

# 02460 – Week 2 Normalising flows

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# Menu of the day

## Module 1: Generative models

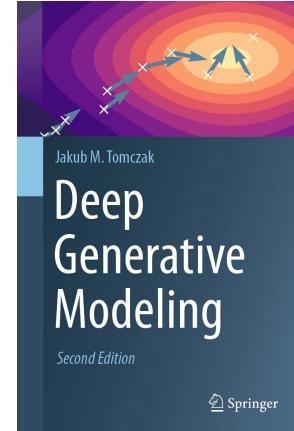
- Week 1: DLVMs
- Week 2: Flows
- Week 3: DDPMs
- Week 4: Mini-project 1

## Lecture

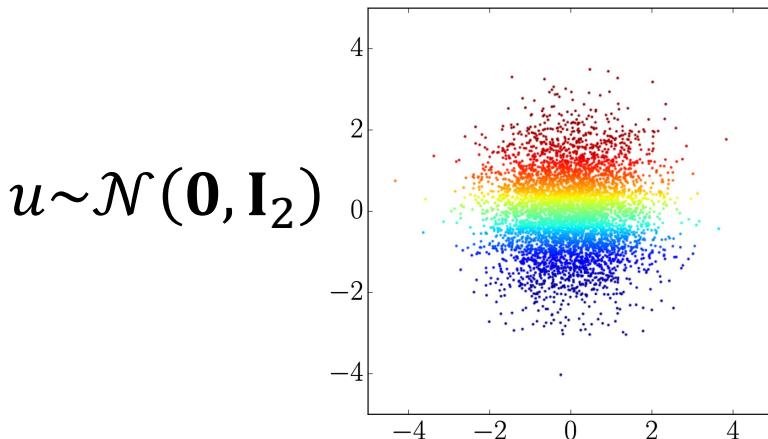
- Intro to Flows
- Flow priors in VAEs
  - Chapter 3
  - Sec. 4.4.1.6 and intro of 4.4.2

## Exercises

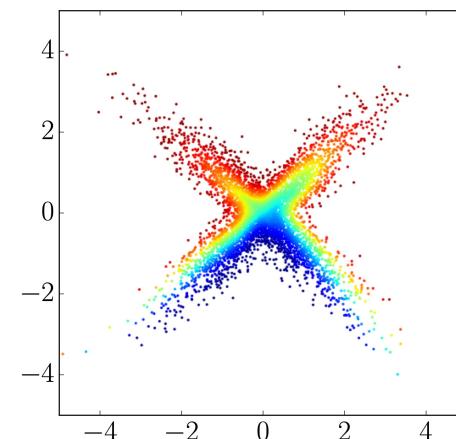
- **Theoretical**: Invertible transformations and Jacobians
- **Programming**: Implement the masked coupling layer and flow prior for a VAE



# Flow-based models



$\downarrow T(\mathbf{u})$

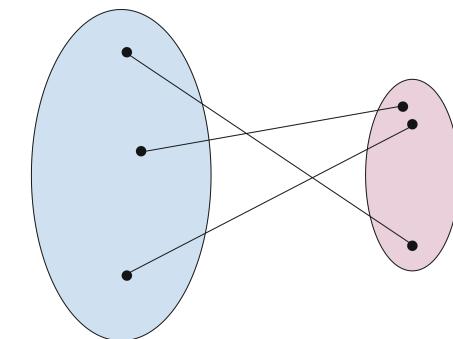


Generative process is  
 $\mathbf{u} \sim p(\mathbf{u})$   
 $\mathbf{x} = f(\mathbf{u})$

VAE generative process  
 $\mathbf{z} \sim p(\mathbf{z})$   
 $\eta = f(\mathbf{z})$   
 $\mathbf{x} \sim p(\mathbf{x}|\eta)$

How is that different from a VAE?

- If we want to calculate the density of  $\mathbf{x}$ , we need to use the **change-of-variable formula** for probability densities
- This requires  $f$  to be **invertible** (bijection) and **differentiable**



In VAEs  $\dim \mathbf{z} < \dim \mathbf{x}$ , hence  $f$  not bijective

# A simple (well-known) example

For  $u \in \mathbb{R}$ , let  $p(u) = \mathcal{N}(u|0,1)$  and  $x = T(u) = 2u + 1$

Q: What is the density of  $x$ ?

A: The density is  $p_x(x) = \mathcal{N}(x|1,2^2)$

The **change of variable formula** for scalar densities

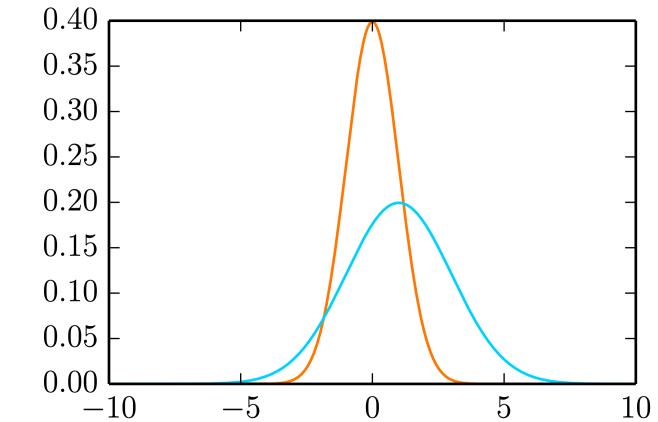
$$p_x(x) = p_u(u) \left| \frac{du}{dx} \right| = p_u(T^{-1}(x)) \left| \frac{d}{dx} T^{-1}(x) \right|$$

We have that

$$T^{-1}(x) = \frac{x - 1}{2} \quad \text{and} \quad \left| \frac{d}{dx} T^{-1}(x) \right| = \frac{1}{2}$$

$$p_x(x) = p_u\left(\frac{x - 1}{2}\right) \cdot \frac{1}{2} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{1}{2} \frac{(x - 1)^2}{2^2}\right) = \mathcal{N}(x|1,2^2)$$

How did  
we get  
there?

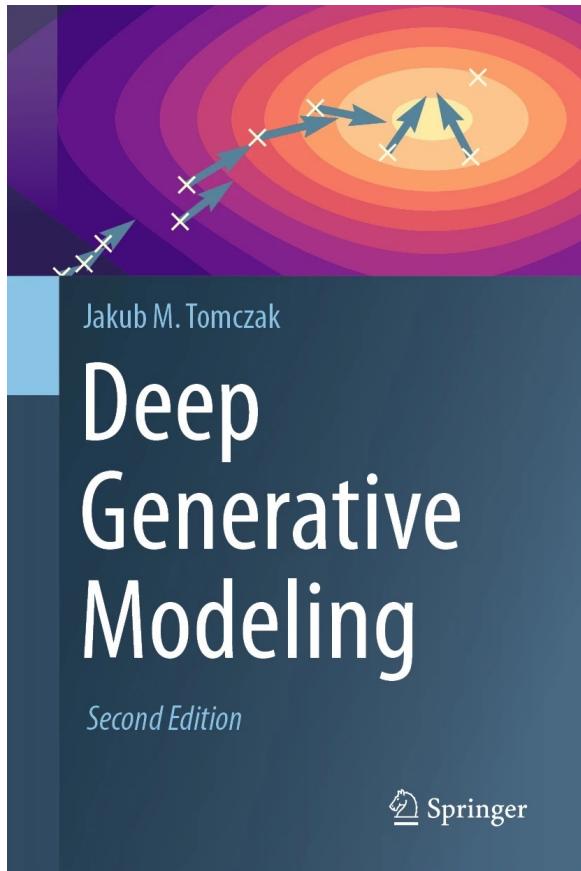


$$\mathcal{N}(u|0,1) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} u^2\right)$$

# Lecture outline

- Introduction to **normalising flows**
- **Coupling layers** and **permutation layers** (RealNVP)
- **RealNVP** and **Glow**
- Flows as **VAE priors**

# Literature



## Normalizing Flows for Probabilistic Modeling and Inference

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**Editor:** Ryan P. Adams

### Abstract

Normalizing flows provide a general mechanism for defining expressive probability distributions, only requiring the specification of a (usually simple) base distribution and a series of bijective transformations. There has been much recent work on normalizing flows, ranging from improving their expressive power to expanding their application. We believe the field has now matured and is in need of a unified perspective. In this review, we attempt to provide such a perspective by describing flows through the lens of probabilistic modeling and inference. We place special emphasis on the fundamental principles of flow design, and discuss foundational topics such as expressive power and computational trade-offs. We

# Normalizing Flows (NFs)<sup>1,2</sup>

Let  $\mathbf{u}, \mathbf{x} \in \mathbb{R}^D$  be random variables driven by the model:

$$\mathbf{u} \sim p_{\mathbf{u}}(\mathbf{u}) \quad \text{and} \quad \mathbf{x} = \mathcal{T}(\mathbf{u})$$

where

- $p_{\mathbf{u}}(\mathbf{u})$  is the **base distribution**
- The **transformation  $\mathcal{T}$  is a diffeomorphism** (invertible and  $\mathcal{T}, \mathcal{T}^{-1}$  differentiable)
- $p_{\mathbf{u}}$  is parametrized by  $\phi$
- $\mathcal{T}$  is parametrized by  $\psi$

...and it **evaluable!**  
“Exact likelihood model”

The density of  $\mathbf{x}$  is well-defined by the change of variable

$$p_{\mathbf{x}}(\mathbf{x}) = p_{\mathbf{u}}(\mathbf{u}) |\det J_{\mathcal{T}}(\mathbf{u})|^{-1} \quad \text{where} \quad \mathbf{u} = \mathcal{T}^{-1}(\mathbf{x})$$

<sup>1</sup>Esteban TG, Vanden-Eijnden E. Density estimation by dual ascent of the log-likelihood. Commun. Math. Sci., 2010.

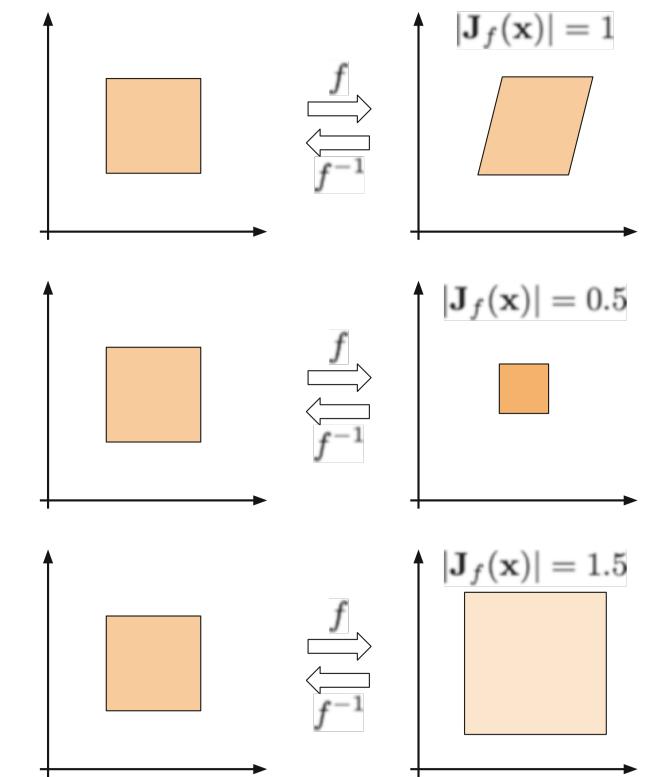
<sup>2</sup>Papamakarios G, Nalisnick E, Rezende DJ, Mohamed S, Lakshminarayanan B. Normalizing Flows for Probabilistic Modeling and Inference. JMLR, 2021.

# Flows: the Jacobian

- The **inverse function theorem**,  $J_{T^{-1}} = J_T^{-1}$ , gives the equivalent formulations

$$p_x(\mathbf{x}) = p_u(\mathbf{u}) \underbrace{|\det J_T(\mathbf{u})|^{-1}}_{= |\det J_{T^{-1}}(\mathbf{x})|}$$

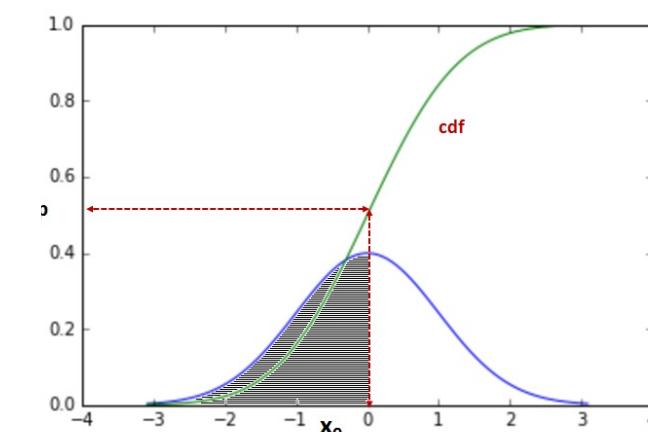
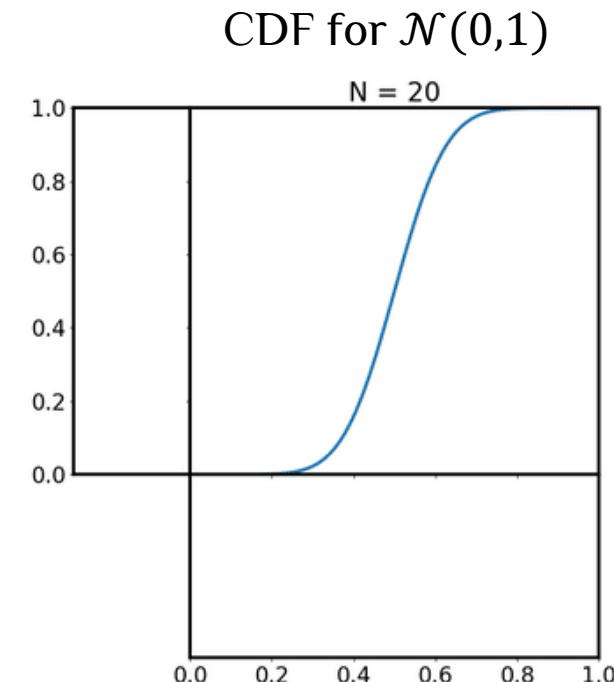
- $|\det J_T(\mathbf{u})|$  quantifies the **relative change of volume** around  $\mathbf{u}$  due to  $T$
- When  $|\det J_T(\mathbf{u})| = 1$ , then transformation is “volume preserving”



# Another simple (well-known) example

- Recall **inverse transform sampling**:
  - Procedure from for sampling from  $p(x)$
  - $p(x)$  is **any\* continuous univariate probability distribution**
  - Utilize the cumulative distribution function (CDF):  $F(x) = \int_{-\infty}^x p(x') dx'$
- We obtain **samples  $x$  from  $p(x)$**  by the procedure
 
$$u \sim U(0,1)$$

$$x = F^{-1}(u)$$
- This is a flow with  $p(x) = U(0,1)$  and  $T(u) = F^{-1}(u)$ !
- Assuming CDF is invariable, transforms  $U(0,1)$  to any distribution
- **So, a flow can represent nearly any distribution!**
  - A similar argument can be in **multiple dimensions**



# Learning NFs from data

- We want to **learn the parameters  $\psi$**  of  $T$  and possibly  $\phi$  of  $p_u$
- Given observations  $\{x_1, \dots, x_N\}$ , a natural objective is the **log-likelihood function**

$$\ell(\psi, \phi) = \sum_{n=1}^N \log p_u(T^{-1}(x_n; \psi); \phi) + \log |\det J_{T^{-1}}(x_n; \psi)|$$

- We would like to find the **ML estimate**:  $\hat{\psi}, \hat{\phi} = \arg \max_{\psi, \phi} \ell(\psi, \phi)$ .
- We can do that by SGD, but we need to:
  - Evaluate  $T^{-1}(x_n; \psi)$  and its **log Jacobian-determinant**
  - Evaluate  $p_u(u; \phi)$
  - ... and **their gradients** (i.e., backprop through them)

$$u \sim p_u(u)$$

$$x = T(u)$$

Note: For MLE, we just need:

- $T^{-1}$
- $J_{T^{-1}}$  (or  $J_T$ )

We don't need  $T$

- But  $T$  is need for sampling

# Challenge in specifying the transformation

- We usually use a standard Gaussian as base,  $p_{\mathbf{u}}(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\mathbf{0}, I_D)$
- We would like a flexible **transformation  $T$** , i.e., a neural net (NN)
- But how do we specify a **NN**, where
  1. The **function is invertible**
  2. The **log Jacobian-determinant is easy to evaluate**
- These properties are **not** fulfilled by **standard feedforward NN**
- However, we formulate **simple NN-based layers** fulfilling these
  - ... and then **we can stack them** to get expressive power!





# Composable transformation

- We can construct a flow by composing **simpler transformations**

$$\textcolor{blue}{T} = \textcolor{orange}{T}_K \circ \dots \circ \textcolor{orange}{T}_1$$

Composition is also invertible

- If each transformation  $\textcolor{orange}{T}_k$  fulfil the properties above (invertible and Jacobian)
- We can iteratively evaluate both the **forward** and **inverse** transformations

$$\mathbf{z}_k = T_k(\mathbf{z}_{k-1}) \quad \text{for } k = 1, \dots, K$$

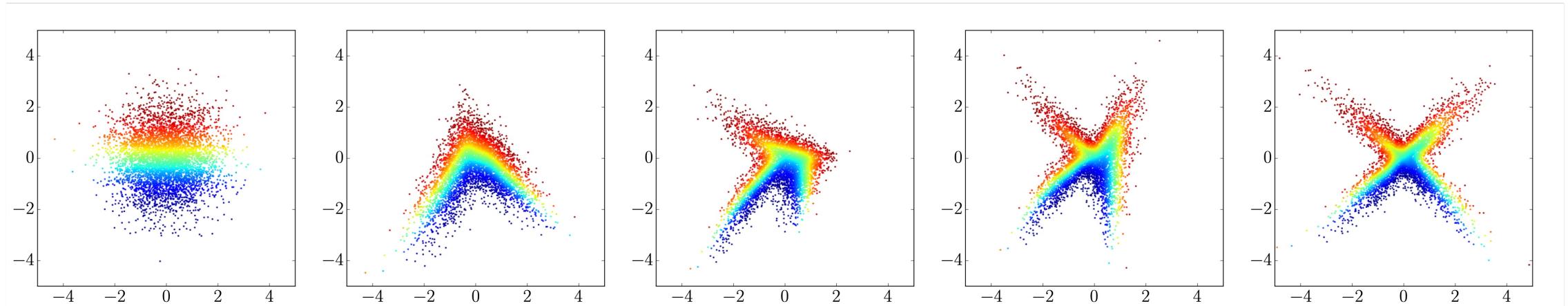
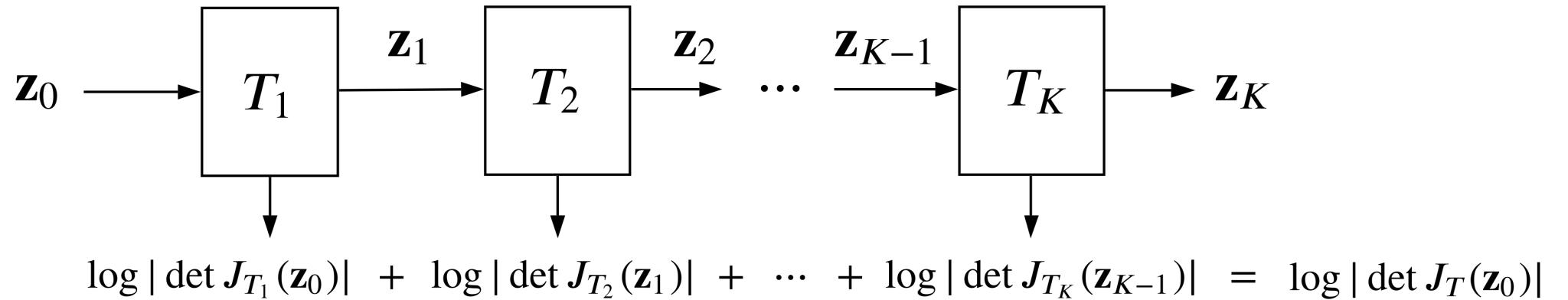
$$\mathbf{z}_{k-1} = T_k^{-1}(\mathbf{z}_k) \quad \text{for } k = K, \dots, 1$$

- ... and the log Jacobian-determinant

$$\log|\det J_{\textcolor{blue}{T}}(\mathbf{x})| = \log \left| \prod_{k=1}^K \det \textcolor{brown}{J}_{T_k}(\mathbf{x}) \right| = \sum_{k=1}^K \log|\det \textcolor{brown}{J}_{T_k}(\mathbf{x})|$$

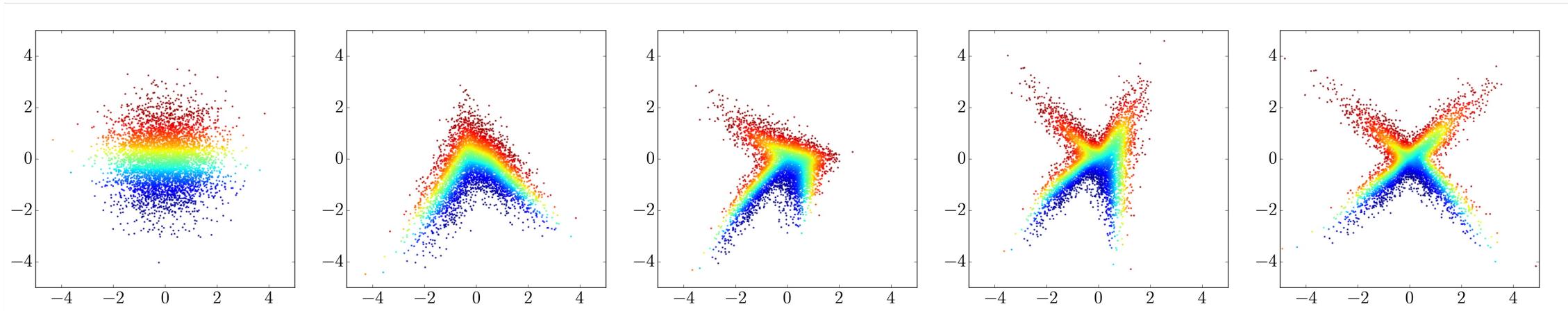
Chain rule for Jacobian

# Composable transformation



# Why are they called “Normalizing Flows”?

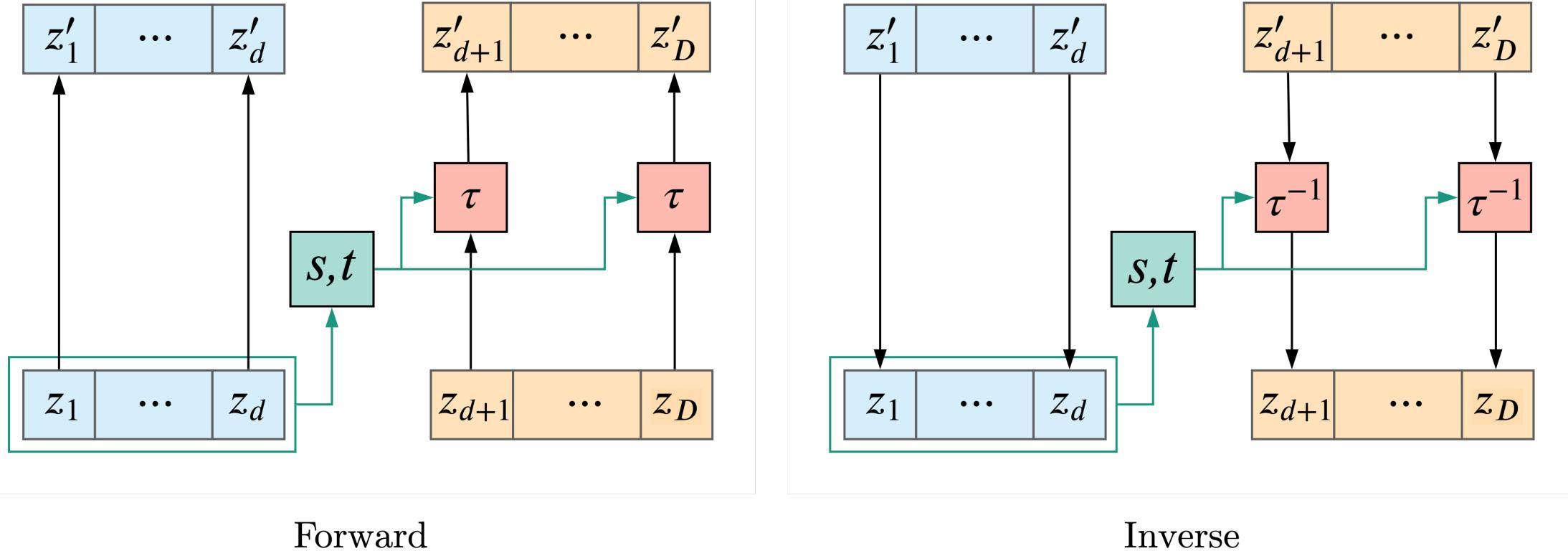
- “Flow”: Refers to the **sequence** of transformation  $T = T_K \circ \dots \circ T_1$  where a sample  $\mathbf{u}$  *flows* from the base to the output  $\mathbf{x}$
- “Normalising”: Refers to the **reverse flow** where a datum  $\mathbf{x}$  *flows* back to a **normal distributed base**, i.e., **data is normalised**



# How to construct the transformations?

- Using a **neural net**, we want to construct a transformation that is
  - **Invertible**
  - **Jacobian is easy evaluate**
- We will go in **details** with to such transformations
  - **Affine coupling layers**
  - **Permutation layers**

# Affine coupling layers



Forward

Inverse

$\tau$  is the affine transformation

$s$  and  $t$  are the scaling and translation

# Affine coupling layers

$$\forall i \leq d : z'_i = z_i$$

$$\forall i > d : z'_i = \exp(s(z_{\leq d}))_i z_i + t(z_{\leq d})_i$$

- Affine coupling layers were introduced by Dinh et al. (2015)
  - Key components in RealNVP<sup>2</sup> (Real-valued Non-Volume Preserving flows)
- The transformation  $T: \mathbf{z} \rightarrow \mathbf{z}'$  partitions  $\mathbf{z} = [\mathbf{z}_{\leq d}, \mathbf{z}_{>d}]$  at  $d < D$ :

$$\mathbf{z}'_{\leq d} = \mathbf{z}_{\leq d}$$

$$\mathbf{z}'_{>d} = \exp(s(\mathbf{z}_{\leq d})) \odot \mathbf{z}_{>d} + t(\mathbf{z}_{\leq d})$$

Arbitrary  
neural nets

$$s : \mathbb{R}^d \rightarrow \mathbb{R}^{D-d}$$

$$t : \mathbb{R}^d \rightarrow \mathbb{R}^{D-d}$$

- Since  $\mathbf{z}'_{>d}$  is an affine transformation of  $\mathbf{z}_{>d}$ , its easily invertible

$$\mathbf{z}_{\leq d} = \mathbf{z}'_{\leq d}$$

$$\mathbf{z}_{>d} = \exp(-s(\mathbf{z}_{\leq d})) \odot (\mathbf{z}'_{>d} - t(\mathbf{z}_{\leq d}))$$

$$\mathbf{z}'_{>d} = \exp(s(\mathbf{z}_{\leq d})) \odot \mathbf{z}_{>d} + t(\mathbf{z}_{\leq d})$$

$$\mathbf{z}'_{>d} - t(\mathbf{z}_{\leq d}) = \exp(s(\mathbf{z}_{\leq d})) \odot \mathbf{z}_{>d}$$

$$\exp(-s(\mathbf{z}_{\leq d})) \odot (\mathbf{z}'_{>d} - t(\mathbf{z}_{\leq d})) = \mathbf{z}_{>d}$$

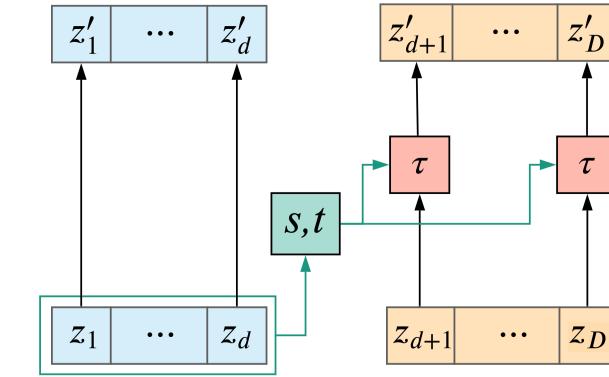
<sup>1</sup>Dinh L, Krueger D, and Bengio Y. NICE: Non-linear independent components estimation. ICLR workshop track, 2015.

<sup>2</sup>Dinh L, Sohl-Dickstein J, Bengio S. Density estimation using Real NVP. ICLR, 2017.

# Affine coupling layers: the Jacobian (1)

- It turns out, that **the Jacobian is easy**
- Let's write it on the following block form

$$J_T(\mathbf{z}) = \begin{bmatrix} \frac{\partial \mathbf{z}'_{\leq d}}{\partial \mathbf{z}_{\leq d}} & \frac{\partial \mathbf{z}'_{\leq d}}{\partial \mathbf{z}_{>d}} \\ \frac{\partial \mathbf{z}'_{>d}}{\partial \mathbf{z}_{\leq d}} & \frac{\partial \mathbf{z}'_{>d}}{\partial \mathbf{z}_{>d}} \end{bmatrix}$$



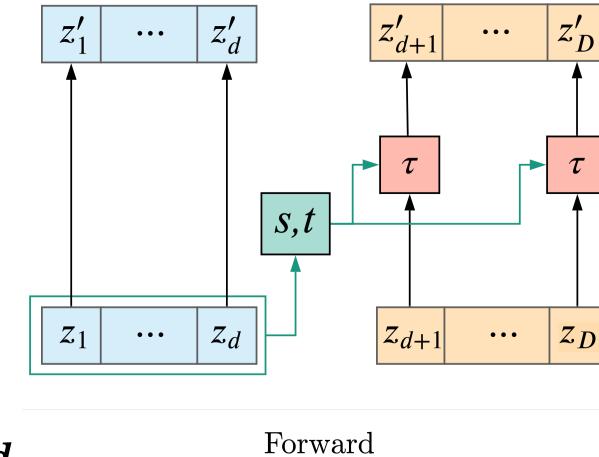
Forward

# Affine coupling layers: the Jacobian (2)

Recall that  $\mathbf{z}'_{\leq d} = \mathbf{z}_{\leq d}$ , and so we find

$$\frac{\partial \mathbf{z}'_{\leq d}}{\partial \mathbf{z}_{\leq d}} = \begin{bmatrix} \frac{\partial z'_1}{\partial z_1} & \dots & \frac{\partial z'_1}{\partial z_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial z'_d}{\partial z_1} & \dots & \frac{\partial z'_d}{\partial z_d} \end{bmatrix} = \begin{bmatrix} 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1 \end{bmatrix} = I_{d \times d}$$

$$\frac{\partial \mathbf{z}'_{\leq d}}{\partial \mathbf{z}_{>d}} = \begin{bmatrix} \frac{\partial z'_1}{\partial z_{d+1}} & \dots & \frac{\partial z'_1}{\partial z_D} \\ \vdots & \ddots & \vdots \\ \frac{\partial z'_d}{\partial z_{d+1}} & \dots & \frac{\partial z'_d}{\partial z_D} \end{bmatrix} = \begin{bmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix} = 0_{d \times (D-d)}$$



# Affine coupling layers: the Jacobian (3)

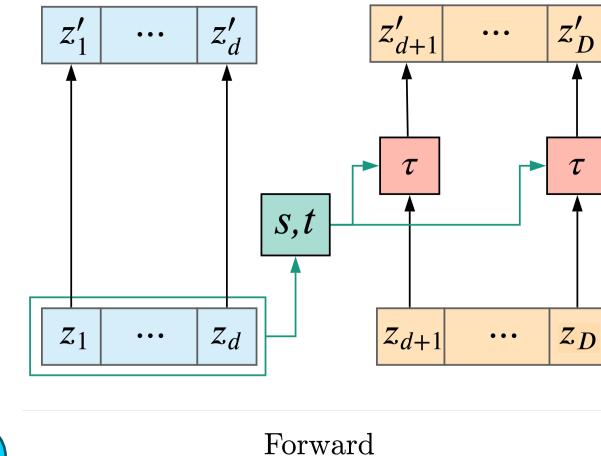
Recall that  $\forall i > d : z'_i = \exp(s(z_{\leq d}))_i z_i + t(z_{\leq d})_i$

$$\frac{\partial \mathbf{z}'_{>d}}{\partial \mathbf{z}_{>d}} = \begin{bmatrix} \frac{\partial z'_{d+1}}{\partial z_{d+1}} & \dots & \frac{\partial z'_{d+1}}{\partial z_D} \\ \vdots & \ddots & \vdots \\ \frac{\partial z'_D}{\partial z_{d+1}} & \dots & \frac{\partial z'_D}{\partial z_D} \end{bmatrix}$$

Q: What is this block of the Jacobian?

$$= \begin{bmatrix} \exp(s(\mathbf{z}_{\leq d}))_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \exp(s(\mathbf{z}_{\leq d}))_{D-d} \end{bmatrix}$$

$$= \text{diag}(\exp(s(\mathbf{z}_{\leq d})))$$



# Affine coupling layers: the Jacobian (3)

- This mean that

$$J_T(\mathbf{z}) = \begin{bmatrix} I_{d \times d} & 0_{d \times (D-d)} \\ \frac{\partial \mathbf{z}'_{>d}}{\partial \mathbf{z}_{\leq d}} \text{ diag}(\exp(s(\mathbf{z}_{\leq d}))) \end{bmatrix}$$

Q: Is this easy?

- Since  $J_T(\mathbf{z})$  is triangular, we have

$$\det J_T(\mathbf{z}) = \prod_{i=1}^{D-d} \exp(s(\mathbf{z}_{\leq d}))_i = \exp\left(\sum_{i=1}^{D-d} s(\mathbf{z}_{\leq d})_i\right)$$

Recall, for triangular matrix  $A$   
we have  $\det A = \prod_i a_{i,i}$

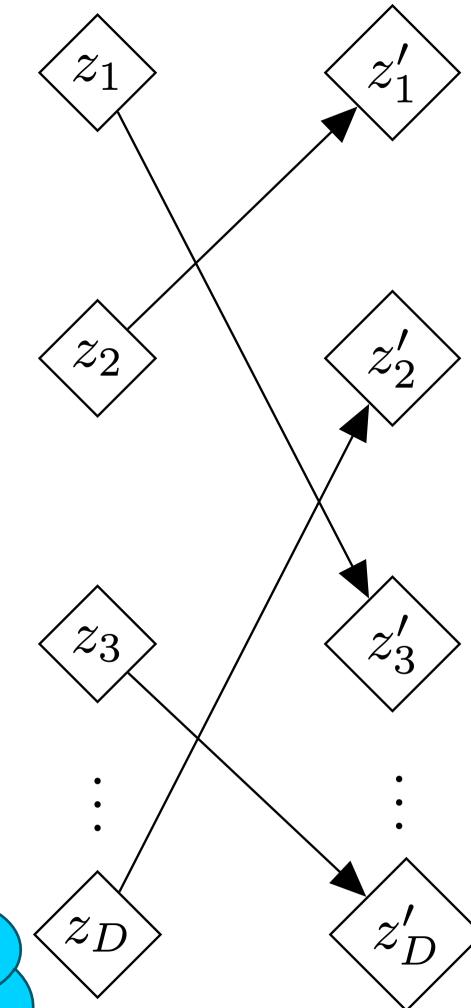
# Permutation layer

- With coupling layers, we need to **permute** the variables
  - If the partitioning is fixed, e.g.,  $d = \frac{D}{2}$ , some variables will never be transformed
  - A permutation is **invertible**
  - A permutation is **volume preserving**, i.e.,  $|\det J_T(\mathbf{z})| = 1$

Q: What is  $|\det J_T(\mathbf{u})|$  for a permutation?

Hint: A permutation is a linear transformation  $T(\mathbf{z}) = A\mathbf{z}$ , where  $A$  is a permutation matrix and  $J_T(\mathbf{z}) = A$ .

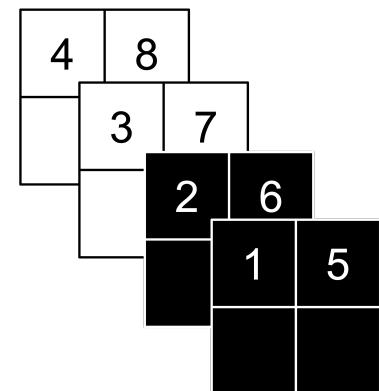
Hint: Recall, if we swap two rows (or columns) in a matrix, the determinant change sign.



# RealNVP<sup>1</sup>

- RealNVP employ affine coupling layers
- The partitioning is implemented by masking:
  - Masking variables in a **checkerboard** pattern (alternating)
    - This helps to learn **spatial dependencies**
  - Masking **channel-wise**
    - Ensures the checkerboard masking is **not redundant**
  - Use **squeezing**: reshape input tensor
    - Converts special dimensions to channels
    - Gives a **multi-scale** behaviour

1	2	5	6
3	4	7	8



<sup>1</sup>Dinh L, Sohl-Dickstein J, Bengio S. Density estimation using Real NVP. ICLR, 2017. Figures from <sup>1</sup>.



# RealNVP<sup>1</sup>: Factoring out variables

- At regular intervals, **half of the dimensions** are “factored out”
  - i.e. they are **not transformed anymore**
- Different pixels are **Gaussianized**
  - In an **earlier layer** (fine scale)
  - In a **later layer** (coarser scale)

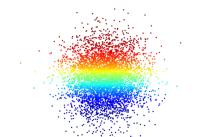
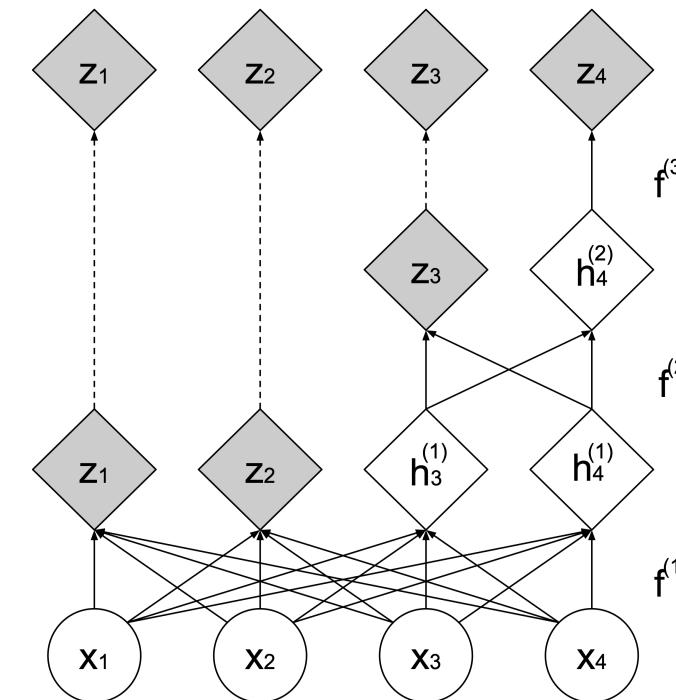
$$h^{(0)} = x$$

abstraction

$$(z^{(i+1)}, h^{(i+1)}) = f^{(i+1)}(h^{(i)})$$

$$z^{(L)} = f^{(L)}(h^{(L-1)})$$

$$z = (z^{(1)}, \dots, z^{(L)})$$



<sup>1</sup>Dinh L, Sohl-Dickstein J, Bengio S. Density estimation using Real NVP. ICLR, 2017. Figures from <sup>1</sup>.

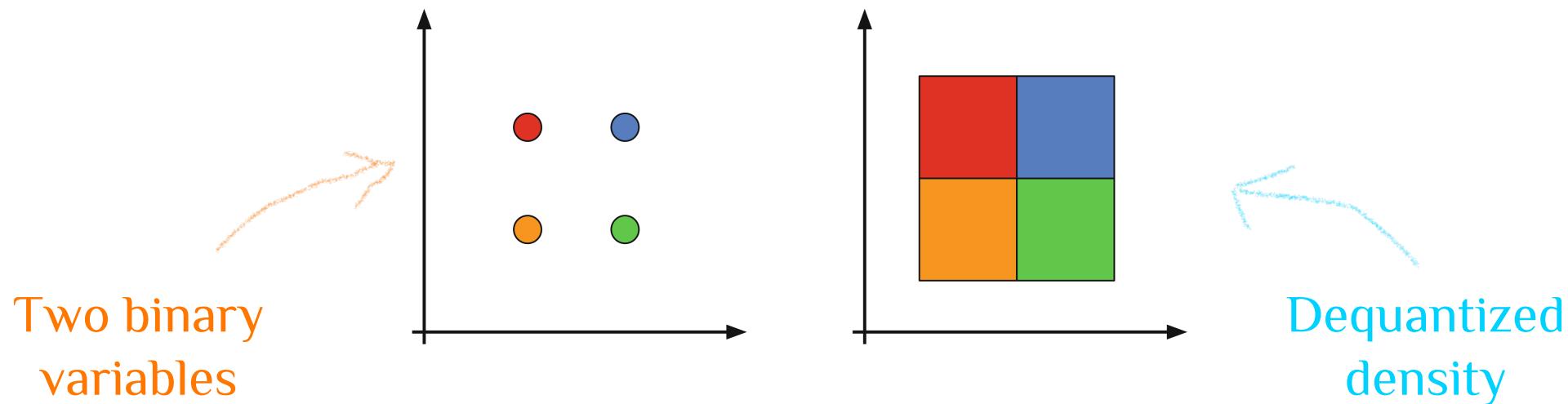
# Dequantization

In flows we assume that  $\mathbf{x} \in \mathbb{R}^D$ , i.e., real-valued

**Q: How can we model images  $\tilde{\mathbf{x}} \in \{0, 1, \dots, 255\}^D$**

**A: We can add noise (dequantize) to  $\tilde{\mathbf{x}}$**

$$x_i = \tilde{x}_i + u \quad \text{where} \quad u \sim U(-0.5, 0.5)$$



# RealNVP<sup>1</sup>

Data

Samples

Imagenet  
(64x64)



CelebA



LSUN  
(bedroom)



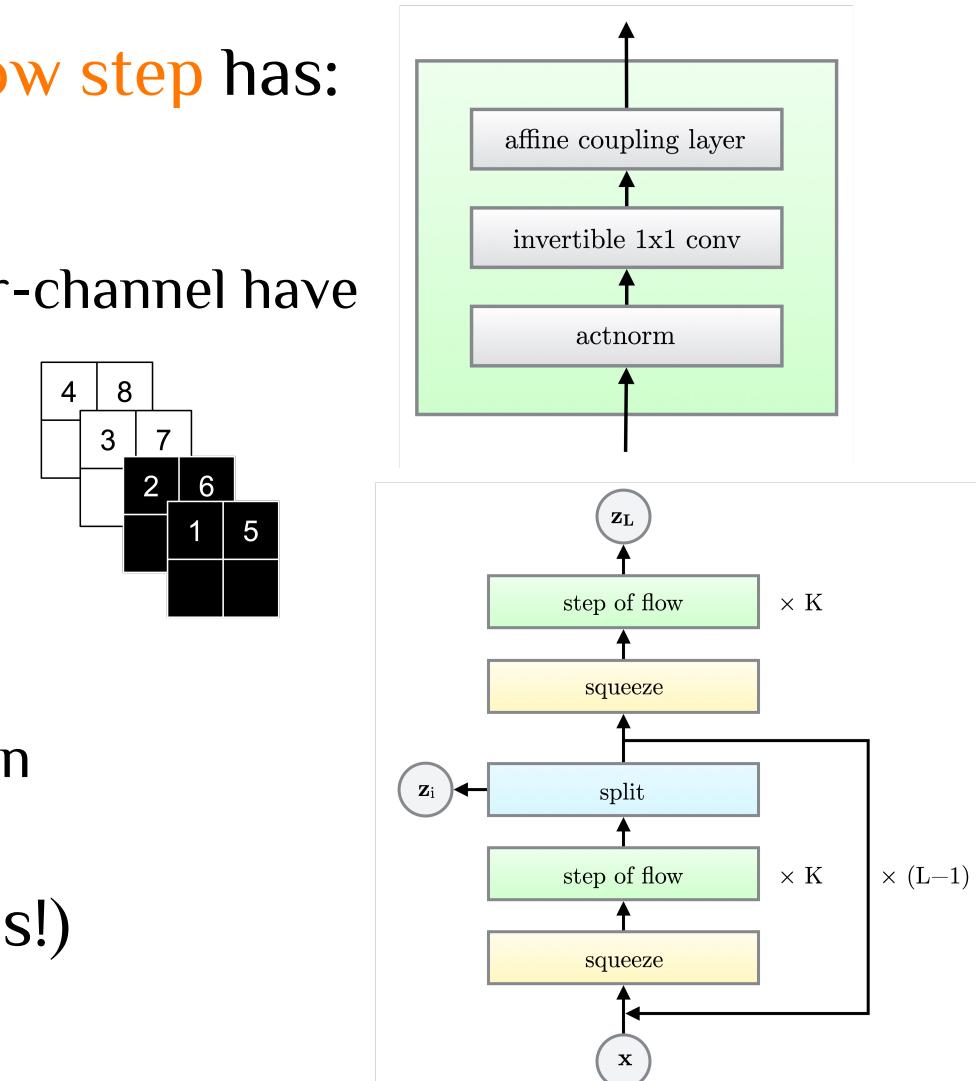
# Glow: Generative flow with $1 \times 1$ convolutions<sup>1</sup>

Glow: an evolution of RealNVP, where each **flow step** has:

- **Actnorm** (a simplified batch norm)
  - **Per channel learned scale and bias layer**
  - Initialized such that post-actnorm activations per-channel have zero mean and unit variance on a mini batch
- **Affine coupling layers**
  - Only split: **channels dimension into two halves**
- **Invertible  $1 \times 1$  convolution**
  - A **channel wise linear transformation**
  - A “generalization” of a permutation
  - Invertibility ensured by  $W = PLU$  parametrisation

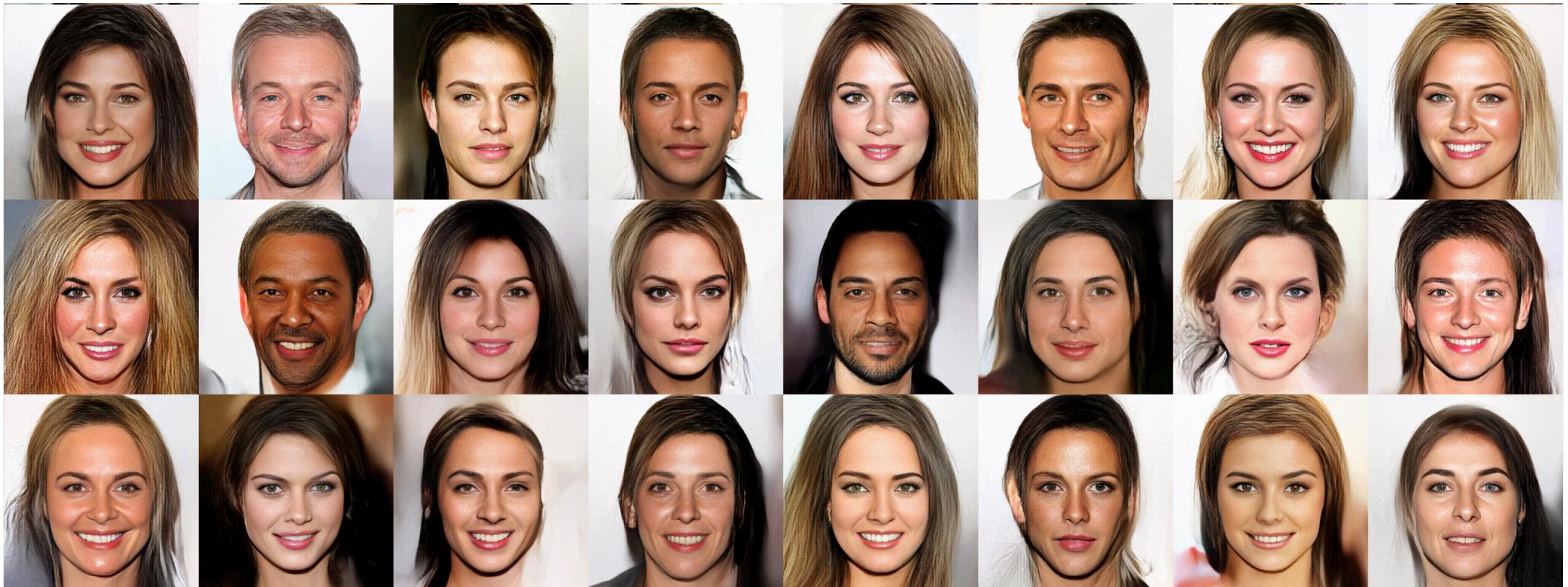
Use a **multi scale architecture** as RealNVP

- For CelebA:  $L = 6$  and  $K = 32$  (192 flow steps!)



<sup>1</sup> Kingma DP, Dhariwal P. Glow: generative flow with invertible  $1 \times 1$  convolutions. NeurIPS, 2018.

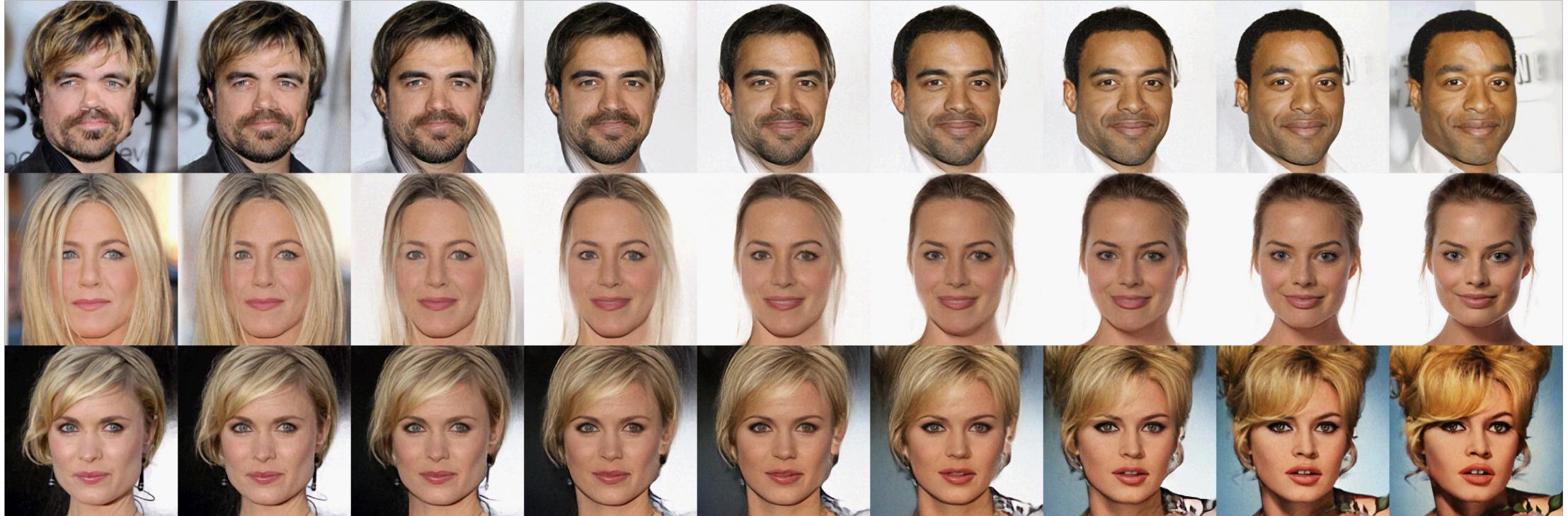
# Glow: samples from model on CelebA HQ<sup>1</sup>



<sup>1</sup> Kingma DP, Dhariwal P. Glow: generative flow with invertible  $1 \times 1$  convolutions. NeurIPS, 2018.

# Glow: Linear interpolation in “latent space” between real images<sup>1</sup>

Q: Why the quotation marks?



<sup>1</sup> Kingma DP, Dhariwal P. Glow: generative flow with invertible  $1 \times 1$  convolutions. NeurIPS, 2018.

# Classes of flows (1)<sup>1</sup>

- **Linear flows**

$$\mathbf{z}' = W\mathbf{z}$$

- Main challenge **parametrizing  $W$**  so it's **invertible**
- **Permutation** is a special case

- **Autoregressive flows**

$$z'_i = \tau(z_i; \mathbf{h}_i) \text{ where } \mathbf{h}_i = c_i(z_{<i})$$

where  $\tau$  is strictly monotonic (inevitable) and  $c_i$  is any neural net

- **Jacobian** is triangular and **tractable**
- **Affine coupling layers** is a special case

# Classes of flows (2)<sup>1</sup>

- **Residual flows**

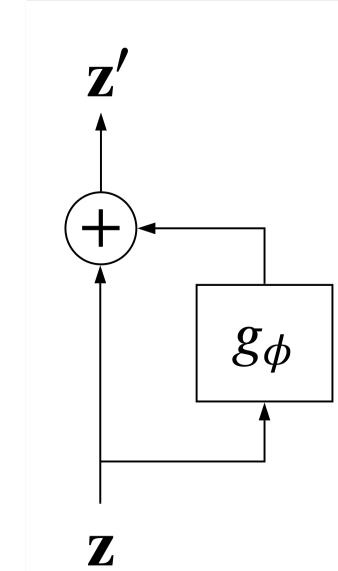
$$\mathbf{z}' = \mathbf{z} + g_\phi(\mathbf{z})$$

Invertible if  $g_\phi(\mathbf{z})$  is **contractive**, i.e.,

$$\exists L < 1, \forall z, \tilde{z} \in \mathbb{R}^d : \delta(F(z), F(\tilde{z})) \leq L \delta(z, \tilde{z})$$

where  $\delta$  is a **distance function**

- A contractive map brings inputs closer together
- **Contractive: Lipschitz continuous**, with the additional constraint  $L < 1$ 
  - **Composition** of  $K$  Lipschitz functions **are Lipschitz** with  $L = \prod_{k=1}^K L_k$
  - Standard **nonlinearities are Lipschitz** with  $L \leq 1$ , e.g., logistic sigmoid and ReLU
  - **Linear layer** can be made **contractive** using **spectral normalization**
- **The Jacobian is difficult** (autodiff or power series approximation)



# What can we use them for?

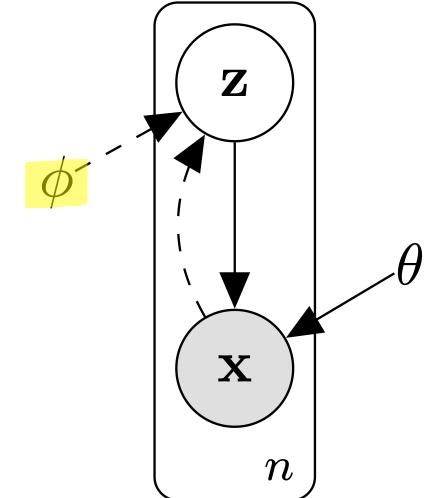
- **Density estimation**
  - With **exact likelihood**
  - Can **approximate any distribution**
  - But, layers are simple, so many are required (c.f. Glow)
- **Variational inference**
  - A flow can be a very **flexible approximate posterior**
- **Flexible priors in VAEs**
- ... and more (see section 6 in Papamakarios et al.<sup>1</sup>)



# Let's revisit the VAE and ELBO

likelihood prior

- Recall the model  $p_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})$
- Learn model by optimizing **ELBO wrt.  $\theta, \phi$**



$$\begin{aligned}
 \log p_\theta(\mathbf{x}) &\geq \mathcal{L}(\theta, \phi) = \mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})} \left[ \log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{x}|\mathbf{z})} \right] \quad \text{tractable objective} \\
 &= \mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z})} [\log p_\theta(\mathbf{x}|\mathbf{z})] - \text{KL}[q_\phi(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z})] \\
 &= \log p_\theta(\mathbf{x}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})) \quad \text{gap}
 \end{aligned}$$

variational distribution

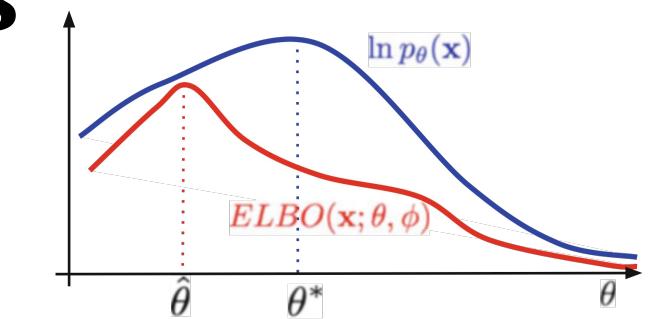
- Gradients are calculated from the **reparameterized ELBO**

$$\mathcal{L}(\theta, \phi) = \mathbb{E}_{\epsilon \sim \mathcal{N}(\epsilon|0, I_M)} [\log p_\theta(\mathbf{x} | \mu_\phi(\mathbf{x}) + \sigma_\phi(\mathbf{x}) \odot \epsilon)] - \text{KL}[q_\phi(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z})]$$

# Inference suboptimality in VAEs<sup>1</sup>

- We can write the **ELBO  $\mathcal{L}$**  as

$$\log p_\theta(\mathbf{x}) = \mathcal{L}(\theta, \phi) + \overbrace{\text{KL}\left(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right)}^{\geq 0}$$



- The KL-term is the gap between ELBO and true log-likelihood

- Approximation gap:**

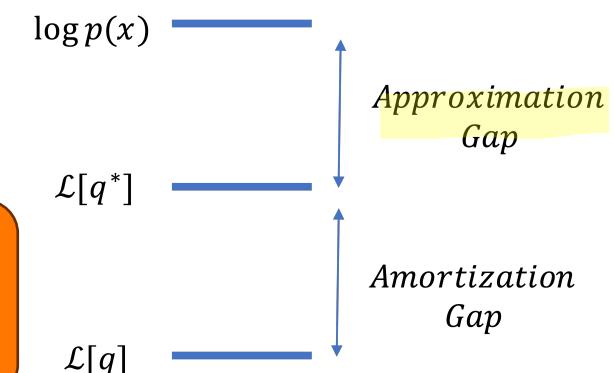
tight when the true posterior belongs to the variational family

- Amortisation gap:**

tight when encoder has large capacity

- We can tighten **approximation gap** with a more expressive variational family!

We can use a flow as the variational distribution in a VAE



Figures from 1,2

<sup>1</sup>Cremer C, Li X, Duvenaud D. Inference suboptimality in variational autoencoders. ICML, 2018.

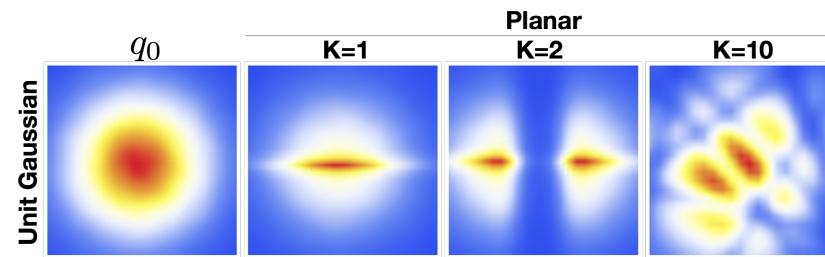
<sup>2</sup>Tomczak JM. Deep generative modeling. Springer, 2022.

# Variational inference with flows<sup>1</sup>

- Rezende and Mohamed (2015)<sup>1</sup> use a **residual flow**, called planar

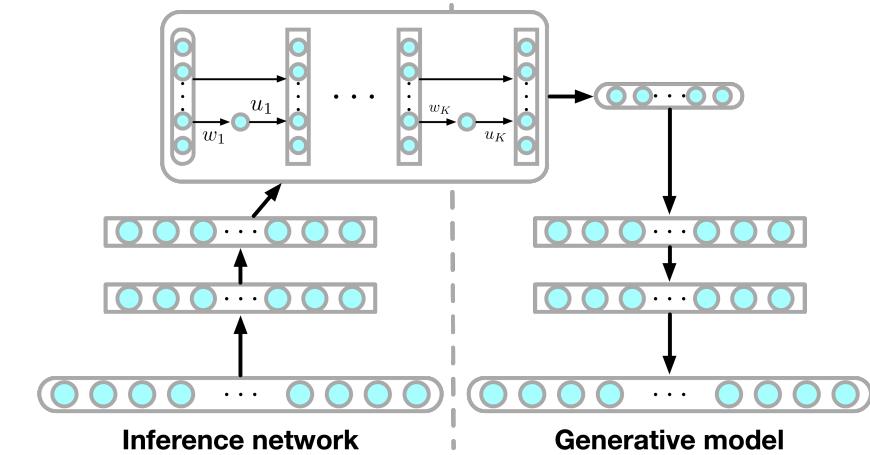
$$T_k(\mathbf{u}) = \mathbf{u} + \mathbf{v}\sigma(\mathbf{w}^T\mathbf{u} + b)$$

- $\sigma$  is an activation function and invertible if  $\mathbf{w}^T\mathbf{v} > -\left(\sup_x \sigma(x)\right)^{-1}$



**Test set ELBO** on binarized  
MNIST using  $k$  transformation

Model	$-\ln p(\mathbf{x})$
DLGM diagonal covariance	$\leq 89.9$
DLGM+NF ( $k = 10$ )	$\leq 87.5$
DLGM+NF ( $k = 20$ )	$\leq 86.5$
DLGM+NF ( $k = 40$ )	$\leq 85.7$
DLGM+NF ( $k = 80$ )	$\leq 85.1$



# Recall: Improving the prior of a VAE

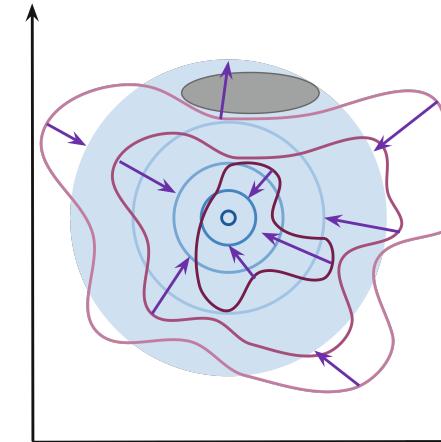
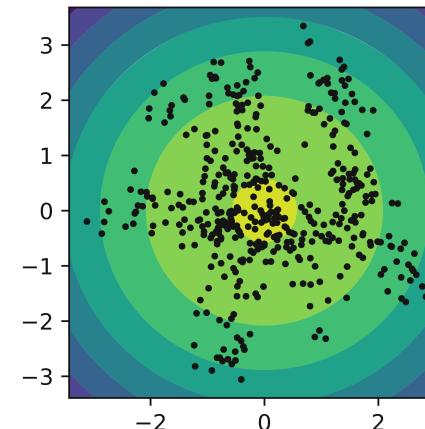
$$\mathcal{L}(\theta, \phi) = \underbrace{\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}|\mathbf{z})]}_{\text{reconstruction term}} - \underbrace{\text{KL}[q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p_{\lambda}(\mathbf{z})]}_{\text{regularisation term}}$$

- We can rewrite the **regularization** term as

$$\mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} \left[ -\text{KL}[q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p_{\lambda}(\mathbf{z})] \right] = -\mathbb{C}\mathbb{E}[q_{\phi}(\mathbf{z}) \parallel p_{\lambda}(\mathbf{z})] + \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} \left[ \mathbb{H}[q_{\phi}(\mathbf{z}|\mathbf{x})] \right]$$

where  $q_{\phi}(\mathbf{z}) = \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} [q_{\phi}(\mathbf{z}|\mathbf{x})] \approx \frac{1}{N} \sum_n q_{\phi}(\mathbf{z}|\mathbf{x}_n)$  is the **aggregated posterior**

- Difficulties in optimising the CE** wrt.  $q_{\phi}$  for a fixed prior gives rise **holes**
- The cross entropy, is minimised wrt.  $p_{\lambda}(\mathbf{z})$  when  $p_{\lambda}(\mathbf{z}) = q_{\phi}(\mathbf{z})$
- This can be addressed by learning the prior  $p_{\lambda}(\mathbf{z})$



# Flow-based prior

- Let's write the ELBO (again) for a learnable prior flow-based prior  $p_{\lambda}(\mathbf{z}) = p_{\mathbf{z}}(\mathbf{z}) = p_{\mathbf{u}}(\mathbf{u})|\det J_T(\mathbf{u})|^{-1}$  and  $\mathbf{u} = T^{-1}(\mathbf{z})$ :

$$\begin{aligned}
 \mathcal{L} &= \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[ \log \frac{p_{\theta, \lambda}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \\
 &= \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[ \log p_{\theta}(\mathbf{x}|\mathbf{z}) + \log p_{\lambda}(\mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x}) \right] \\
 &= \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[ \log p_{\theta}(\mathbf{x}|\mathbf{z}) + \log \left( p_{\mathbf{u}}(T^{-1}(\mathbf{z})) |\det J_T(T^{-1}(\mathbf{z}))|^{-1} \right) - \log q_{\phi}(\mathbf{z}|\mathbf{x}) \right] \\
 &= \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[ \log p_{\theta}(\mathbf{x}|\mathbf{z}) - \log |\det J_T(T^{-1}(\mathbf{z}))| \right] + \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[ \log \frac{p_{\mathbf{u}}(T^{-1}(\mathbf{z}))}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right]
 \end{aligned}$$

- We recover the usual ELBO, we one additional term  

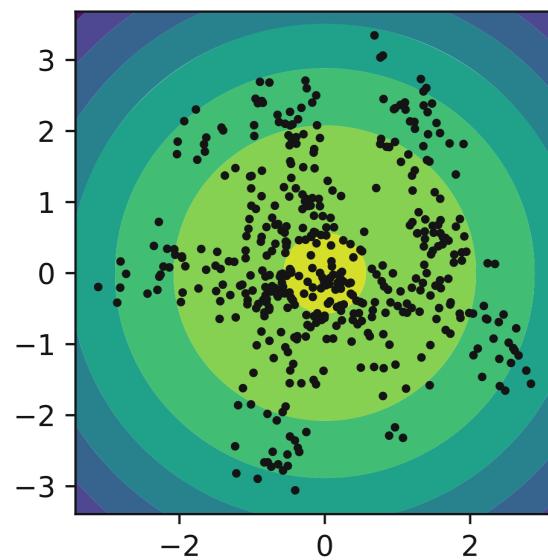
$$-\text{KL}\left(q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p_{\mathbf{u}}(T^{-1}(\mathbf{z}))\right)$$
- Gradients are straight forward

# Flow-based prior on digits dataset<sup>1</sup>

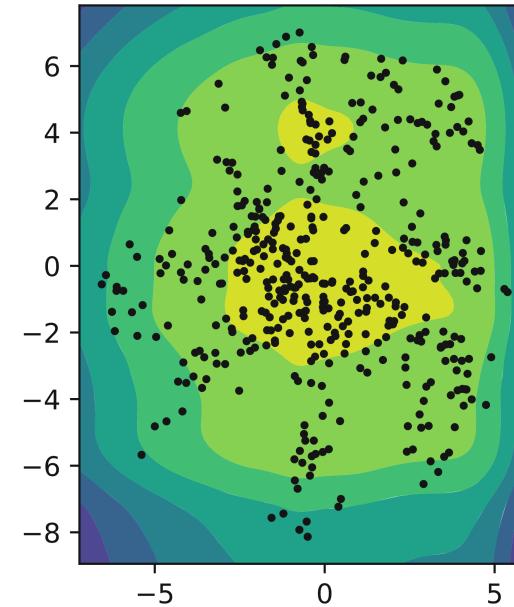


Examples from Jakub's book

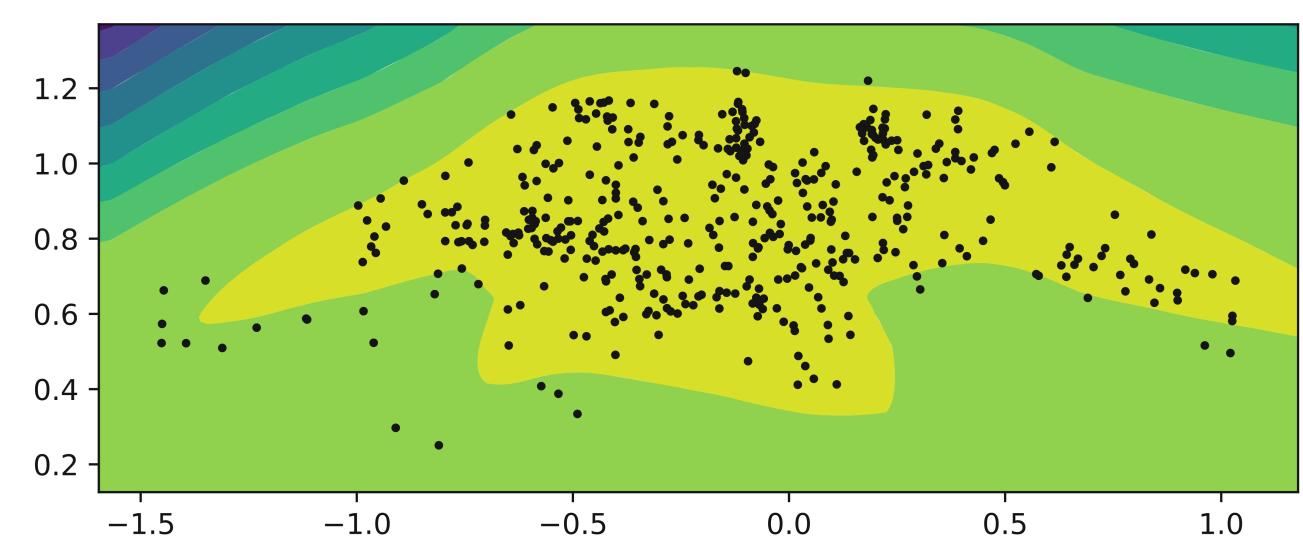
Standard Gaussian prior



MoG prior



RealNVP prior



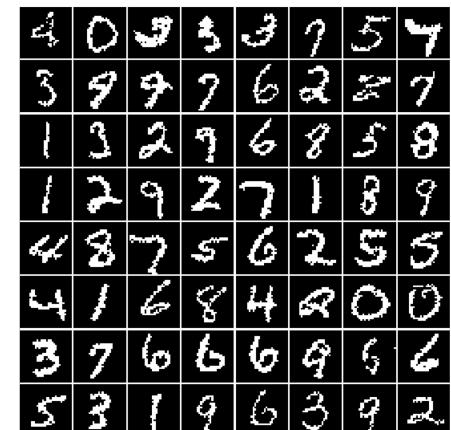
<sup>1</sup>Tomczak JM. Deep generative modeling. Springer, 2022.

# To learn prior or variational posterior?

- Flow prior and flow var. posterior have the same computational cost
- You have a more expressive model with a flow prior
  - Therefore, Chen et al. (2017)<sup>1</sup> argues for using a flow prior
- Empirical validation<sup>1</sup>, using
  - Inverse autoregressive flow (IAF) variational posterior
  - Autoregressive flow (AF) prior

Table 1: Statically Binarized MNIST

Model	NLL Test
Normalizing flows (Rezende & Mohamed, 2015)	85.10
DRAW (Gregor et al., 2015)	< 80.97
Discrete VAE (Rolle, 2016)	81.01
PixelRNN (van den Oord et al., 2016a)	79.20
IAF VAE (Kingma et al., 2016)	79.88
AF VAE	79.30
VLAЕ	<b>79.03</b>



(b) Samples from VLAЕ

<sup>1</sup>Chen X, Kingma DP, Salimans T, Duan Y, Dhariwal P, Schulman J, Sutskever I, Abbeel P. Variational Lossy Autoencoder. ICLR, 2017.

# Flows vs VAEs<sup>1</sup>

## Flows

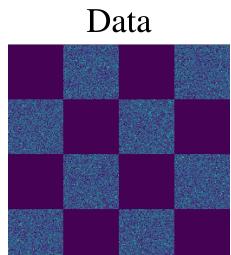
- Exact likelihood
- No dimensionality reduction
- Don't model discrete data or discrete nature data (well)

Performs a bijective transformation of the prior

## VAEs

- Approximate likelihood
- Dimensionality reduction
- Can model discrete data or discrete nature data

Performs a stochastic transformation of the prior



# Take-away!

- Flow are models for density estimation
  - With exact likelihood
  - Can approximate any distribution
  - However, layers are simple, so many are required (c.f., Glow)
- We can use them for
  - Flexible posteriors in variational inference
  - Flexible priors in VAEs
  - ... and more
- In a VAE, it is preferable to use a flow prior

# Thank you!