d \times (D-d)} \\ \frac{\partial \mathbf{y}_{d+1:D}}{\partial \mathbf{x}_{1:d}} & \text{diag}(\exp(s(\mathbf{x}_{1:d}))) \end{bmatrix}$$

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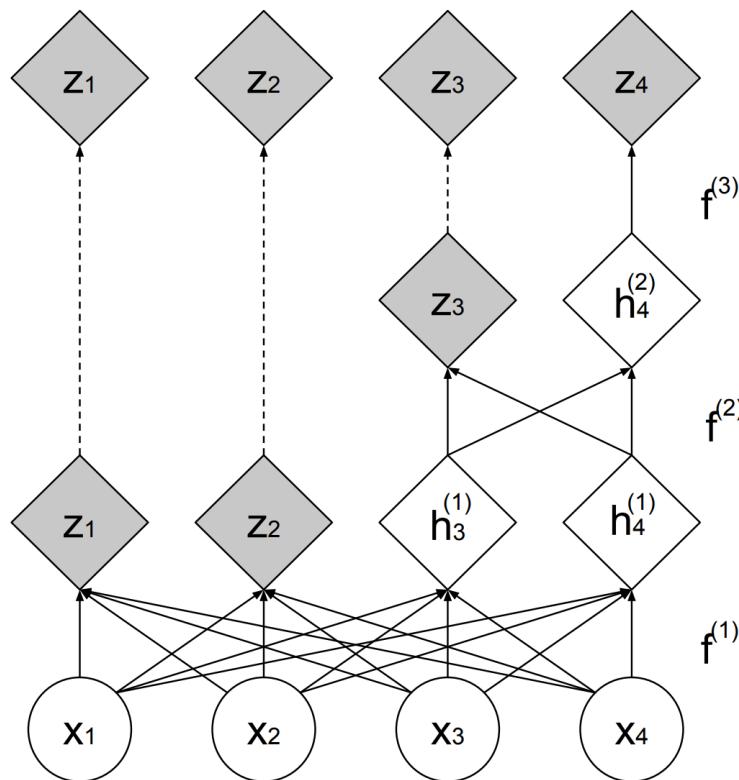
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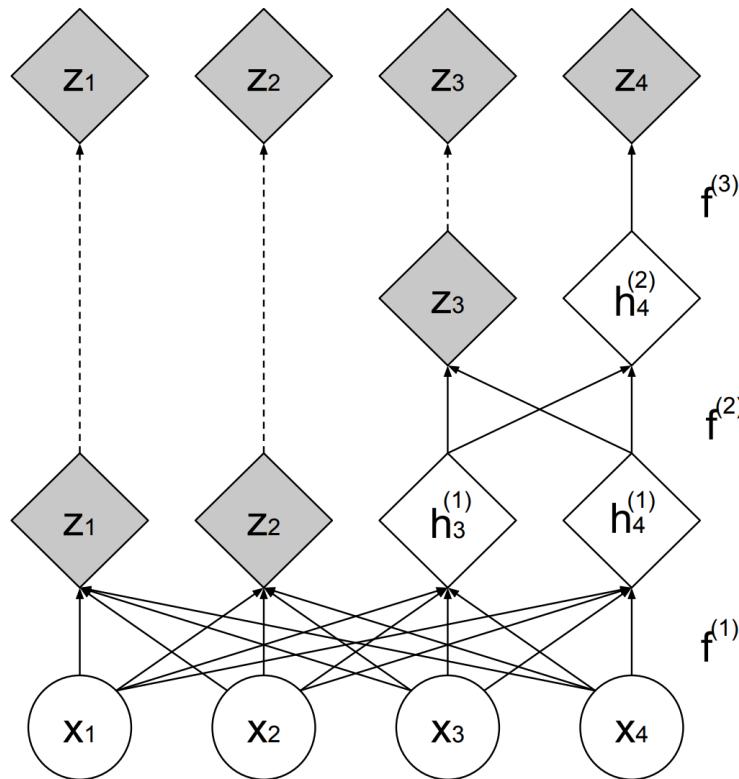
Easy to calculate!

We can also introduce the idea of autoregressive modeling here as well:



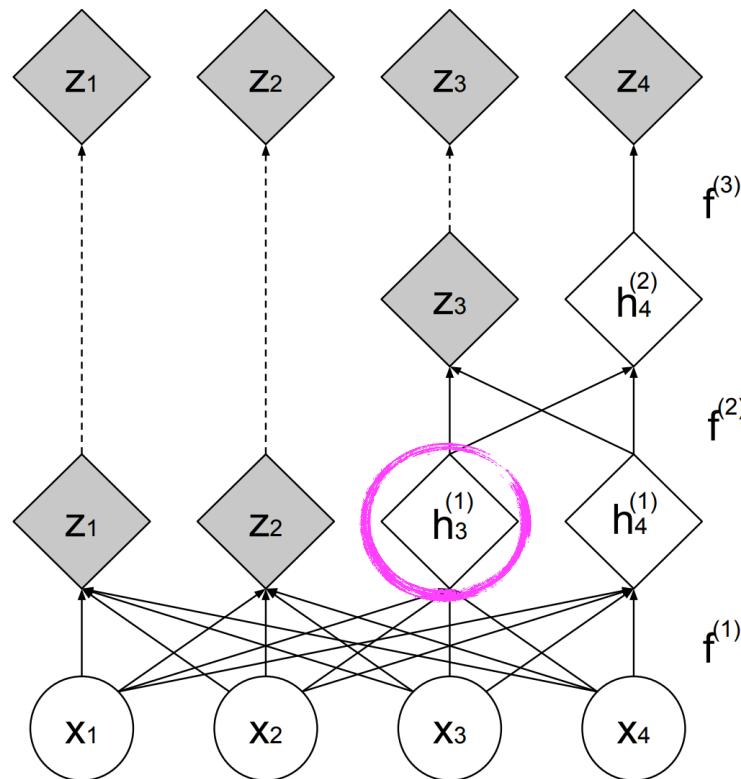
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$$p(z_1)p(z_2)p(z_3 | z_1, z_2)p(z_4 | z_1, z_2, z_3)$$

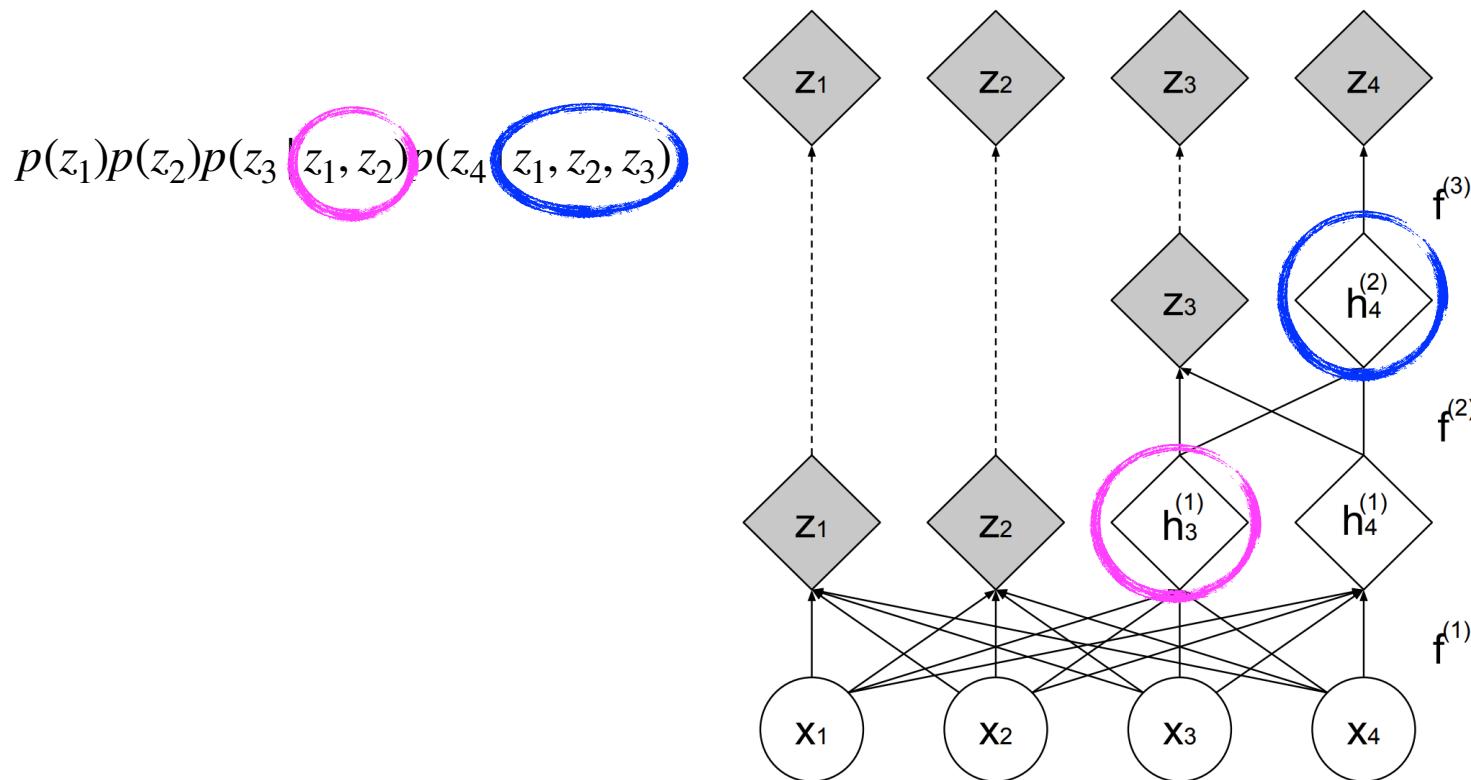


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We can also introduce the idea of autoregressive modeling here as well:



Moreover, we can use additional transformations:

1. **Permutations** of variables (this is invertible).

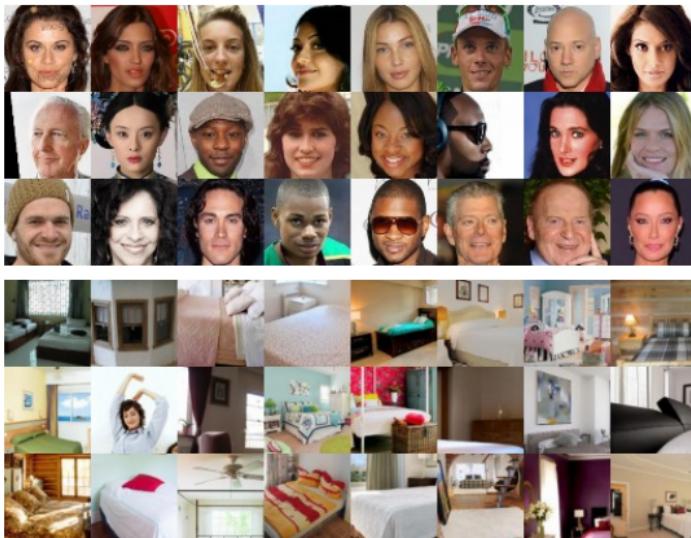
→ this helps to “mix” variables.

2. Divide variables using a **checkerboard pattern**.

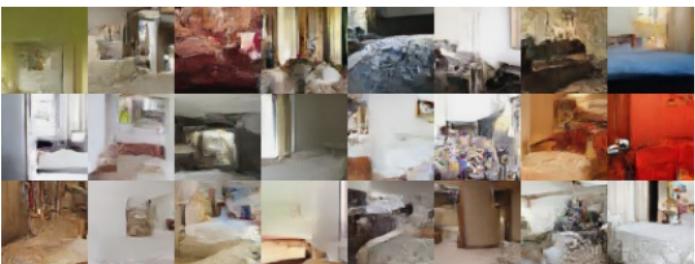
→ this helps to learn higher-order dependencies.

3. Use **squeezing**: reshape input tensor

→ reshaping can help to “mix” variables.



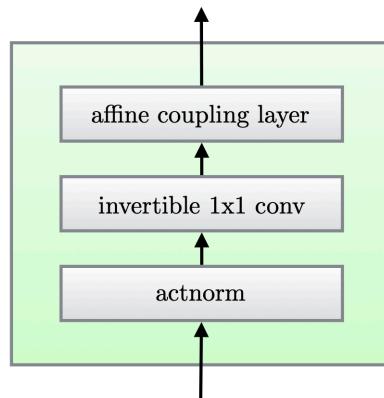
REALNVP



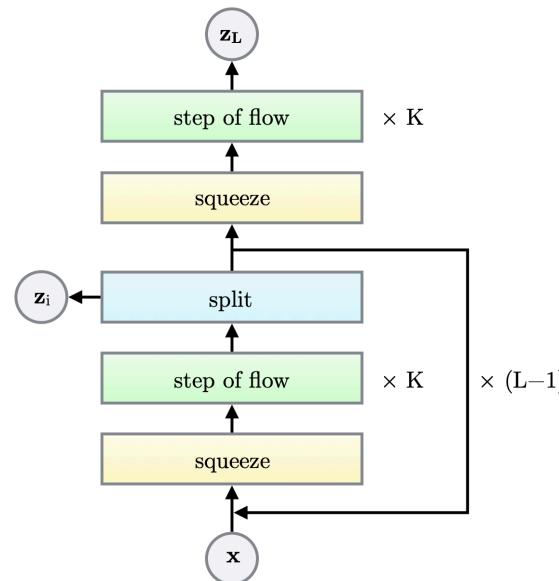
GLOW: REALNVP WITH 1X1 CONVOLUTIONS

A model contains ~1000 convolutions.

A new component: 1x1 convolution instead of a permutation matrix.

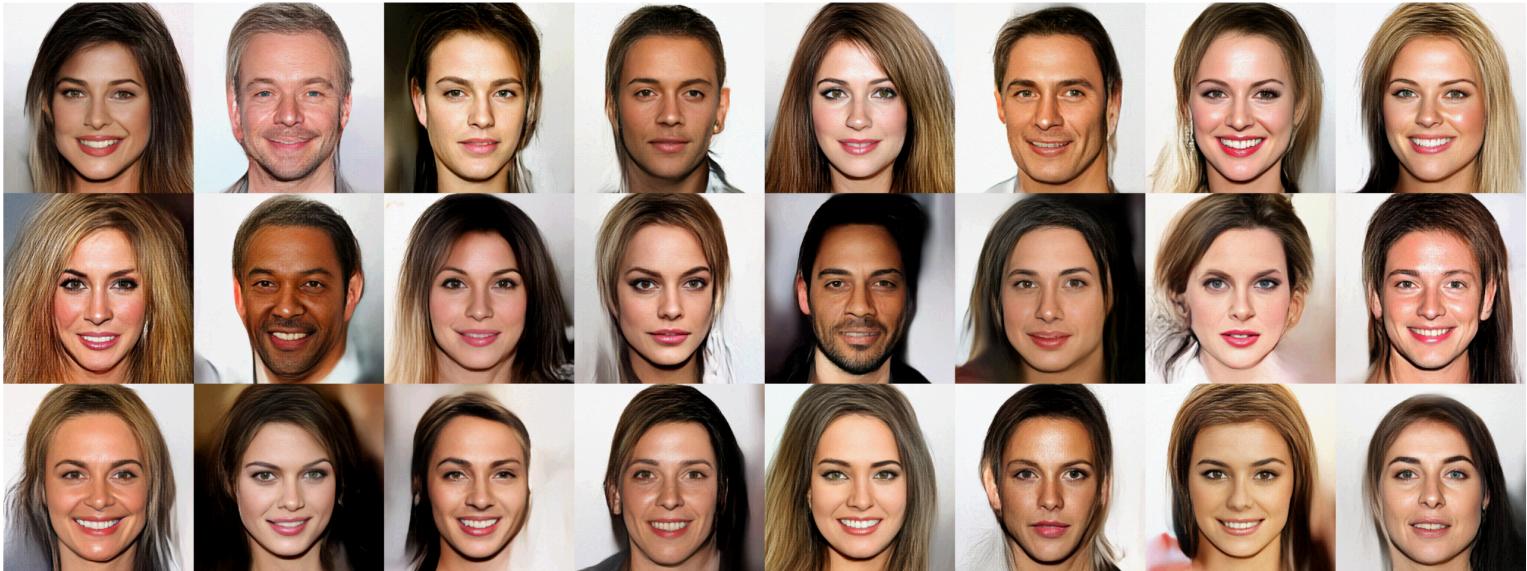


(a) One step of our flow.

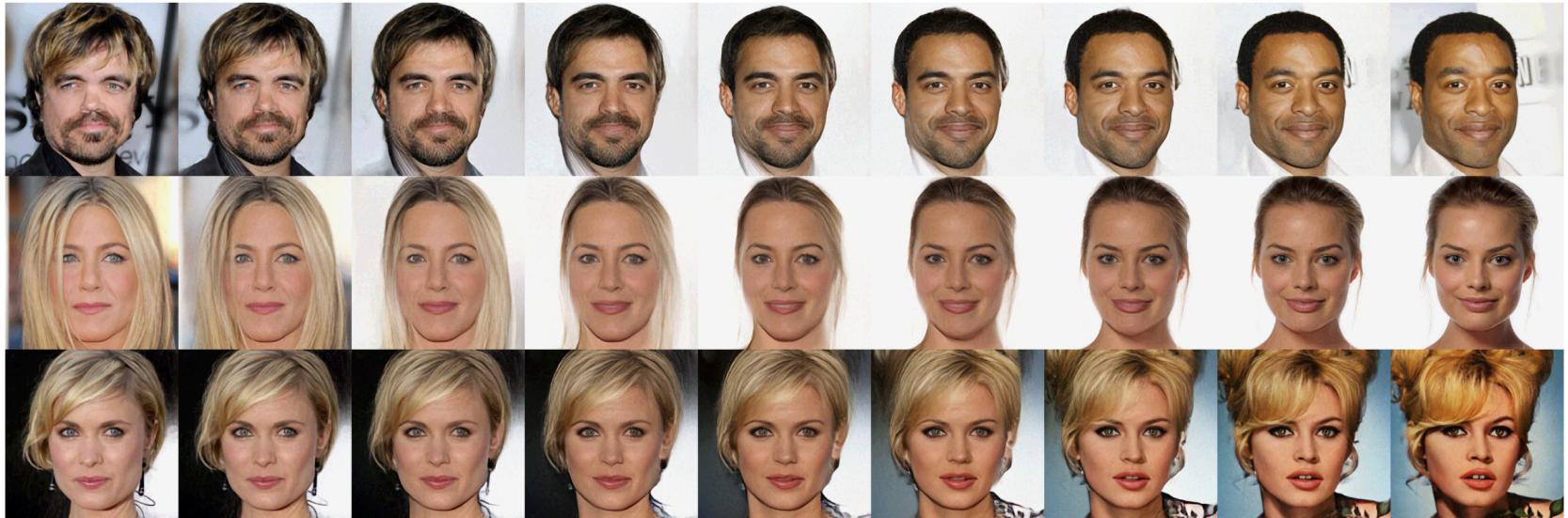


(b) Multi-scale architecture (Dinh et al., 2016).

GLOW: SAMPLES

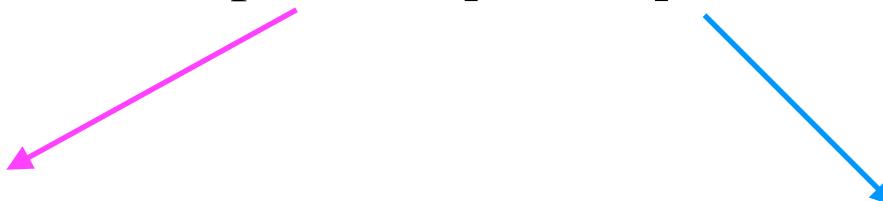


GLOW: LATENT INTERPOLATION



VAES WITH NORMALIZING FLOWS

$$q(\mathbf{z} \mid \mathbf{x}) \propto p(\mathbf{x} \mid \mathbf{z}) p(\mathbf{z})$$



Variational inference with normalizing flows

Rezende & Mohamed. "Variational inference with normalizing flows."

v.d. Berg, Hasenclever, Tomczak, Welling, "Sylvester normalizing flows for variational inference"

Kingma, Salimans, Jozefowicz, Chen, Sutskever, Welling "Improved variational inference with inverse autoregressive flow"

Tomczak, Welling, "Improving variational auto-encoders using householder flow"

Flow-based priors

Chen, Kingma, Salimans, Duan, Dhariwal, Schulman, Abbeel, "Variational lossy autoencoder"

Gatopoulos, Tomczak. "Self-Supervised Variational Auto-Encoders."

Thank you!