Deep generative modeling: ARMs and Normalizing Flows

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Deep Learning

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TYPES OF GENERATIVE MODELS

Generative model

- **Autoregressive** (*e.g.*, PixelCNN)
- **Flow-based** (e.g., RealNVP, GLOW)
- **Latent variable models**
  - **Implicit models** (*e.g.*, GANs)
  - **Prescribed models** (*e.g.*, VAE)

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
Implicit models (e.g., GANs)	Unstable	No	Fast	No
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ARMS: AUTOREGRESSIVE MODELS

REPRESENTING A JOINT DISTRIBUTION

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- Product rule: $p(x, y) = p(y \mid x)\ p(x)$

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

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

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- Sum rule: $p(x) = \sum_{y} p(x, y)$
- Product rule: $p(x, y) = p(y | x)\ p(x)$

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

$$p(\mathbf{x}) = p(x_1) \sum_{d=2}^{D} p(x_d | \mathbf{x}_{<d})$$

where $\mathbf{x}_{<d} = [x_1, x_2, \ldots, x_{d-1}]^\top$

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Can we do better that?

We can assume a **finite dependency**.

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For instance, for two last variables:

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Now, we can model $p(x_d | x_{d-2}, x_{d-1})$ by a **single model**.

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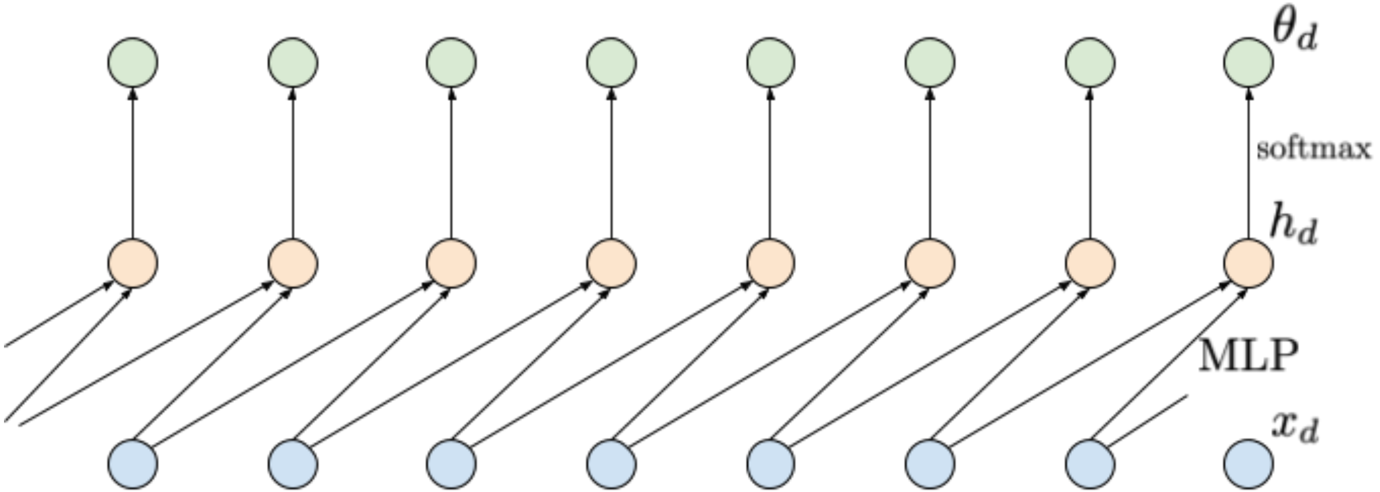

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However, it is still pretty **limiting**, because we need to decide on the length of the dependency.

AUTOREGRESSIVE MODELS (ARM)

Instead, we can use RNNs to model the conditionals:

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

where $h_d = RNN(x_{d-1}, h_{d-1})$.

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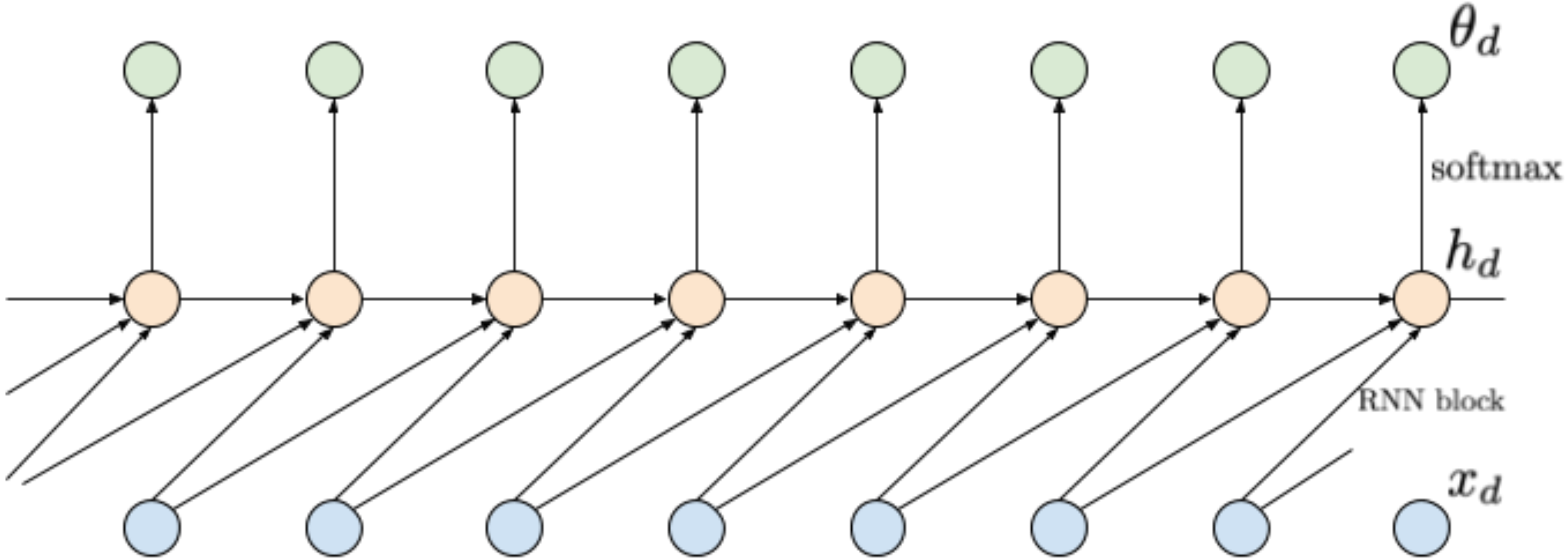

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We assume all observed data are *D*-dimensional.

USING CONVOLUTIONAL NEURAL NETWORKS FOR MODELING SEQUENCES

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

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

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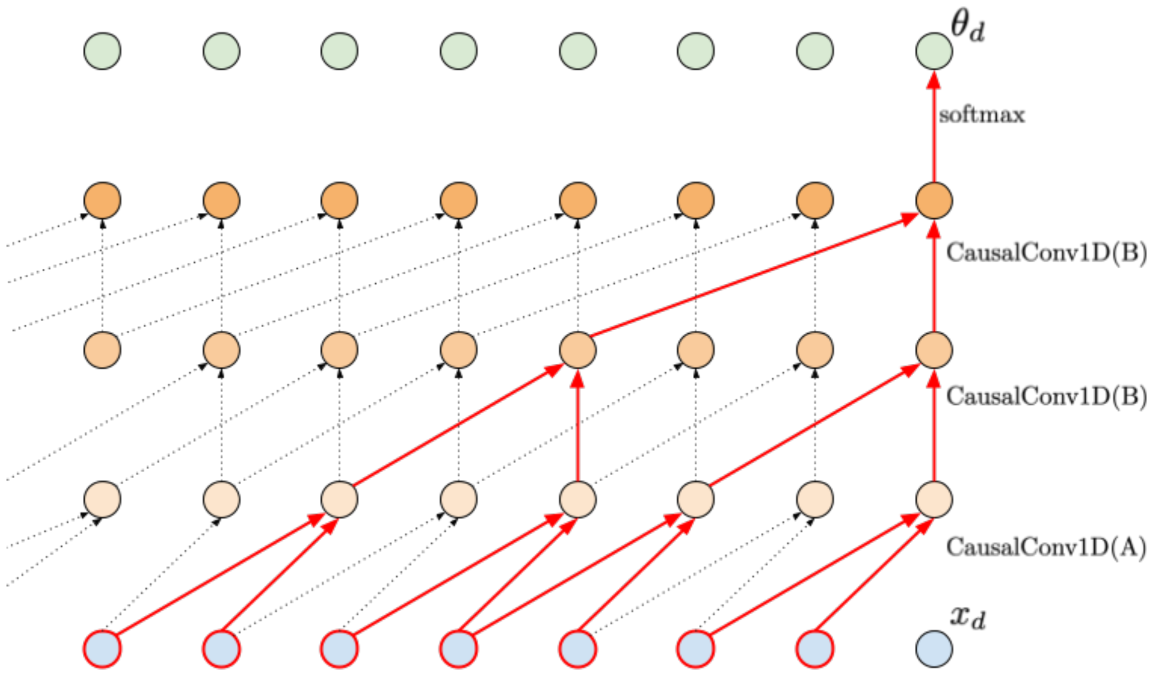

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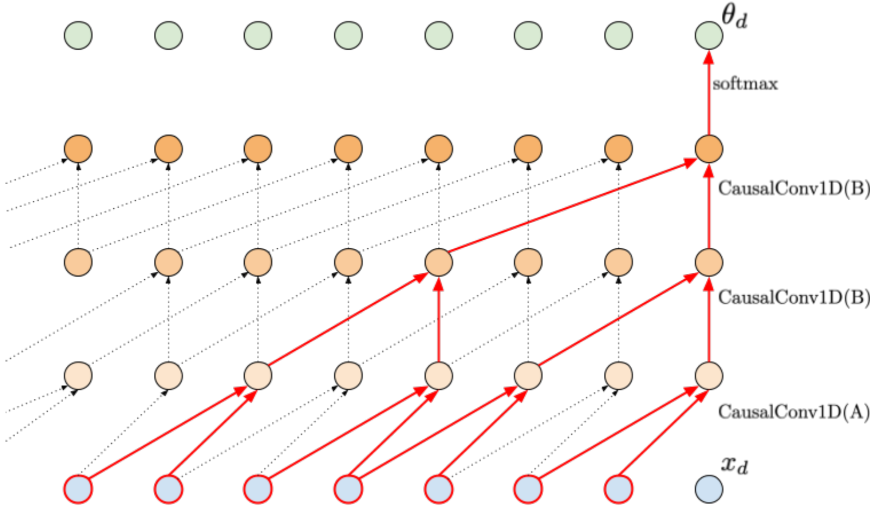

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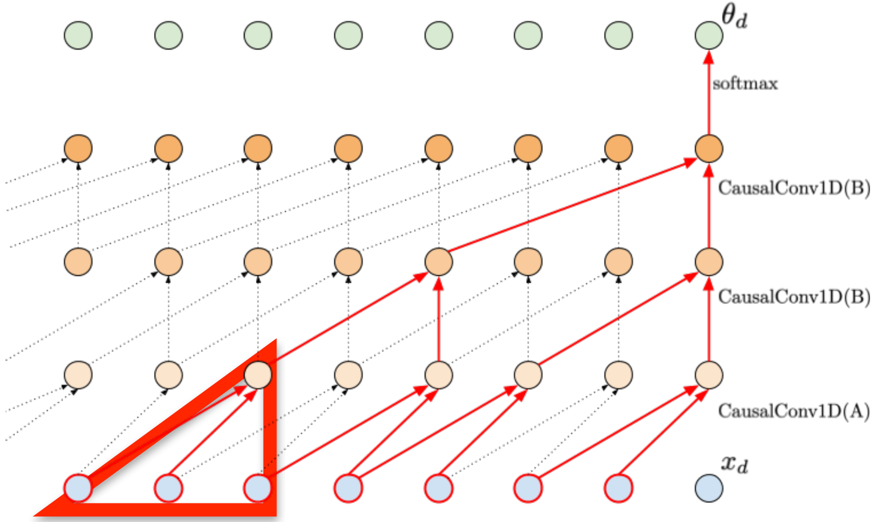

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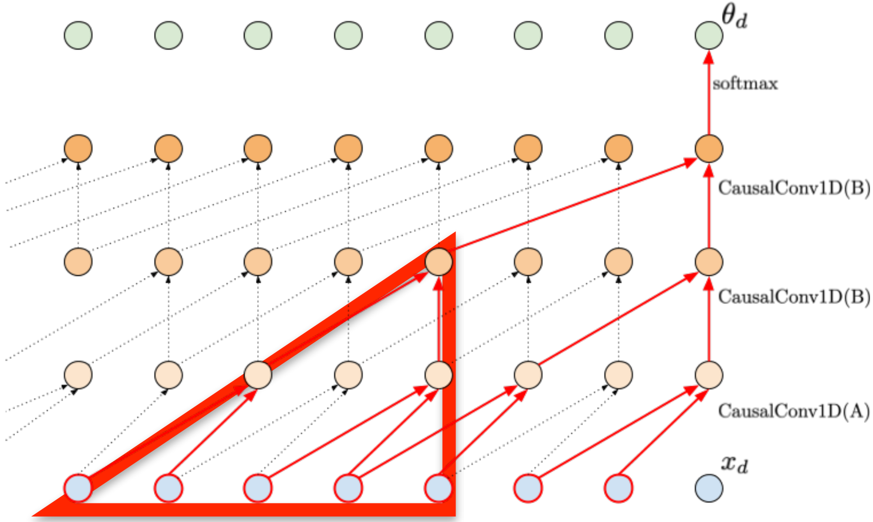

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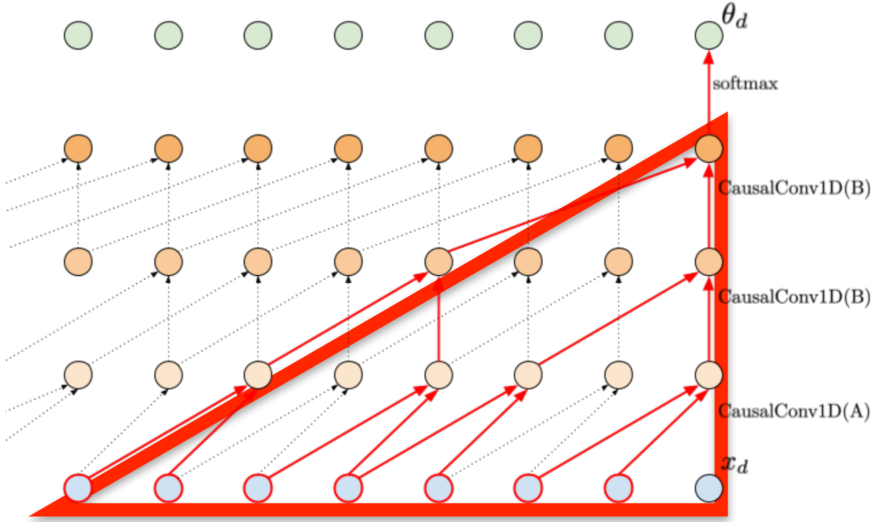

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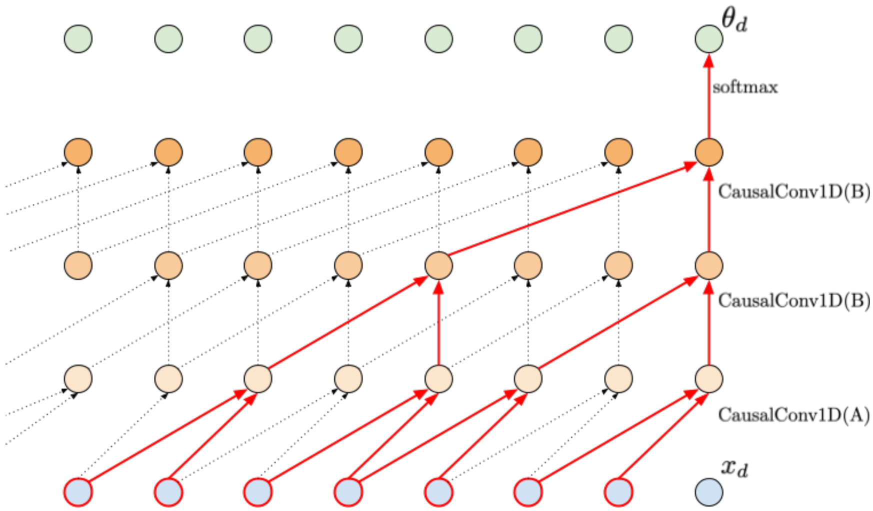

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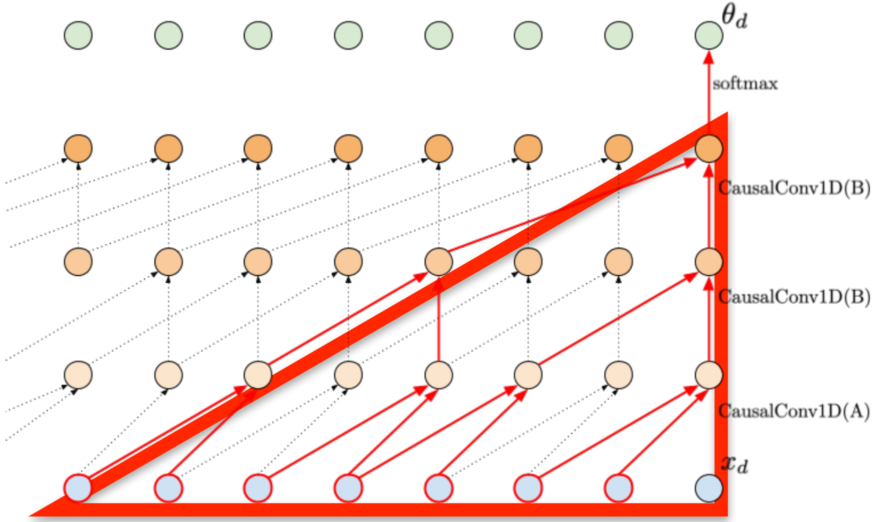

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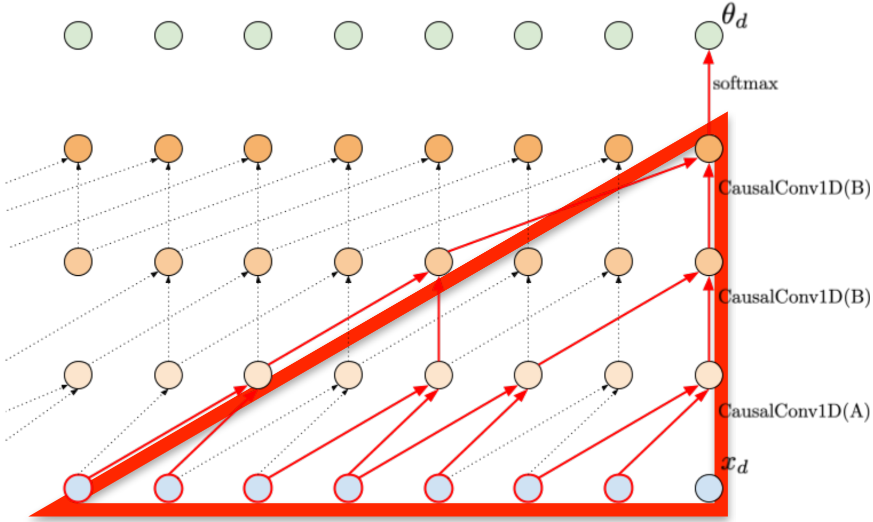

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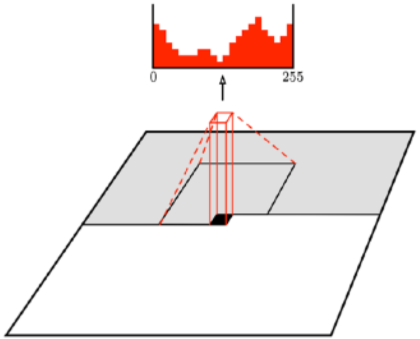
 Oord, Aaron van den, et al. "**Wavenet**: A generative model for raw audio." *arXiv preprint arXiv:1609.03499* (2016).

PIXELCNN

We can utilize the very same idea for images, but using **2D convolutions**.

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



1	1	1	1	1
1	1	1	1	1
1	1	0	0	0
0	0	0	0	0
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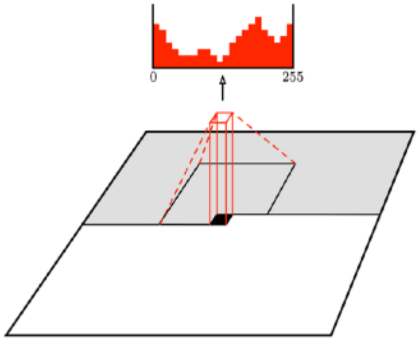

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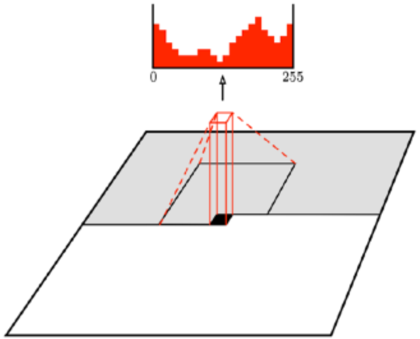

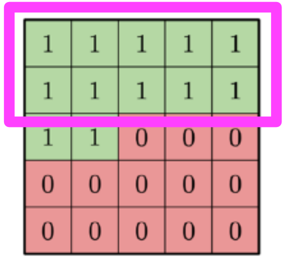

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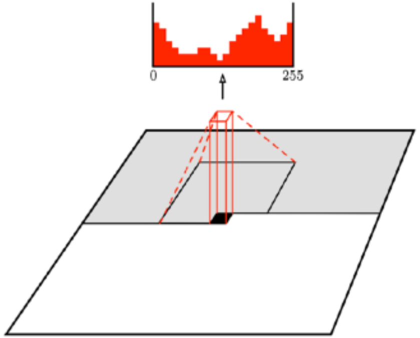

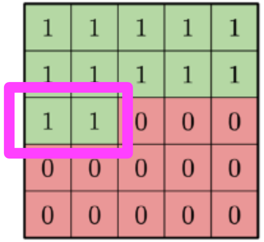

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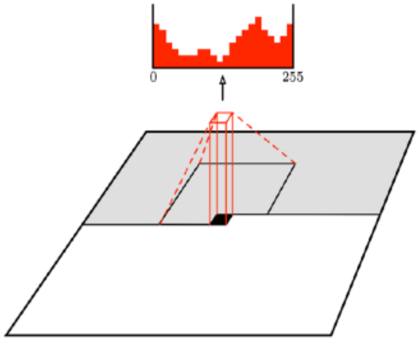

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using masking for kernel weights.

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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:

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

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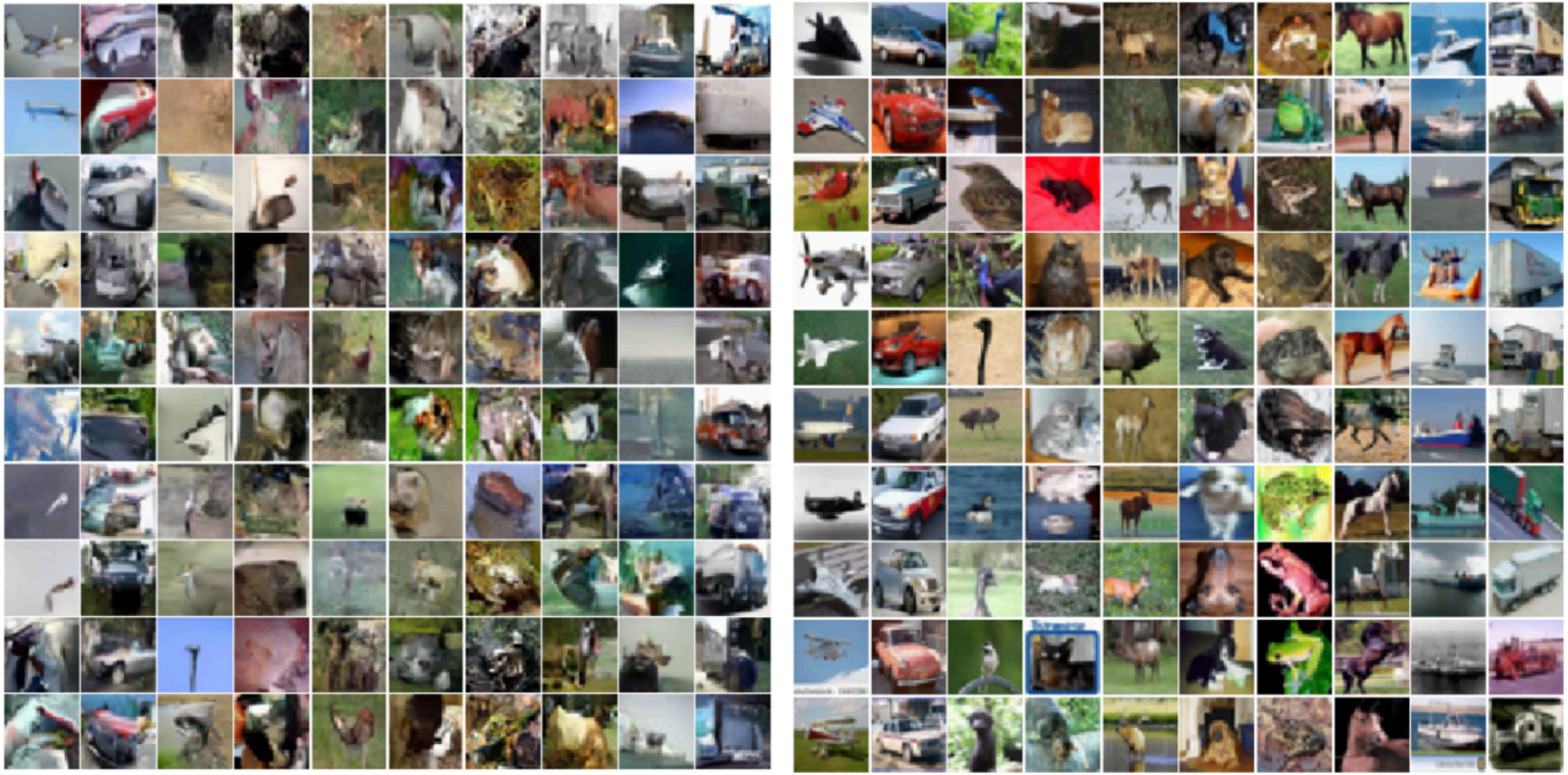

Sampled Real

42 Salimans, Tim, et al. "PixelCNN++: Improving the pixelcnn with discretized logistic mixture likelihood and other modifications." *arXiv* (2017).

Advantages

✓ Exact likelihood.

✓ Stable training.

Disadvantages

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

FLOW-BASED MODELS

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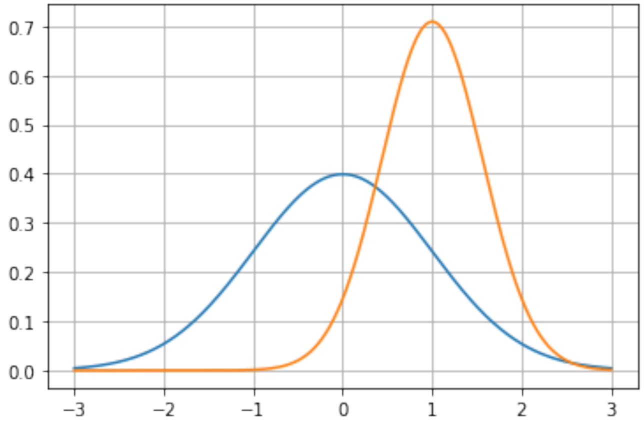
A: The pdf is $p(u) = \mathcal{N}(u \mid 1, 0.75^2)$.



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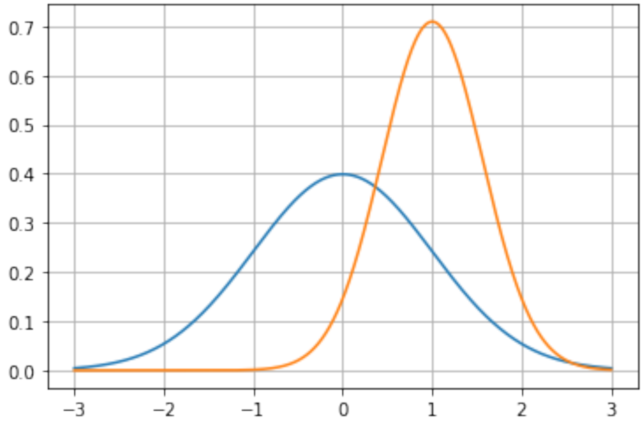

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$$p(u) = p\left(f^{-1}(u)\right)\left|\frac{\partial f^{-1}(u)}{\partial u}\right|$$

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

CHANGE OF VARIABLES

Multidimensional case:

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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 $f_k : \mathbb{R}^D \to \mathbb{R}^D$.

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

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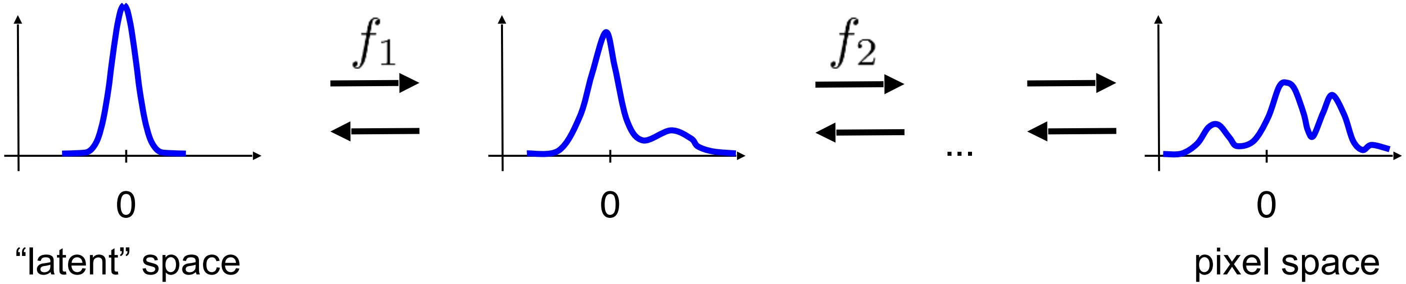

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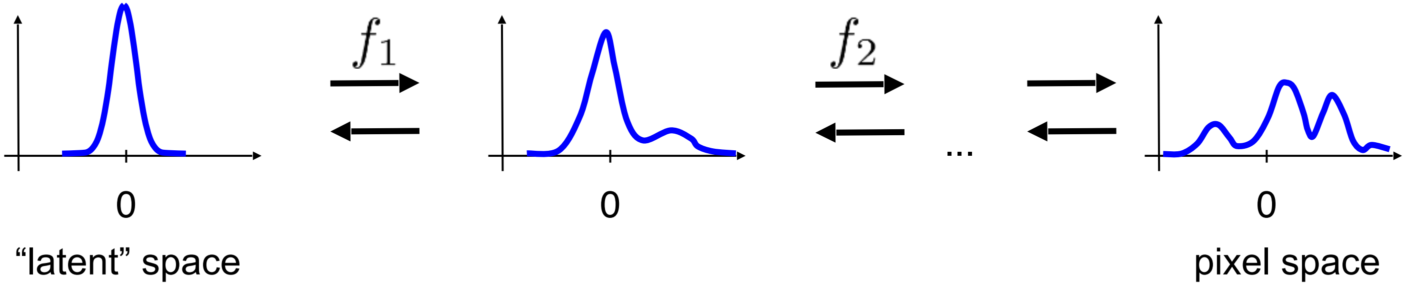
APPLYING CHANGE OF VARIABLES AND INVERTIBLE TRANSFORMATIONS

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

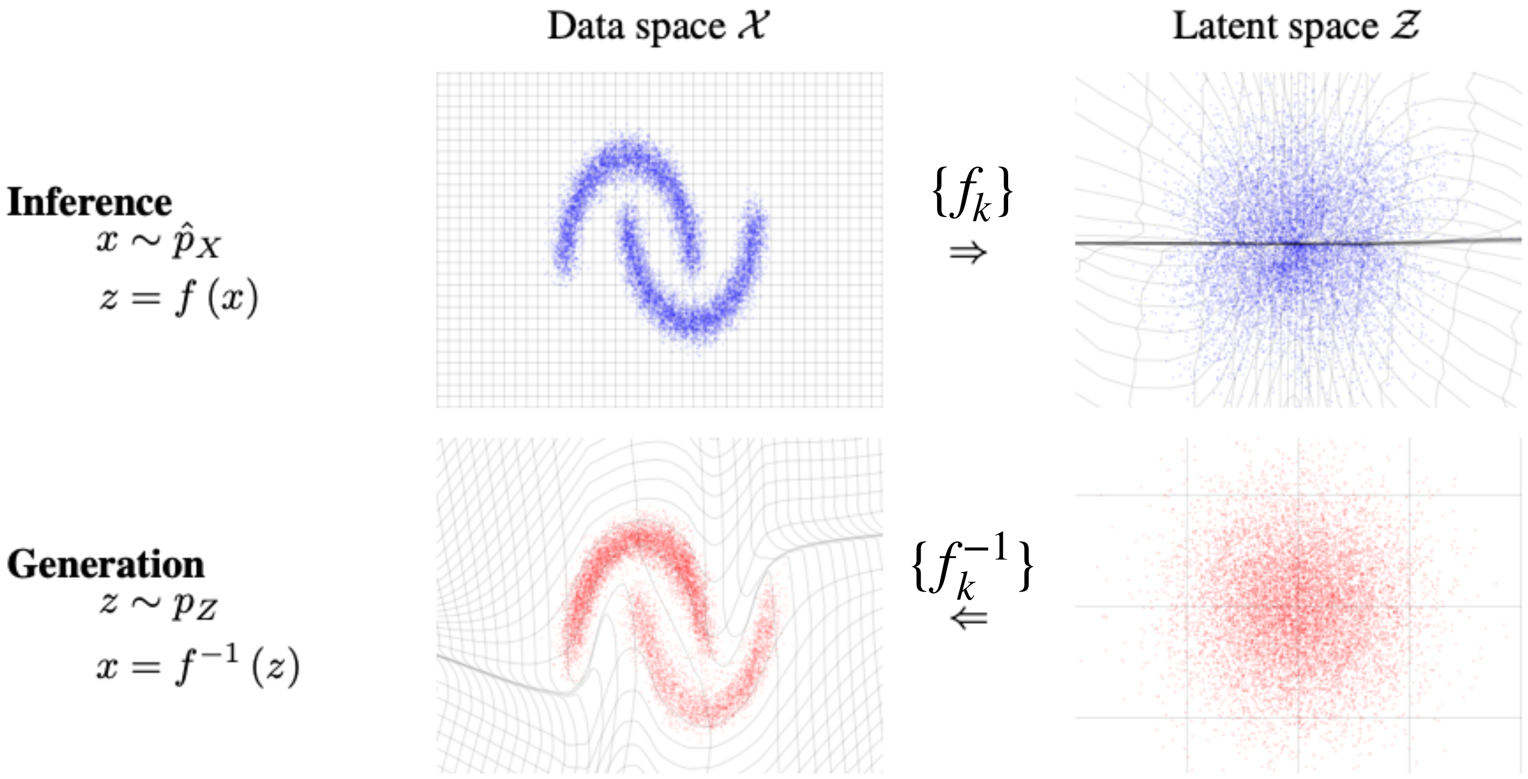
We can start with a *simple* distribution, e.g., $\pi(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$.



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

Rippel, O., & Adams, R. P. (2013). High-dimensional probability estimation with deep density models. arXiv

2D EXAMPLE


Data space $\mathcal{X}$
Latent space $\mathcal{Z}$
Inference
$x \sim \hat{p}_X$
$z = f(x)$
$\{f_k\}$
$\Rightarrow$
Generation
$z \sim p_Z$
$x = f^{-1}(z)$
$\{f_k^{-1}\}$
$\Leftarrow$

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

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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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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.

REALNVP

Design the invertible transformations as follows:

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

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

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

Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using **RealNVP**. arXiv preprint arXiv:1605.08803.

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

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

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Known as
affine coupling layer

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

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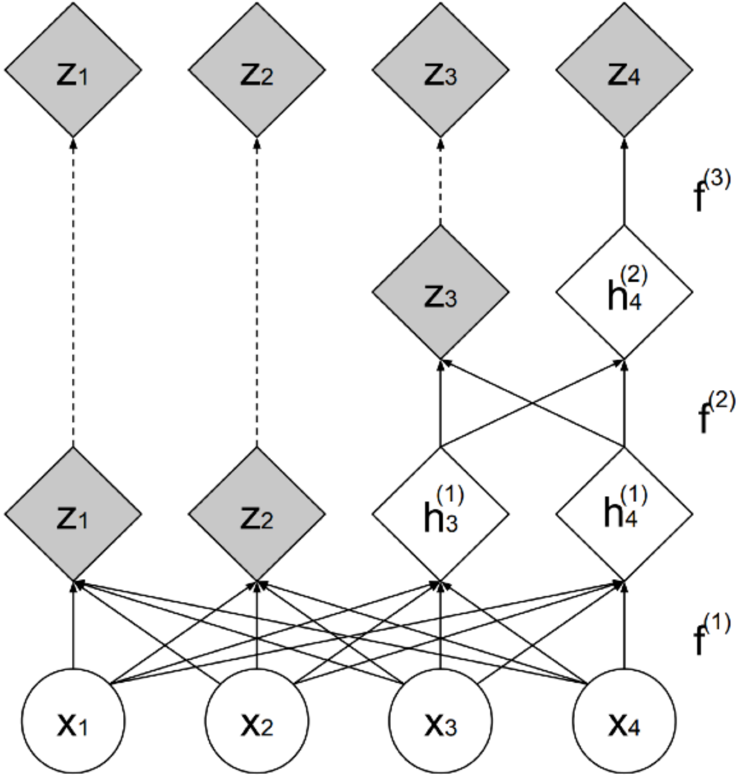
Easy to calculate!

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



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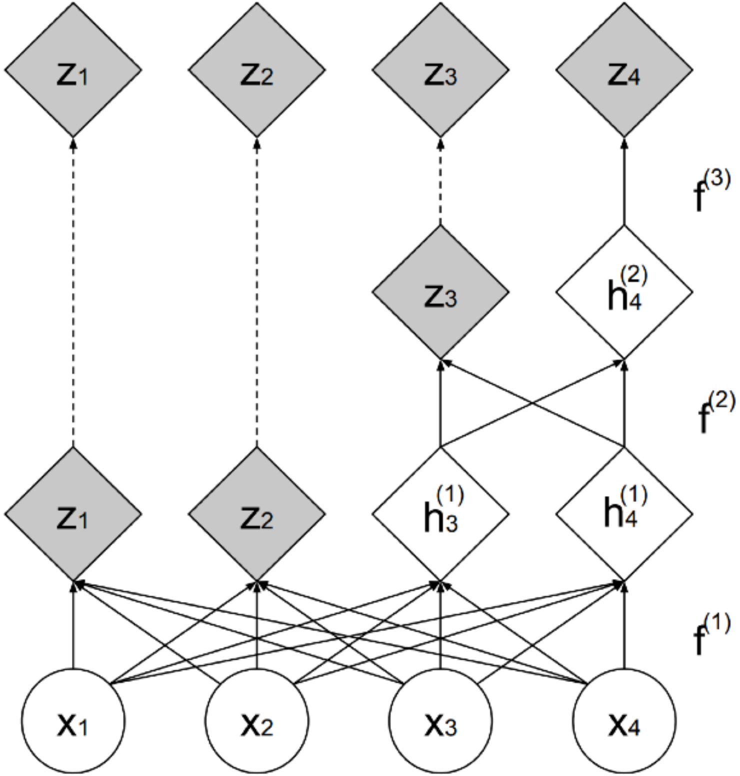
$$p(z_1)p(z_2)p(z_3 \,|\, z_1, z_2)p(z_4 \,|\, z_1, z_2, z_3)$$



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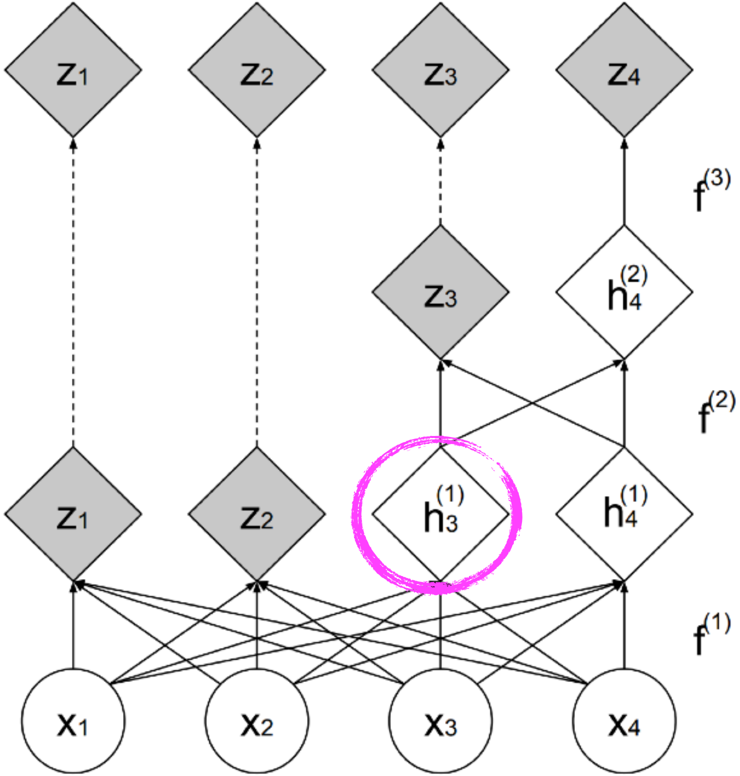
$$p(z_1)p(z_2)p(z_3 \mid z_1, z_2)p(z_4 \mid z_1, z_2, z_3)$$



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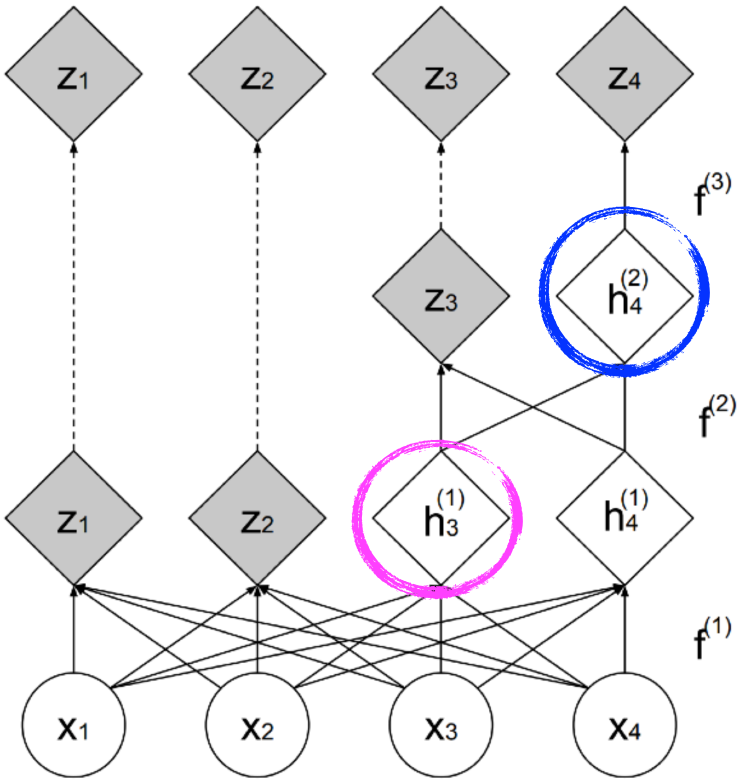


Moreover, we can use additional transformations:

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.

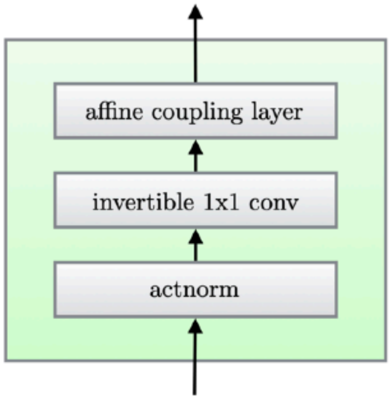
REALNVP

REALNVP

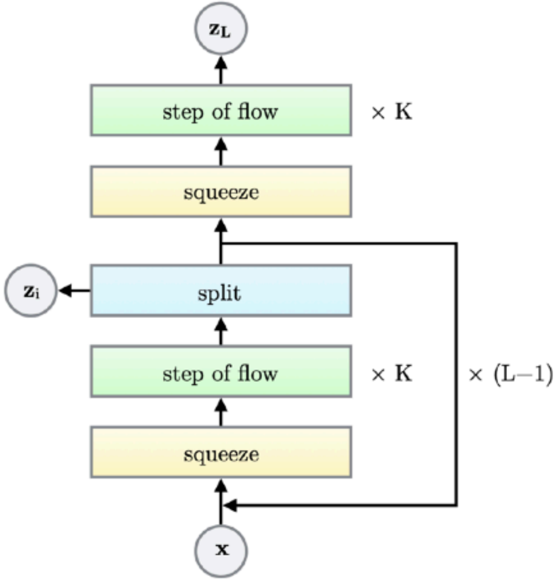
GLOW: REALNVP WITH 1X1 CONVOLUTIONS

A model contains ~1000 convolutions.

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



(a) One step of our flow.



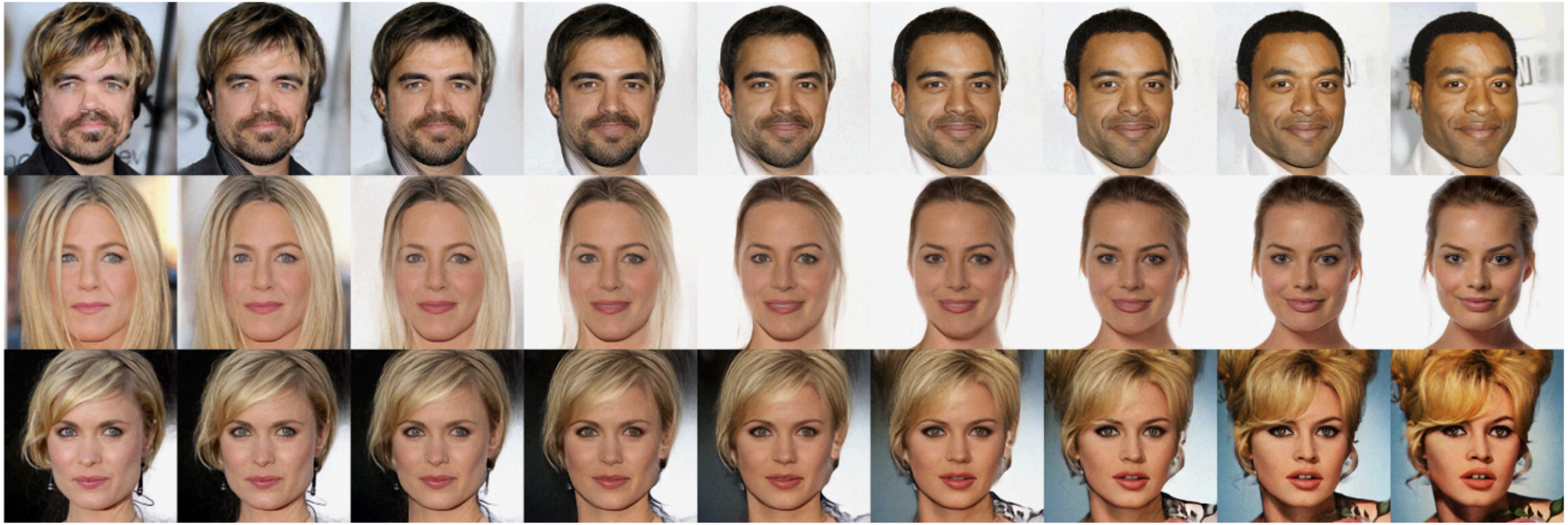
(b) Multi-scale architecture (Dinh et al., 2016).

Kingma, D. P., & Dhariwal, P. (2018). **GLOW**: Generative flow with invertible 1x1 convolutions. *NeurIPS 2018*

GLOW: SAMPLES

CelebAHQ

GLOW: LATENT INTERPOLATION



CelebAHQ

VAES WITH NORMALIZING FLOWS

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

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!