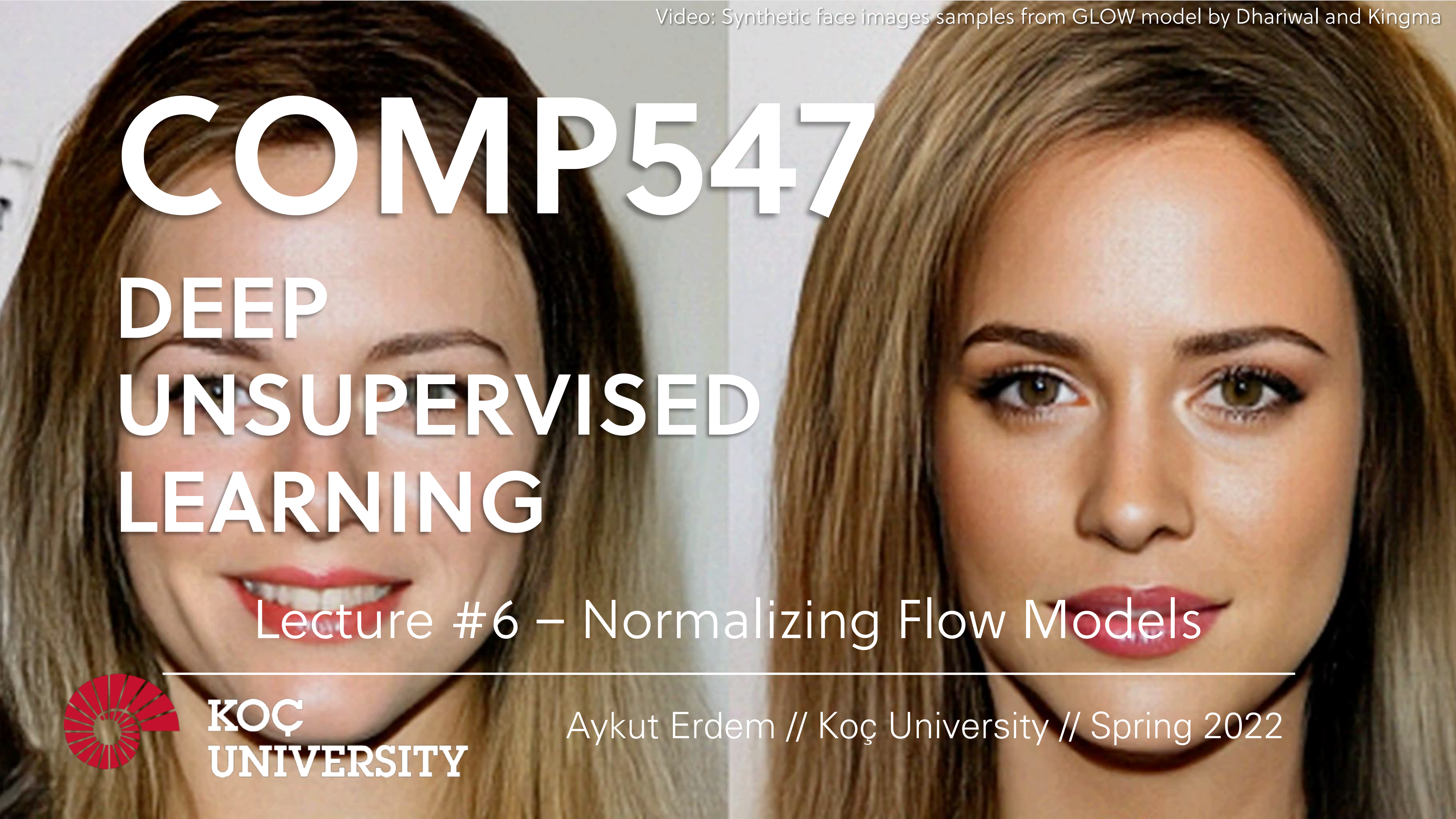

Video: Synthetic face images samples from GLOW model by Dhariwal and Kingma

# COMP547

# DEEP UNSUPERVISED LEARNING

## Lecture #6 – Normalizing Flow Models

KOÇ UNIVERSITY

Aykut Erdem // Koç University // Spring 2022

# Previously on COMP547

- Motivation
- Simple generative models: histograms
- Parameterized distributions and maximum likelihood
- Causal masked neural models
- Other things to be aware of

# Overview

- What do we want from a generative model?
  - Good fit to the training data (really, the underlying distribution!)
  - For new x, ability to evaluate $p_\theta(x)$
  - Ability to sample from $p_\theta(x)$
  - A latent representation / embedding space that's meaningful
- Recall L2 Autoregressive Models?
  - Check many boxes except
    - Sampling is serial (hence slow)
    - Lacks latent representation / embedding space
    - Limited to discrete data (at least in terms of where experimental success has been)
- Flow Models will check all boxes (but performance not as good as other models…)

# Our Goal Today

- How to fit a density model $p_\theta(x)$ with continuous $x \in \mathbb{R}^n$

- What do we want from this model?
  - Good fit to the training data (really, the underlying distribution!)
  - For new $x$, ability to evaluate $p_\theta(x)$
  - Ability to sample from $p_\theta(x)$
  - A latent representation / embedding space that's meaningful

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Differences from Autoregressive Models from last lecture

# Lecture overview

- Foundations of Flows (1-D)
- 2-D Flows
- N-D Flows
- Dequantization

**Disclaimer:** Much of the material and slides for this lecture were borrowed from

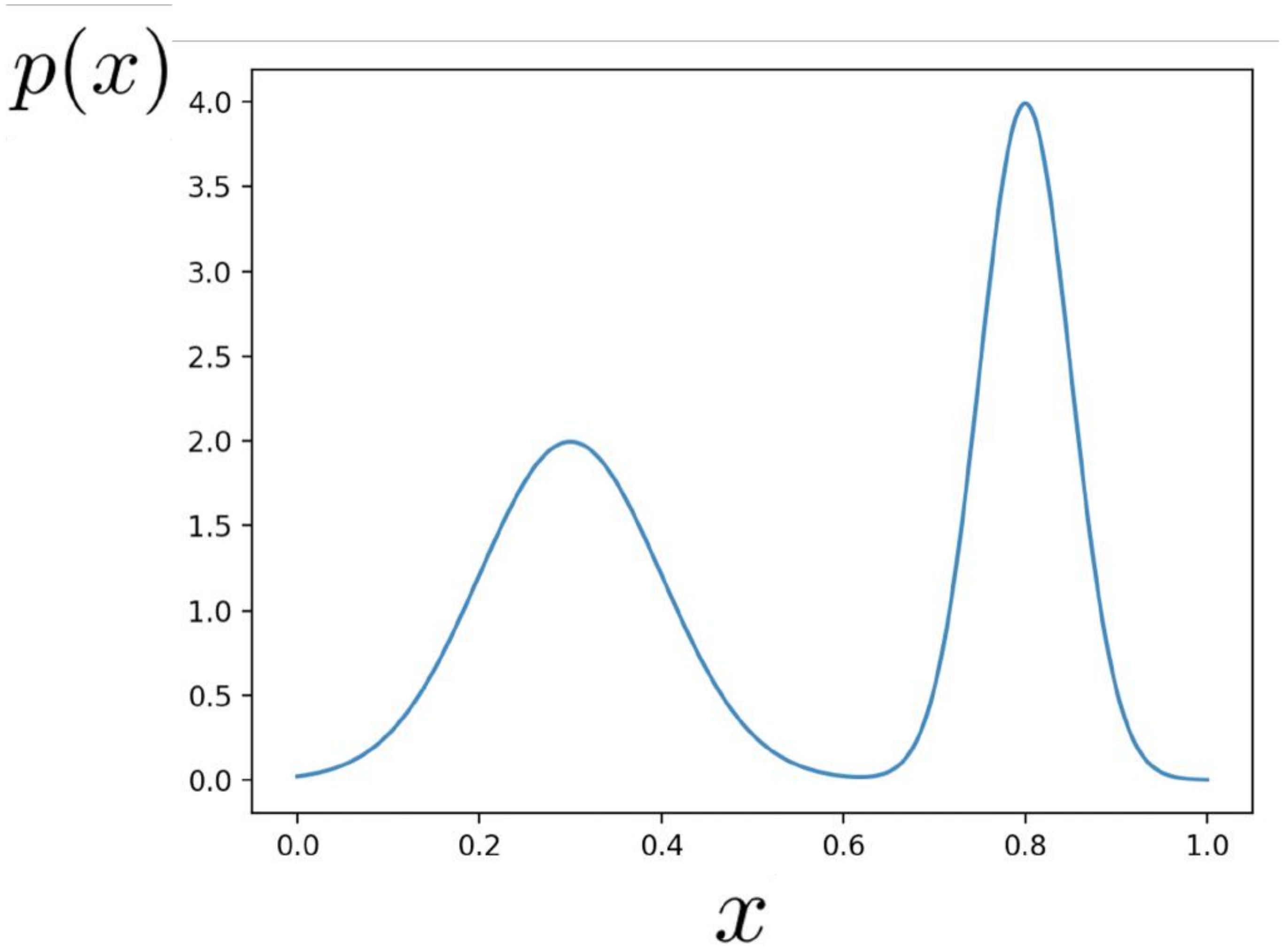
—Pieter Abbeel, Peter Chen, Jonathan Ho, Aravind Srinivas' Berkeley CS294-158 class

—Chin-Wei Huang slides on Normalizing Flows

# Lecture overview

- Foundations of Flows (1-D)
- 2-D Flows
- N-D Flows
- Dequantization

# Quick Refresher: Probability Density Models




$$P(x \in [a,b]) = \int_a^b p(x)dx$$

# How to fit a density model?

## Continuous data

0.22159854, 0.84525919, 0.09121633, 0.364252 , 0.30738086,
0.32240615, 0.24371194, 0.22400792, 0.39181847, 0.16407012,
0.84685229, 0.15944969, 0.79142357, 0.6505366 , 0.33123603,
0.81409325, 0.74042126, 0.67950372, 0.74073271, 0.37091554,
0.83476616, 0.38346571, 0.33561352, 0.74100048, 0.32061713,
0.09172335, 0.39037131, 0.80496586, 0.80301971, 0.32048452,
0.79428266, 0.6961708 , 0.20183965, 0.82621227, 0.367292 ,
0.76095756, 0.10125199, 0.41495427, 0.85999877, 0.23004346,
0.28881973, 0.41211802, 0.24764836, 0.72743029, 0.20749136,
0.29877091, 0.75781455, 0.29219608, 0.79681589, 0.86823823,
0.29936483, 0.02948181, 0.78528968, 0.84015573, 0.40391632,
0.77816356, 0.75039186, 0.84709016, 0.76950307, 0.29772759,
0.41163966, 0.24862007, 0.34249207, 0.74363912, 0.38303383, …

## Maximum Likelihood:

$$\max_\theta \sum_i \log p_\theta(x^{(i)})$$

## Equivalently:

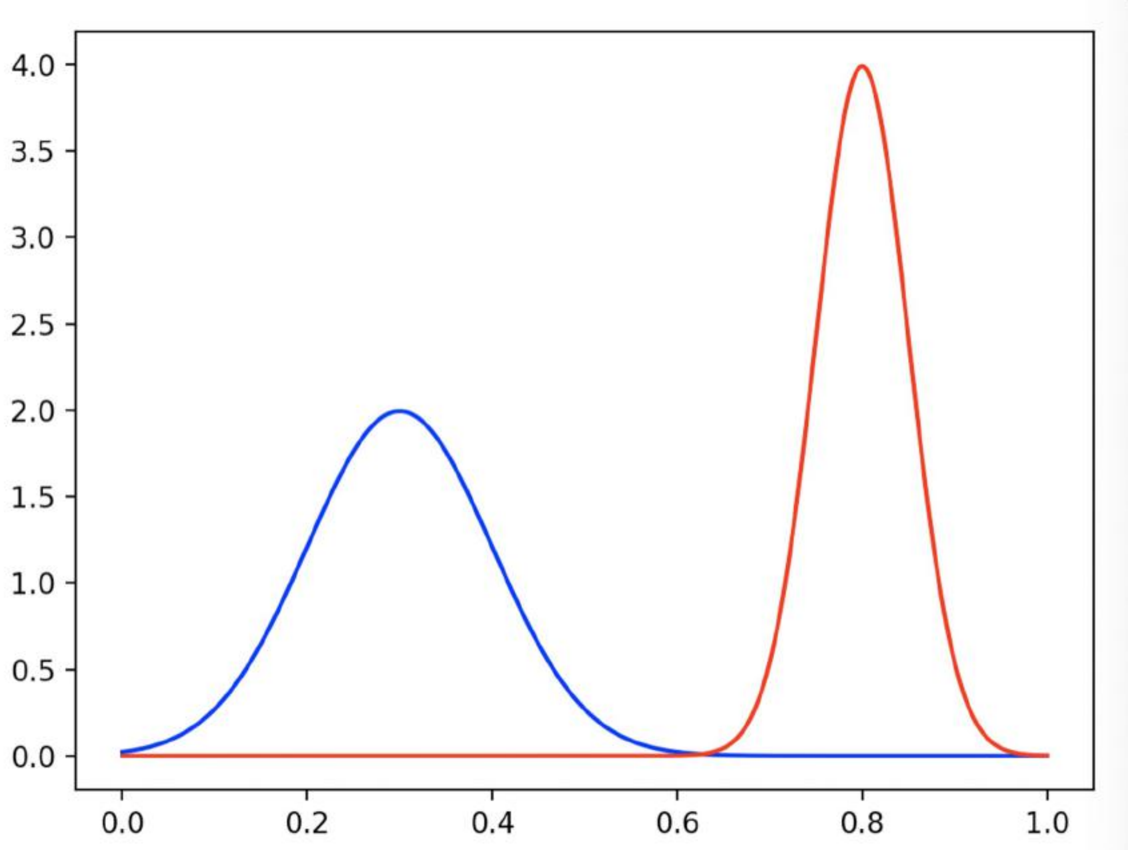
$$\min_\theta \mathbb{E}_x \left[-\log p_\theta(x)\right]$$

# Example Density Model: Mixtures of Gaussians

$$p_\theta(x) = \sum_{i=1}^{k} \pi_i \mathcal{N}(x; \mu_i, \sigma_i^2)$$

Parameters: means and variances of components, mixture weights

$$\theta = (\pi_1, \ldots, \pi_k, \mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k)$$



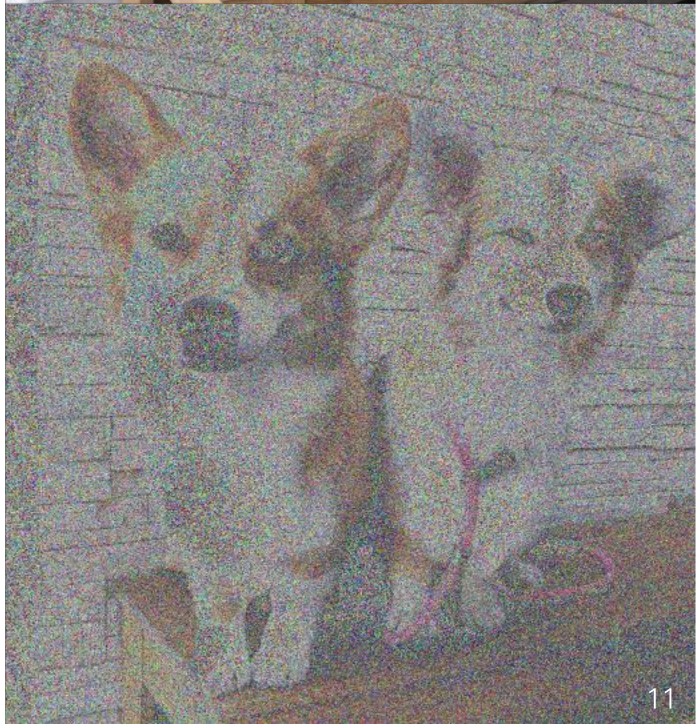
# Aside on Mixtures of Gaussians

Do mixtures of Gaussians work for high-dimensional data?

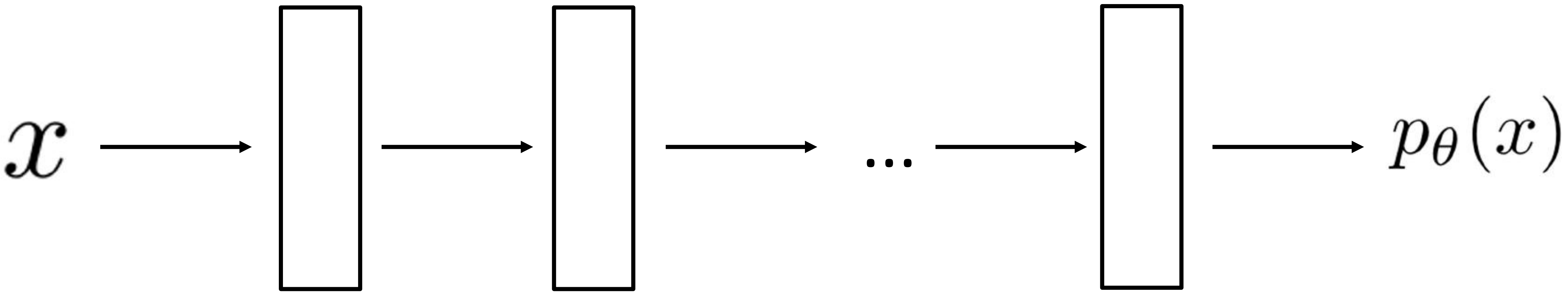
Not really. The sampling process is:

1. Pick a cluster center
2. Add Gaussian noise

Imagine this for modeling natural images! The only way a realistic image can be generated is if it is a cluster center, i.e. if it is already stored directly in the parameters.



# How to fit a general density model?



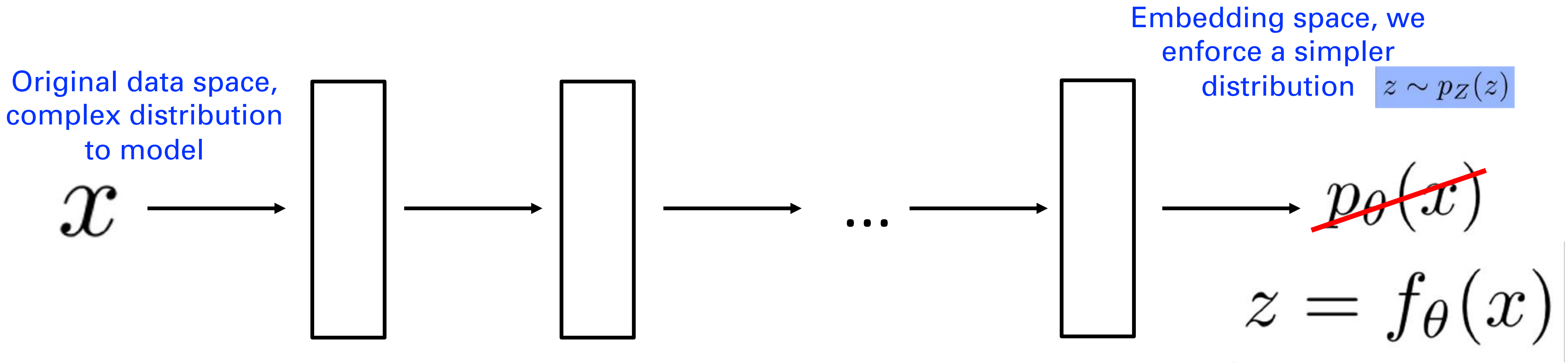

- How to ensure proper distribution?

$$\int_{-\infty}^{+\infty} p_\theta(x)dx = 1 \qquad p_\theta(x) \geq 0 \ \ \forall x$$

- How to sample?
- Latent representation?

Easily achieved for discrete data, using softmax
What about continuous data?

# Flows: Main Idea

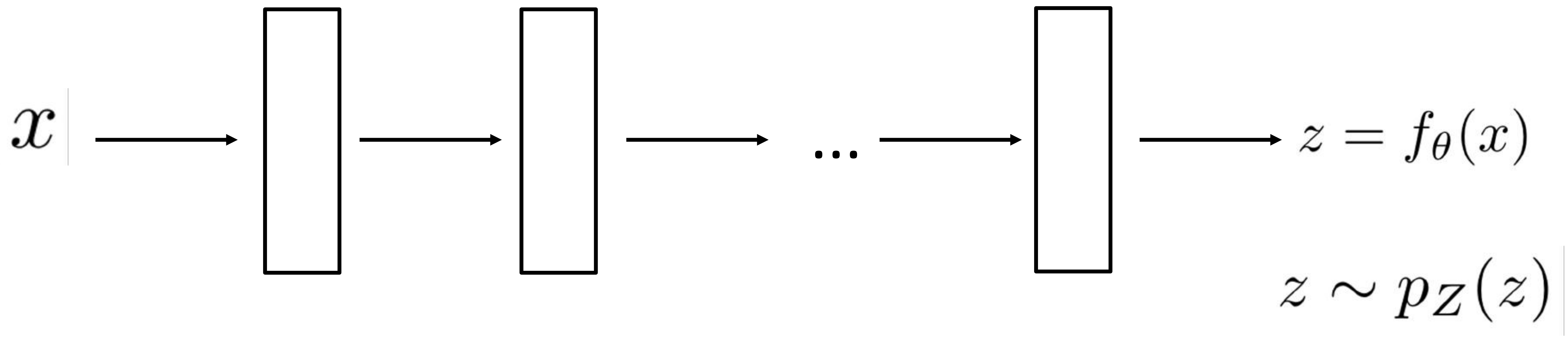



Generally: $z \sim p_Z(z)$

Normalizing Flow: $z \sim \mathcal{N}(0, 1)$

How to train? How to evaluate $p_\theta(x)$? How to sample?

# Flows: Training



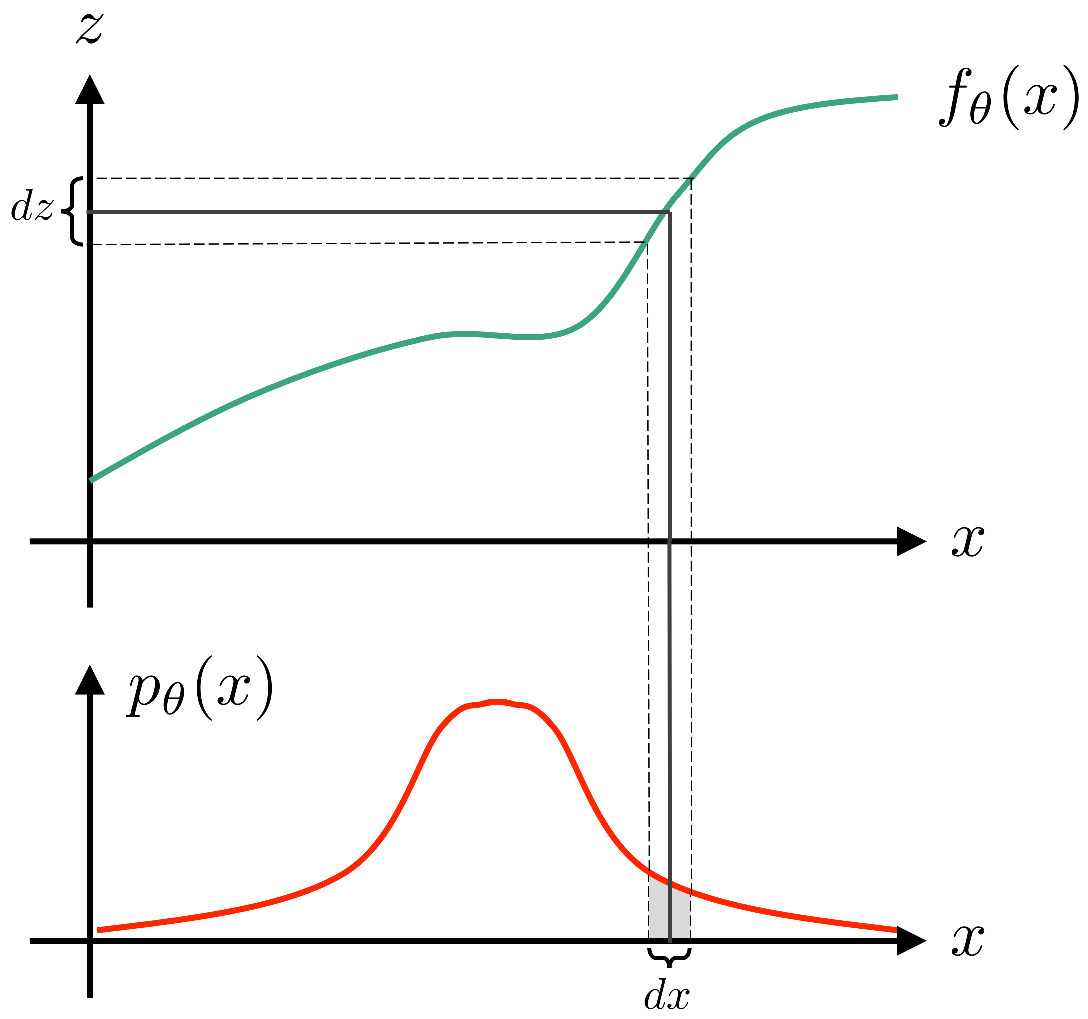

$$\max_\theta \sum_i \log p_\theta(x^{(i)})$$

# Change of Variables

$$z = f_\theta(x)$$

$$p_\theta(x)\,dx = p(z)\,dz$$

$$p_\theta(x) = p(f_\theta(x)) \left| \frac{\partial f_\theta(x)}{\partial x} \right|$$

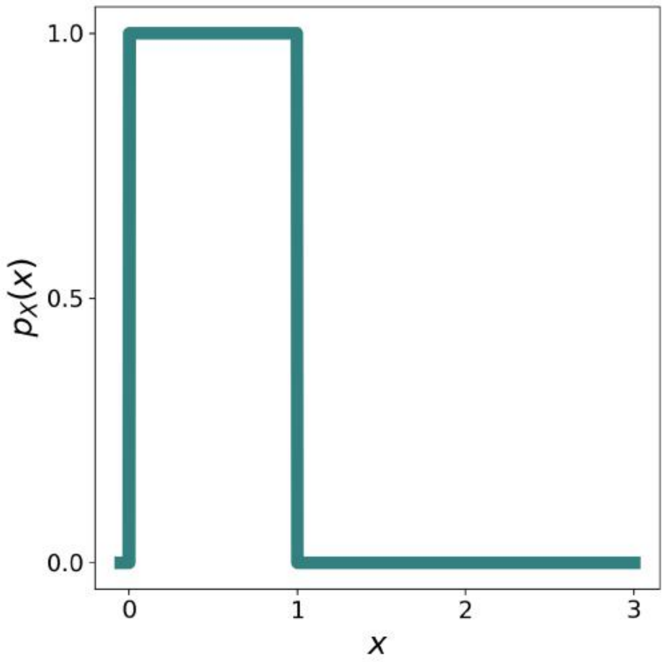


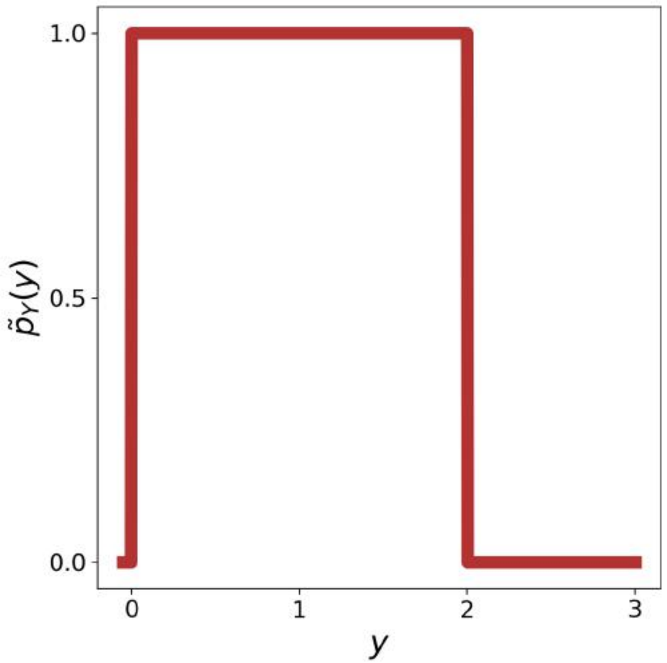

**Note:** requires $f_\theta$ invertible & differentiable

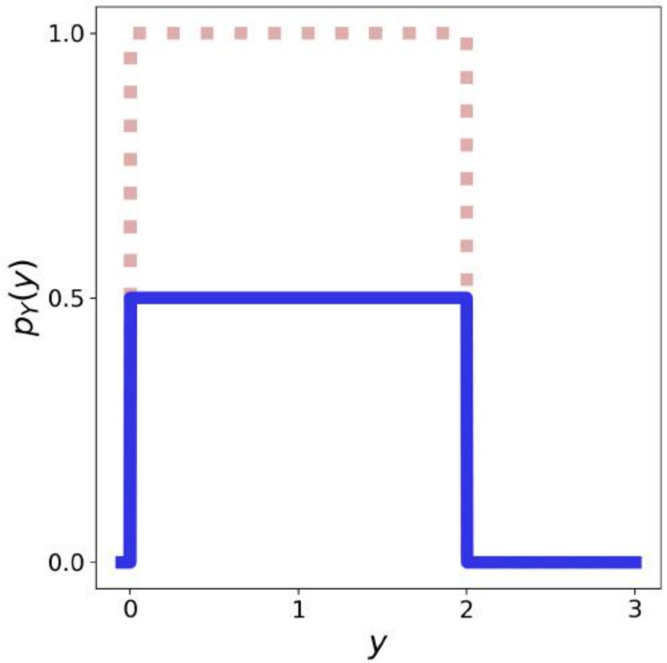
# Change of Variable Density Needs to Be Normalized

$$X \sim p_X \qquad Y := 2X$$

$$p_X(x) = \begin{cases} 1 & \text{for } 0 \leq x \leq 1 \\ 0 & \text{else} \end{cases} \qquad \tilde{p}_Y(y) = p_X(y/2) \qquad p_Y(y) = p_X(y/2)/2$$



# Flows: Training

$$\max_\theta \sum_i \log p_\theta(x^{(i)})$$

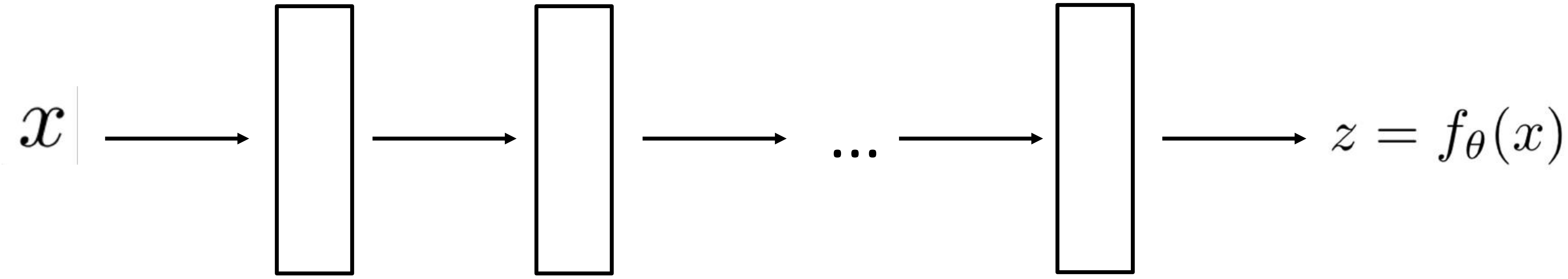
$$z^{(i)} = f_\theta(x^{(i)})$$

$$\begin{aligned} p_\theta(x^{(i)}) &= \quad p_Z(z^{(i)}) \left|\frac{\partial z}{\partial x}(x^{(i)})\right| \\ &= \quad p_Z(f_\theta(x^{(i)})) \left|\frac{\partial f_\theta}{\partial x}(x^{(i)})\right| \end{aligned}$$

$$\max_\theta \sum_i \log p_\theta(x^{(i)}) = \max_\theta \sum_i \log p_Z(f_\theta(x^{(i)})) + \log \left|\frac{\partial f_\theta}{\partial x}(x^{(i)})\right|$$

→ assuming we have an expression for $p_Z$,
this can be optimized with Stochastic Gradient Descent

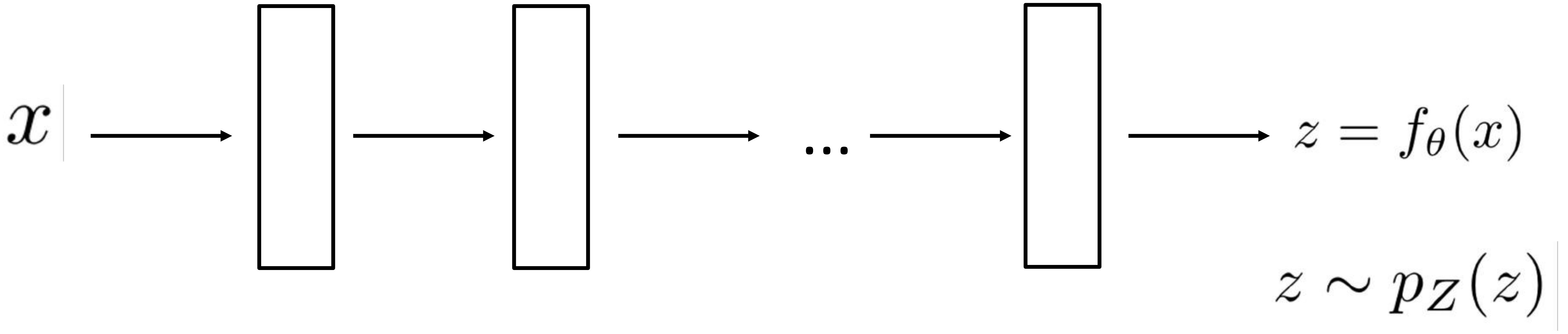
# Flows: Sampling




Step 1: sample $z \sim p_Z(z)$

Step 2: $x = f_\theta^{-1}(z)$

# What do we need to keep in mind for f?



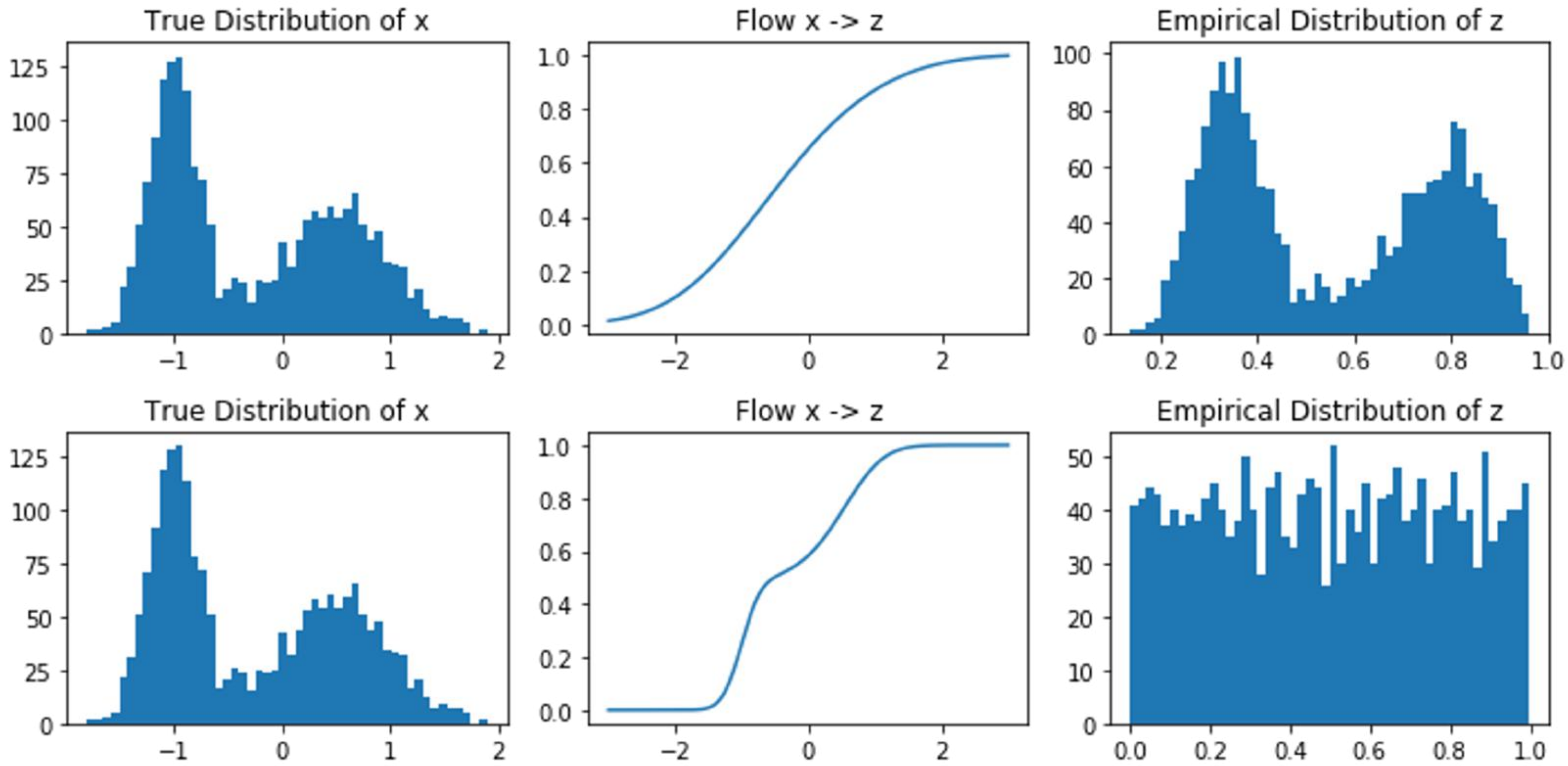

Recall, change of variable formula requires

- $f_\theta$ Invertible & differentiable

# Example: Flow to <u>Uniform</u> z

Before training

After training

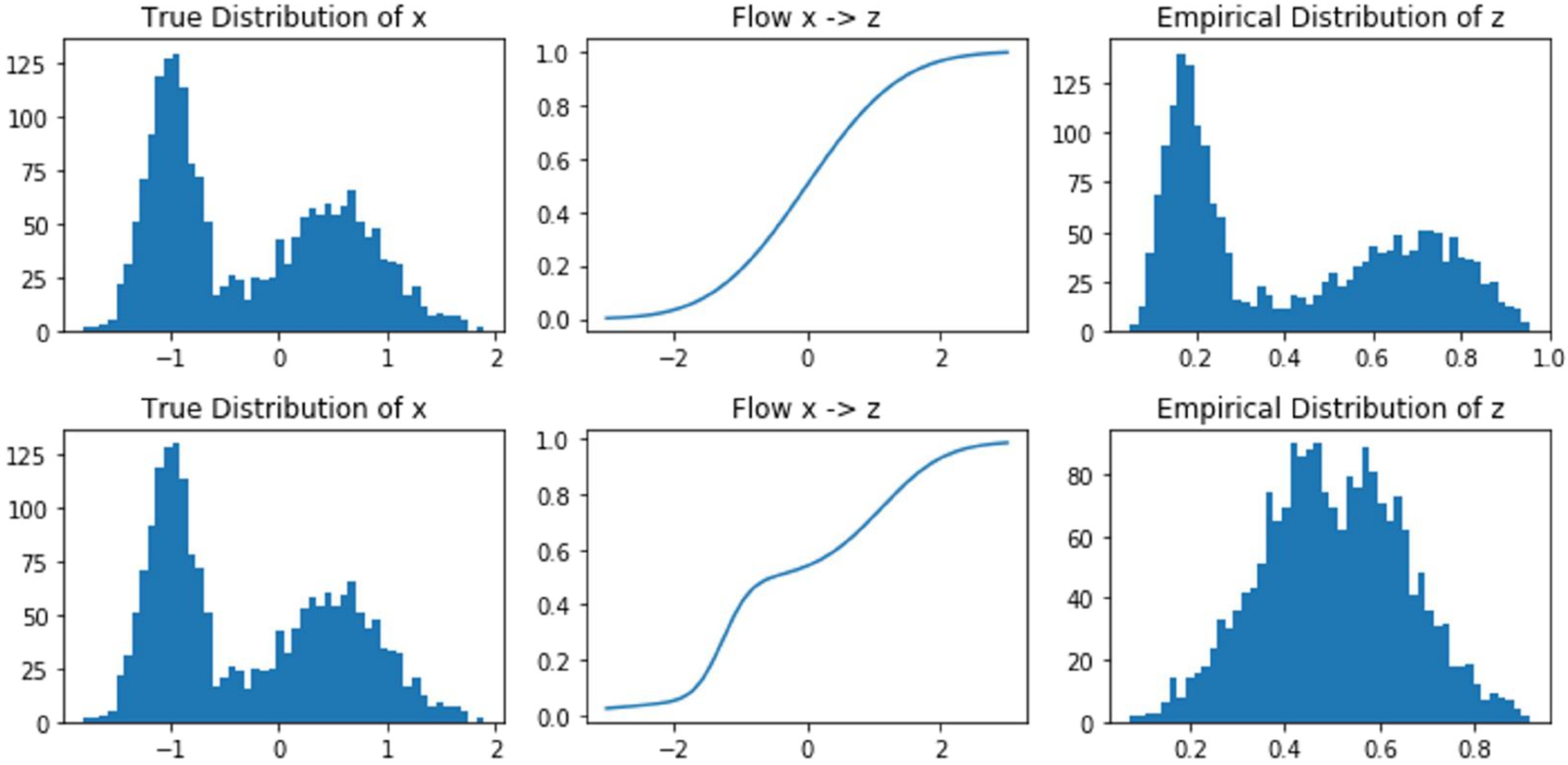



True distribution of x    Flow x → z    Empirical distribution of z

# Example: Flow to Beta(5,5) z

Before training

After training

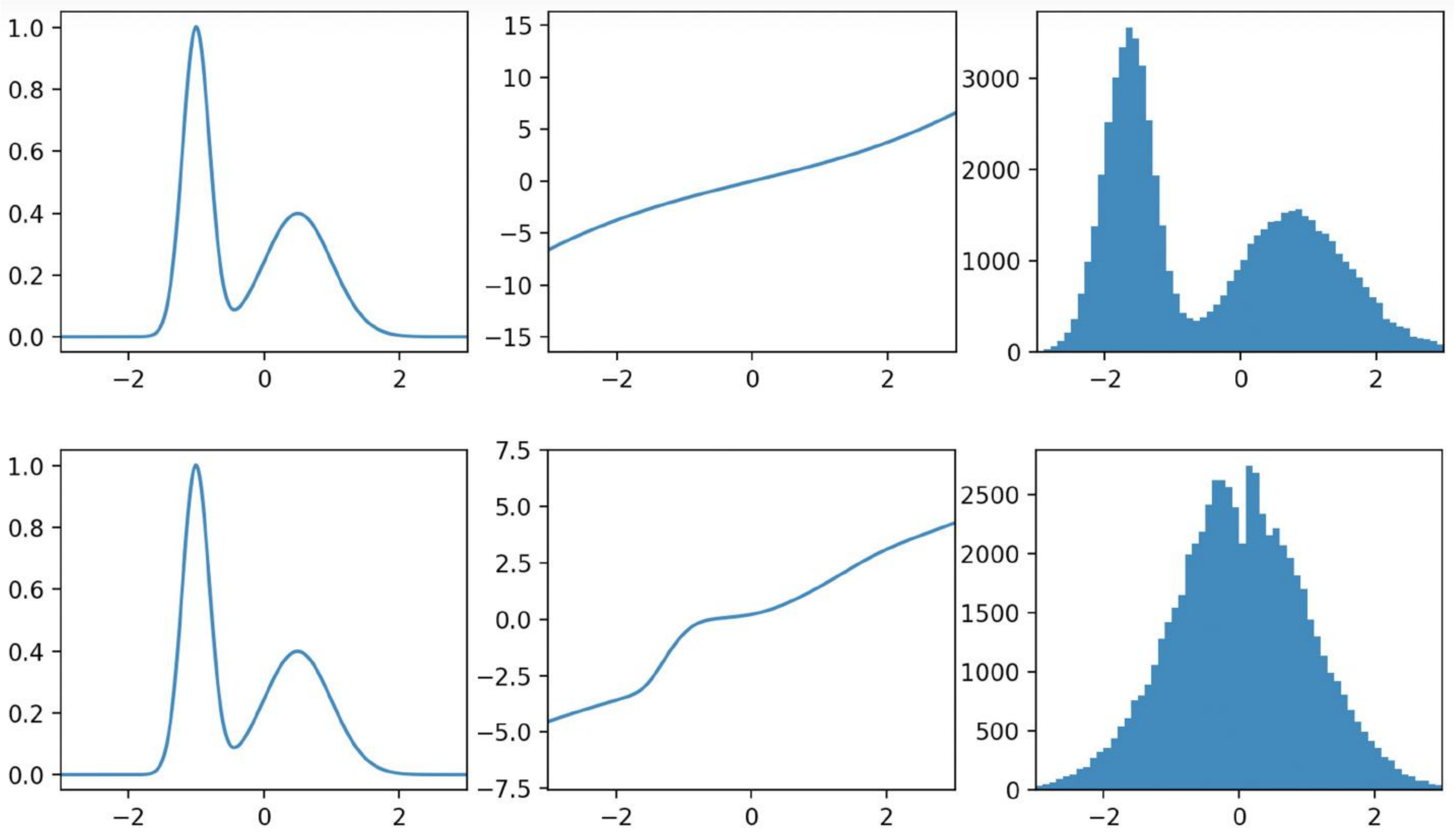



True distribution of x    Flow x → z    Empirical distribution of z

# Example: Flow to Gaussian z

Before training

After training




True distribution of x | Flow x → z | Empirical distribution of z

# Practical Parameterizations of Flows

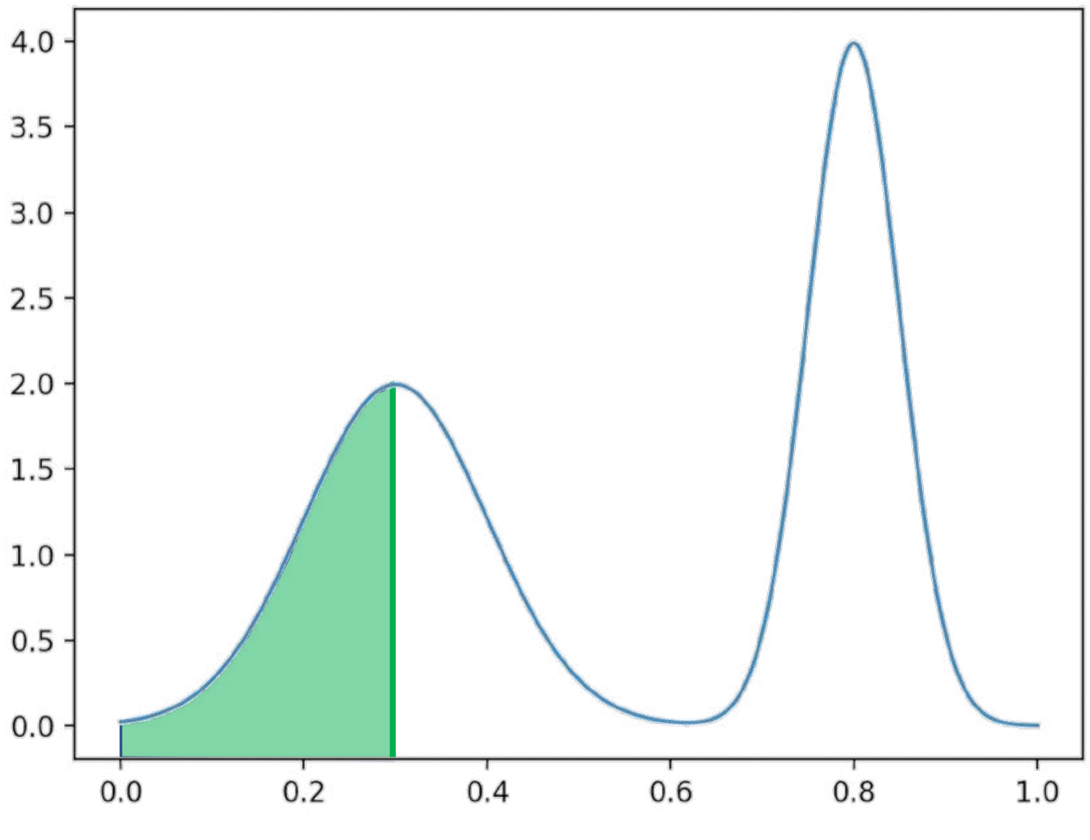
**Requirement:** Invertible and Differentiable

- Cumulative Density Functions
  - E.g. Gaussian mixture density, mixture of logistics
- Neural Net
  - If each layer flow, then sequencing of layers = flow
  - Each layer:
    - ReLU?
    - Sigmoid?
    - Tanh?

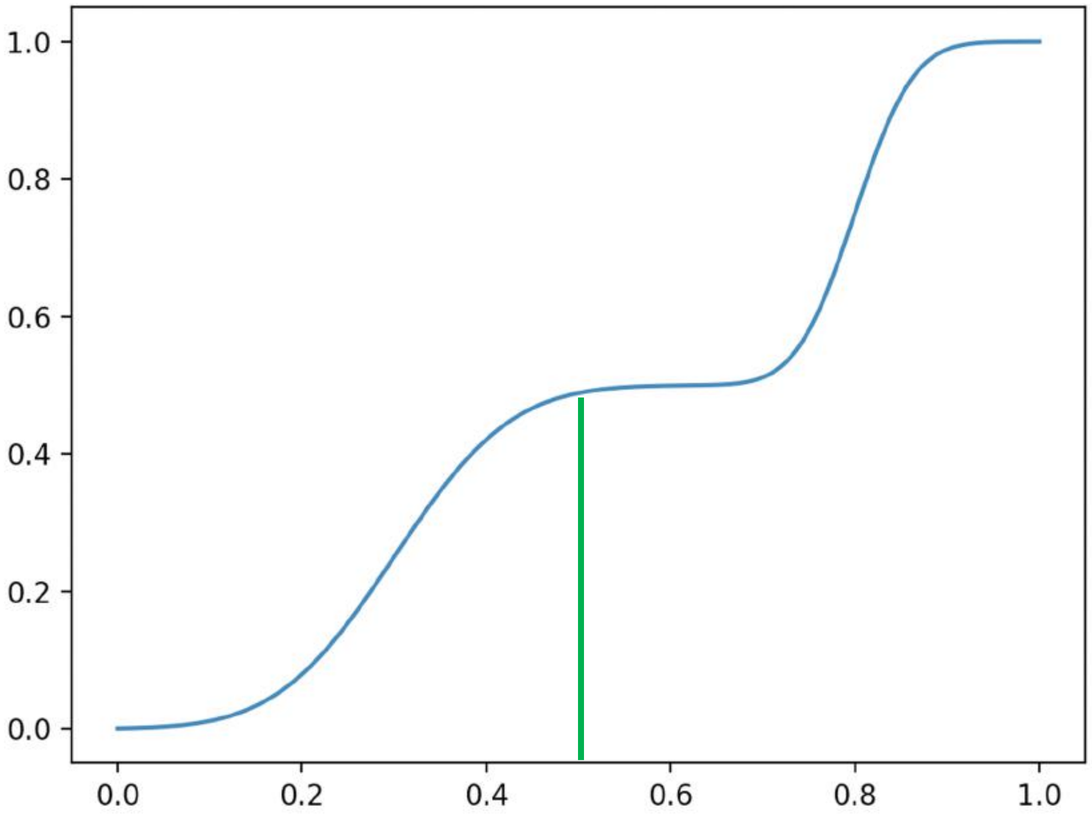
# How general are flows?

- Can every (smooth) distribution be represented by a (normalizing) flow?  [considering 1-D for now]

# Refresher: Cumulative Density Function (CDF)




$$p_\theta(x)$$



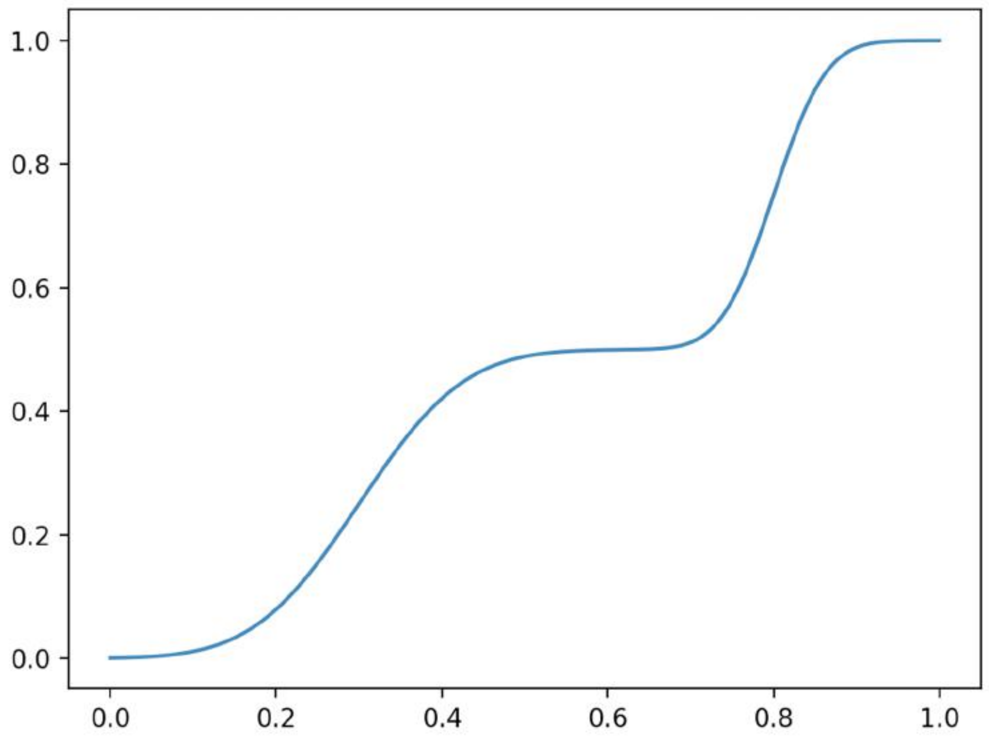

$$f_\theta(x) = \int_{-\infty}^{x} p_\theta(t)\, dt$$

# Sampling via inverse CDF

Sampling from the model:

$$z \sim \text{Uniform}([0,1])$$
$$x = f_\theta^{-1}(z)$$

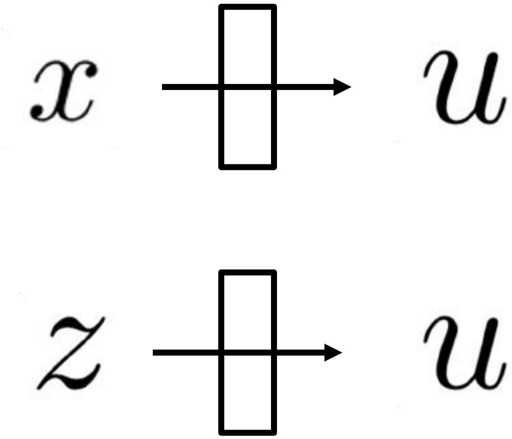
The CDF is an invertible, differentiable map from data to [0, 1]




$$f_\theta(x) = \int_{-\infty}^{x} p_\theta(t)\, dt$$

# How general are flows?

- CDF turns any density into uniform
- Inverse flow is flow





→ can turn any (smooth) p(x) into any (smooth) p(z)

# Lecture overview

- Foundations of Flows (1-D)
- **2-D Flows**
- N-D Flows
- Dequantization

# 2-D Autoregressive Flow

$$x_1 \to z_1 = f_\theta(x_1)$$

$$x_2 \to z_2 = f_\phi(x_1, x_2)$$

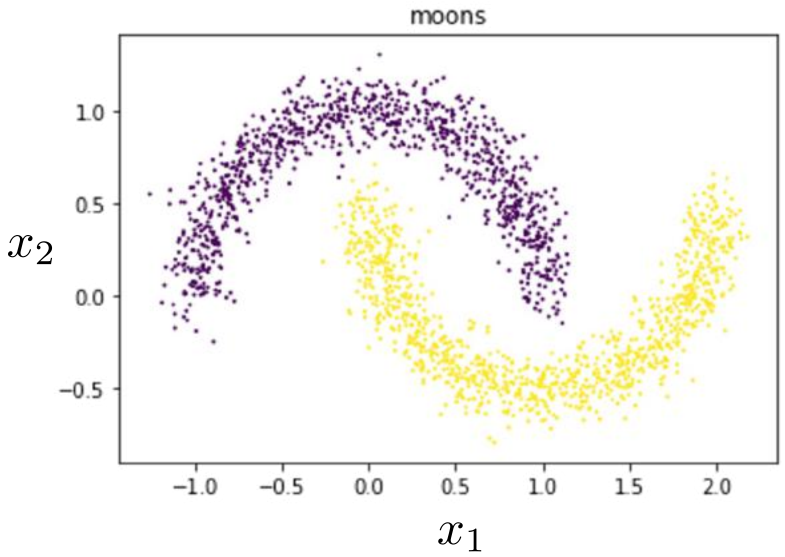
$$\max_{\theta,\phi} \sum_i \log p_{z_1}(f_\theta(x_1)) + \log \left| \frac{dz_1}{dx_1} \right| + \log p_{z_2}(f_\phi(x_1, x_2)) + \log \left| \frac{dz_2}{dx_2} \right|$$

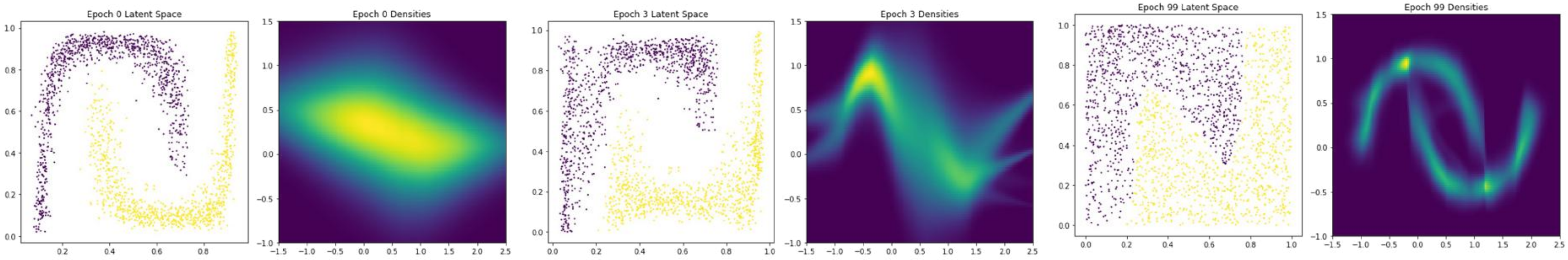
$$\frac{dz_1}{dx_1} = \frac{df_\theta(x_1)}{dx_1}, \frac{dz_2}{dx_2} = \frac{df_\phi(x_1, x_2)}{dx_2}$$

# 2-D Autoregressive Flow: Two Moons

## Architecture:

- Base distribution: $\text{Uniform}[0,1]^2$
- $x_1$: mixture of 5 Gaussians
- $x_2$: mixture of 5 Gaussians, conditioned on $x_1$

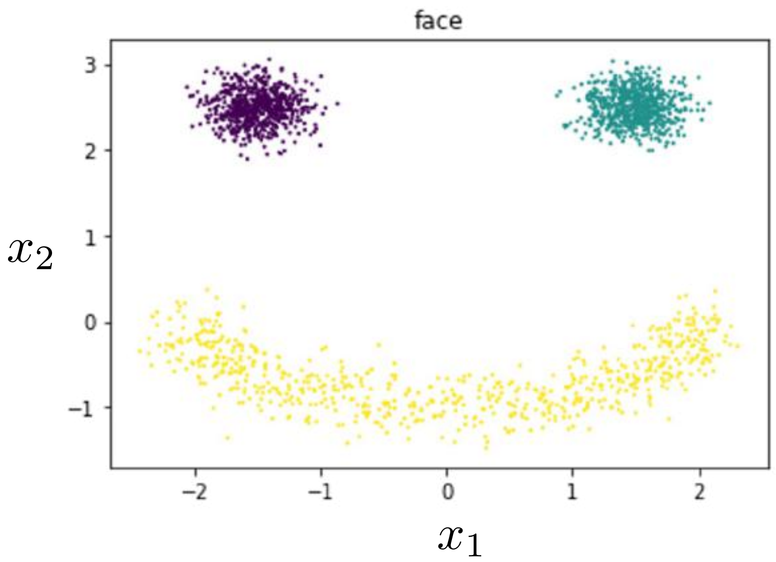


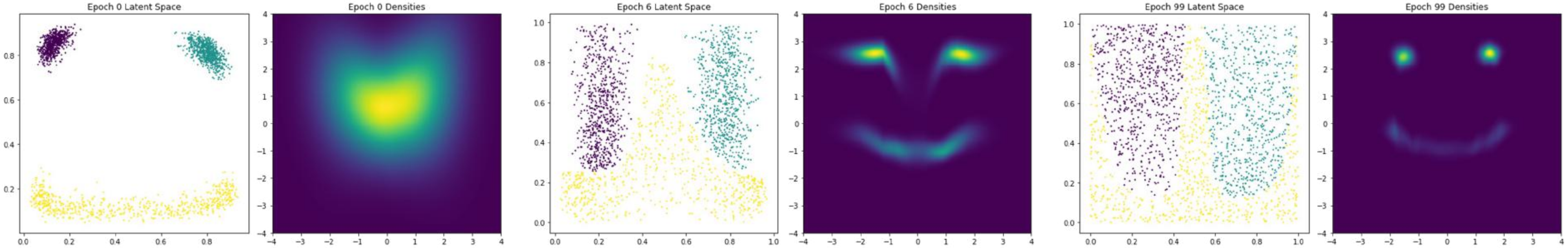



# 2-D Autoregressive Flow: Face

## Architecture:

- Base distribution: Uniform$[0,1]^2$
- $x_1$: mixture of 5 Gaussians
- $x_2$: mixture of 5 Gaussians, conditioned on $x_1$



# Lecture overview

- Foundations of Flows (1-D)
- 2-D Flows
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# Lecture overview

- Foundations of Flows (1-D)
- 2-D Flows
- **N-D Flows**
  - **Autoregressive Flows and Inverse Autoregressive Flows**
  - RealNVP (like) architectures
  - Glow, Flow++, FFJORD
- Dequantization

# Autoregressive flows

- The sampling process of a Bayes net is a flow
  - If autoregressive, this flow is called an **autoregressive flow**

$$
\begin{array}{lll}
x_1 \sim p_\theta(x_1) & x_1 = f_\theta^{-1}(z_1) & z_1 = f_\theta(x_1) \\
x_2 \sim p_\theta(x_2|x_1) & x_2 = f_\theta^{-1}(z_2; x_1) & z_2 = f_\theta(x_1, x_2) \\
x_3 \sim p_\theta(x_3|x_1, x_2) & x_3 = f_\theta^{-1}(z_3; x_1, x_2) & z_3 = f_\theta(x_1, x_2, x_3)
\end{array}
$$

- Sampling is an **invertible** mapping from z to x

# Autoregressive flows

- How to fit autoregressive flows?
  - Map **x** to z
  - Fully parallelizable

$$p_\theta(\mathbf{x}) = p(f_\theta(\mathbf{x})) \left| \det \frac{\partial f_\theta(\mathbf{x})}{\partial \mathbf{x}} \right|$$

- Notice
  - **x** → **z** has the same structure as the **log likelihood** computation of an autoregressive model
  - **z** → **x** has the same structure as the **sampling** procedure of an autoregressive model

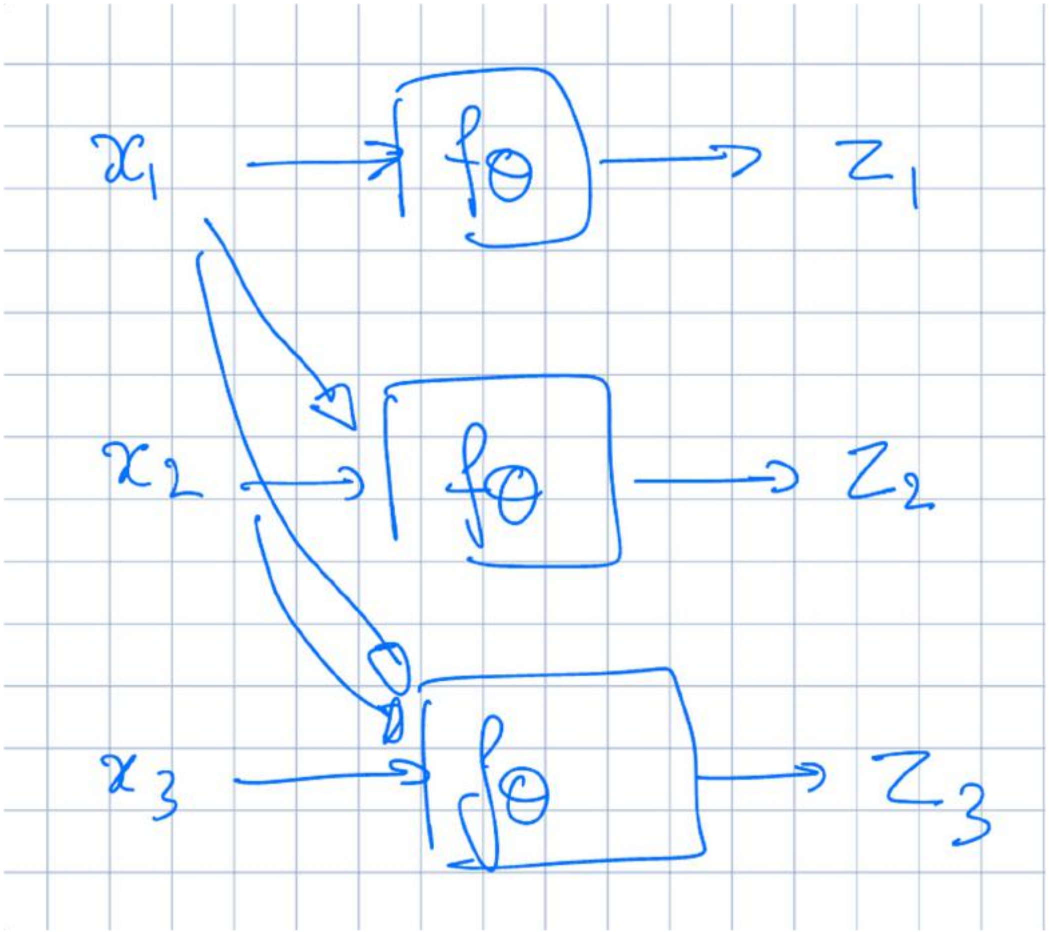
$$\begin{aligned} z_1 &= f_\theta(x_1) \\ z_2 &= f_\theta(x_2; x_1) \\ z_3 &= f_\theta(x_3; x_1, x_2) \end{aligned} \qquad \begin{aligned} x_1 &= f_\theta^{-1}(z_1) \\ x_2 &= f_\theta^{-1}(z_2; x_1) \\ x_3 &= f_\theta^{-1}(z_3; x_1, x_2) \end{aligned}$$

# Inverse autoregressive flows

- The inverse of an autoregressive flow is also a flow, called the **inverse autoregressive flow (IAF)**
  - $\mathbf{x} \rightarrow \mathbf{z}$ has the same structure as the **sampling** in an autoregressive model
  - $\mathbf{z} \rightarrow \mathbf{x}$ has the same structure as **log likelihood** computation of an autoregressive model. So, **IAF sampling is fast**

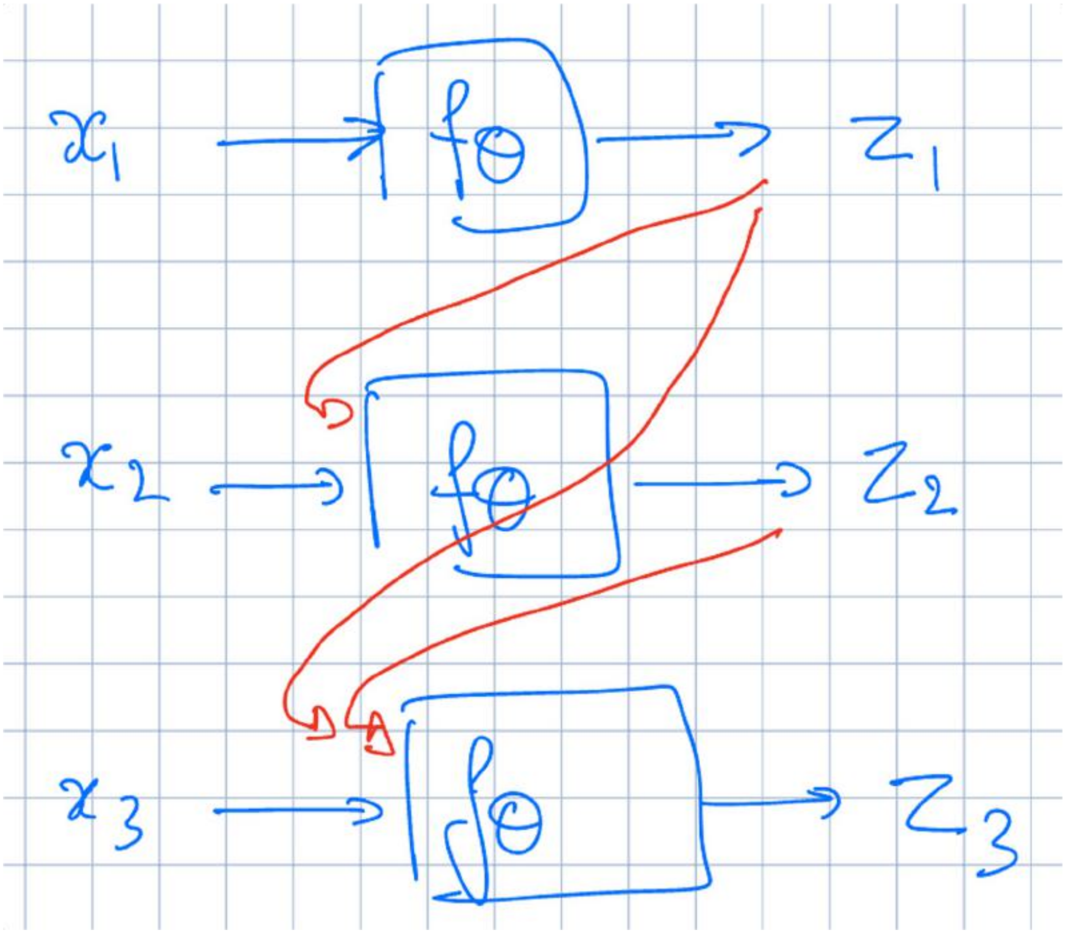
$$z_1 = f_\theta^{-1}(x_1) \qquad\qquad x_1 = f_\theta(z_1)$$
$$z_2 = f_\theta^{-1}(x_2; z_1) \qquad\qquad x_2 = f_\theta(z_2; z_1)$$
$$z_3 = f_\theta^{-1}(x_3; z_1, z_2) \qquad\qquad x_3 = f_\theta(z_3; z_1, z_2)$$

# AF



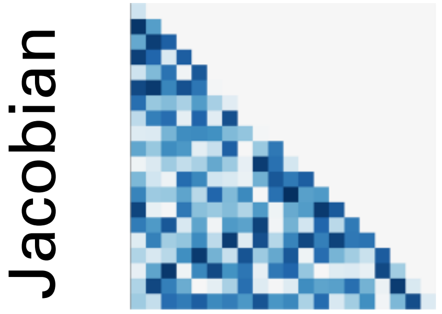

Training: parallel / fast
Sampling: long serial chain

# IAF




Training: long serial chain
Sampling: parallel / fast

# AF vs IAF




(Lower triangular)

- Autoregressive flow
  - Fast evaluation of p(x) for arbitrary x
  - Slow sampling
- Inverse autoregressive flow
  - Slow evaluation of p(x) for arbitrary x, so training directly by maximum likelihood is slow.
  - Fast sampling
  - Fast evaluation of p(x) if x is a sample
- There are models (Parallel WaveNet, IAF-VAE) that exploit IAF's fast sampling

# AF and IAF

Naively, both end up being as deep as the number of variables!

- E.g. 1MP image → 1M layers/sampling steps…

Can do parameter sharing as in Autoregressive Models from previous lecture [e.g. RNN, masking]

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- Foundations of Flows (1-D)
- 2-D Flows
- **N-D Flows**
  - Autoregressive Flows and Inverse Autoregressive Flows
  - **RealNVP (like) architectures**
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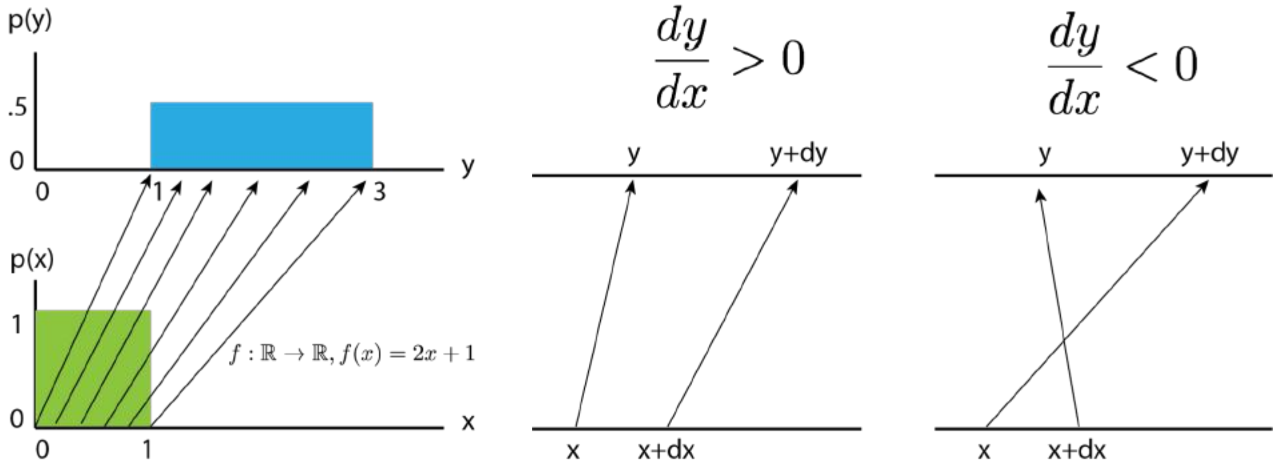
# Refresher: Change of MANY variables

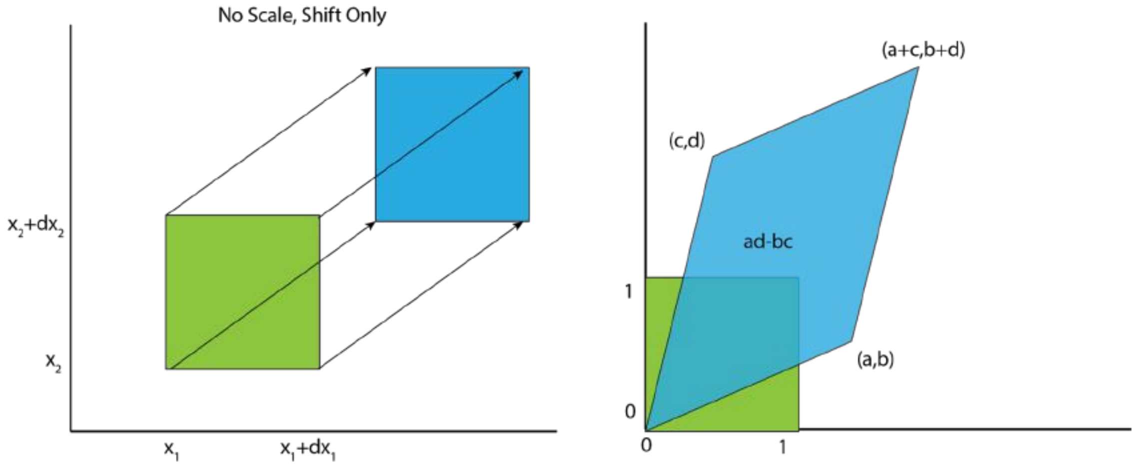
For a multivariable invertible mapping $f : \mathbb{R}^m \rightarrow \mathbb{R}^m \quad X \sim p_X \quad Y := f(X)$

$$p_Y(y) = p_X(f^{-1}(y)) \left| \det \frac{\partial f^{-1}(y)}{\partial y} \right|$$

1-D




2-D




Figures from blog post: Normalizing Flows Tutorial, Part 1: Distributions and Determinants by Eric Jang

# Change of MANY variables

For z ~ p(z), sampling process $f^{-1}$ linearly transforms a small cube dz to a small parallelepiped dx. Probability is conserved:

$$p(x) = p(z)\frac{\mathrm{vol}(dz)}{\mathrm{vol}(dx)} = p(z)\left|\det\frac{dz}{dx}\right|$$

**Intuition**: x is likely if it maps to a "large" region in z space

# Flow models: training

**Change-of-variables formula** lets us compute the density over x:

$$p_\theta(\mathbf{x}) = p(f_\theta(\mathbf{x})) \left| \det \frac{\partial f_\theta(\mathbf{x})}{\partial \mathbf{x}} \right|$$

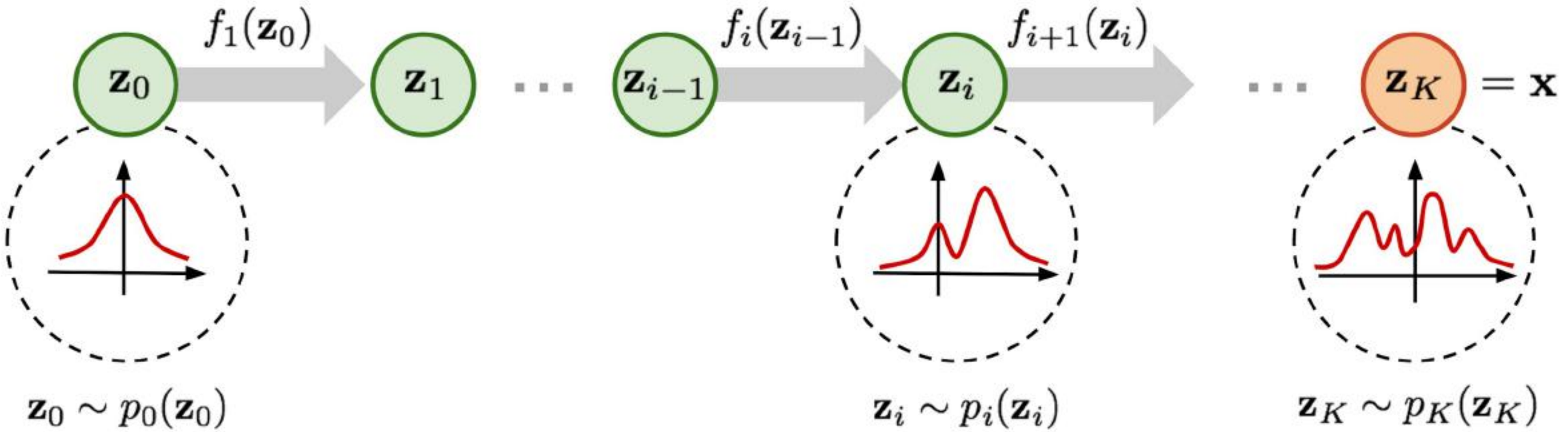
Train with maximum likelihood:

$$\arg\min_\theta \mathbb{E}_\mathbf{x} \left[ -\log p_\theta(\mathbf{x}) \right] = \mathbb{E}_\mathbf{x} \left[ -\log p(f_\theta(\mathbf{x})) - \log \det \left| \frac{\partial f_\theta(\mathbf{x})}{\partial \mathbf{x}} \right| \right]$$

**New key requirement:** the Jacobian determinant must be easy to calculate and differentiate!

# Chaining Invertible Mappings

$$f = f_S \circ \cdots \circ f_2 \circ f_1 \qquad f(x) = f_S(\cdots f_2(f_1(x)))$$




$$\frac{\partial f(x)}{\partial x} = \frac{f_S(x_{S-1})}{\partial x_{S-1}} \cdots \frac{f_2(x_1)}{\partial x_1} \frac{f_1(x_0)}{\partial x_0} \qquad \begin{aligned} x_s &= f_s(x_{s-1}) \\ x_0 &= x \end{aligned}$$

**Chain rule**

$$\det\left(\frac{\partial f(x)}{\partial x}\right) = \det\left(\frac{f_S(x_{S-1})}{\partial x_{S-1}}\right) \cdots \det\left(\frac{f_2(x_1)}{\partial x_1}\right) \det\left(\frac{f_1(x_0)}{\partial x_0}\right)$$

**Determinant of matrix product**

Figure from blog post: Flow-based Deep Generative Models by Lilian Weng, 2018

# Constructing flows: composition

- Flows can be composed

$$x \rightarrow f_1 \rightarrow f_2 \rightarrow \dots f_k \rightarrow z$$

$$z = f_k \circ \cdots \circ f_1(x)$$

$$x = f_1^{-1} \circ \cdots \circ f_k^{-1}(z)$$

$$\log p_\theta(x) = \log p_\theta(z) + \sum_{i=1}^{k} \log \left| \det \frac{\partial f_i}{\partial f_{i-1}} \right|$$

- Easy way to increase expressiveness

# Affine flows

- Another name for affine flow: multivariate Gaussian.
  - Parameters: an invertible matrix A and a vector b
  - $f(x) = A^{-1}(x - b)$
- Sampling: $x = Az + b$, where $z \sim \mathcal{N}(0, I)$ $x \sim \mathcal{N}(b, AA^T)$
- Log likelihood is expensive when dimension is large.
  - The Jacobian of $f$ is $A^{-1}$
  - Log likelihood involves calculating $\det(A)$

# Elementwise flows

$$f_\theta((x_1, \ldots, x_d)) = (f_\theta(x_1), \ldots, f_\theta(x_d))$$

- Lots of freedom in elementwise flow
  - Can use elementwise affine functions or CDF flows.
- The Jacobian is diagonal, so the determinant is easy to evaluate.

$$\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \operatorname{diag}(f'_\theta(x_1), \ldots, f'_\theta(x_d))$$

$$\det \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \prod_{i=1}^{d} f'_\theta(x_i)$$

# NICE/RealNVP

Affine coupling layer

- Split variables in half: $x_{1:d/2}$, $x_{d/2+1:d}$

$$\mathbf{z}_{1:d/2} = \mathbf{x}_{1:d/2}$$

$$\mathbf{z}_{d/2:d} = \mathbf{x}_{d/2:d} \cdot \exp(s_\theta(\mathbf{x}_{1:d/2})) + t_\theta(\mathbf{x}_{1:d/2})$$

- Invertible! Note that $s_\theta$ and $t_\theta$ can be arbitrary neural nets with **no restrictions**.
  - Think of them as **data-parameterized elementwise flows.**

$$\begin{cases} \mathbf{z}_{1:d/2} & = \mathbf{x}_{1:d/2} \\ \mathbf{z}_{d/2:d} & = \mathbf{x}_{d/2:d} \cdot \exp(s_\theta(\mathbf{x}_{1:d/2})) + t_\theta(\mathbf{x}_{1:d/2}) \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_{1:d/2} & = \mathbf{z}_{1:d/2} \\ \mathbf{x}_{d/2:d} & = \left(\mathbf{z}_{d/2:d} - t_\theta\left(\mathbf{z}_{1:d/2}\right)\right) \cdot \exp\left(-s_\theta\left(\mathbf{z}_{1:d/2}\right)\right) \end{cases}$$

# NICE/RealNVP

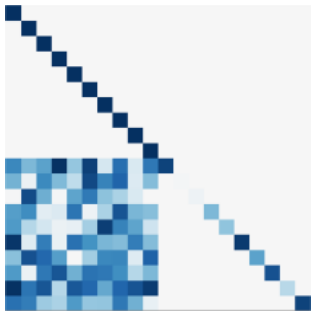
- It also has a tractable Jacobian determinant

$$\mathbf{z}_{1:d/2} = \mathbf{x}_{1:d/2}$$

$$\mathbf{z}_{d/2:d} = \mathbf{x}_{d/2:d} \cdot s_\theta(\mathbf{x}_{1:d/2}) + t_\theta(\mathbf{x}_{1:d/2})$$

$$\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{bmatrix} I & 0 \\ \frac{\partial \mathbf{z}_{d/2:d}}{\partial \mathbf{x}_{1:d/2}} & \mathrm{diag}(s_\theta(\mathbf{x}_{1:d/2})) \end{bmatrix}$$

Jacobian



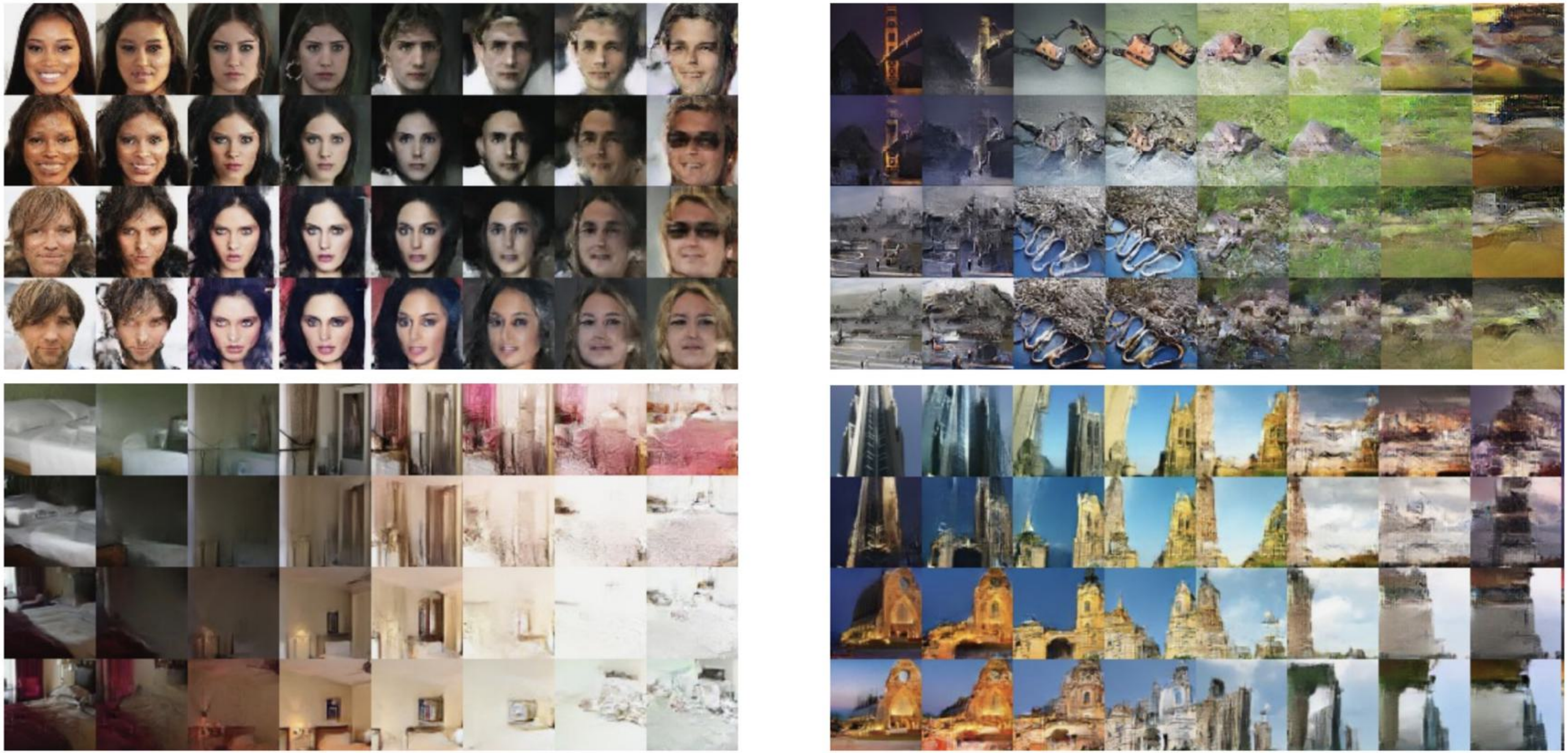
(Lower triangular + structured)

- The Jacobian is triangular, so its determinant is the product of diagonal entries.

$$\det \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \prod_{k=1}^{d} s_\theta(\mathbf{x}_{1:d/2})_k$$

# RealNVP

- Takeaway: coupling layers allow unrestricted neural nets to be used in flows, while preserving invertibility and tractability



[Dinh et al. Density estimation using Real NVP. ICLR 2017]

# RealNVP: How to partition variables?

Partitioning can be implemented using a binary mask b, and using the functional form for y

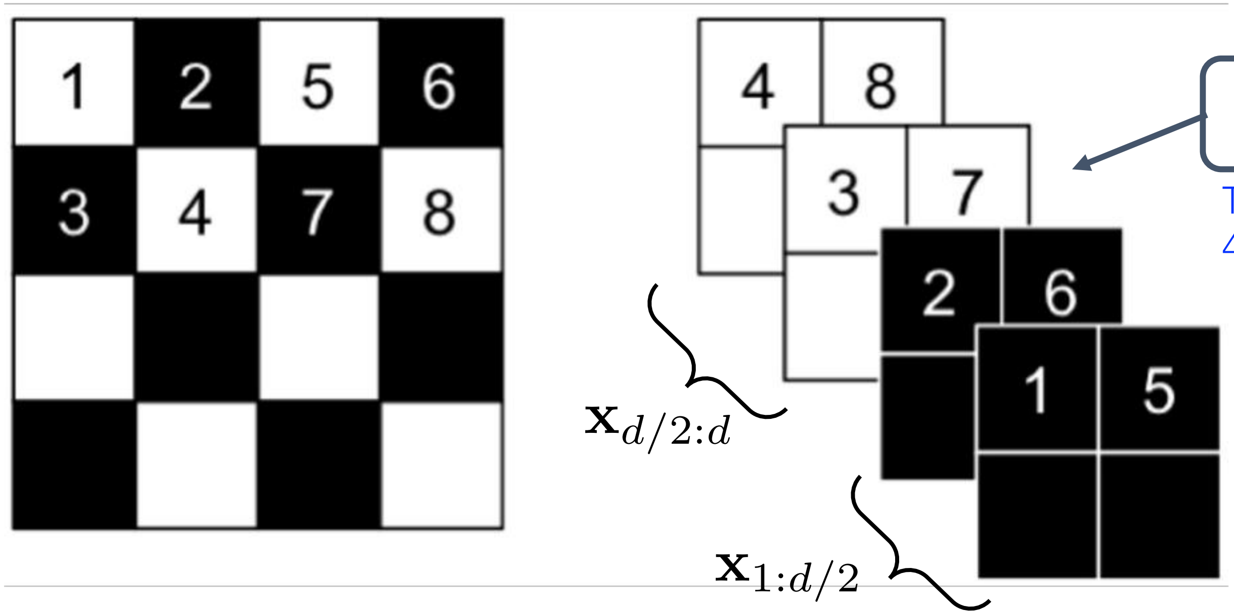
$$f(x) = b \odot x + (1 - b) \odot (x \odot \exp(s\_(b \odot x)) + m(b \odot x))$$

# RealNVP: How to partition variables?

Partitioning can be implemented using a binary mask b, and using the functional form for y

$$f(x) = b \odot x + (1 - b) \odot (x \odot \exp(s\_(b \odot x)) + m(b \odot x))$$

The **spatial checkerboard pattern mask** has value 1 where the sum of spatial coordinates is odd, and 0 otherwise.




After a "**squeeze**" operation

The squeezing operation reduces the $4 \times 4 \times 1$ tensor into a $2 \times 2 \times 4$ tensor

**The channel-wise mask** b is 1 for the first half of the channel dimensions and 0 for the second half.

Figures from Density Estimation Using Real NVP by Dinh et al., 2017

# RealNVP Architecture

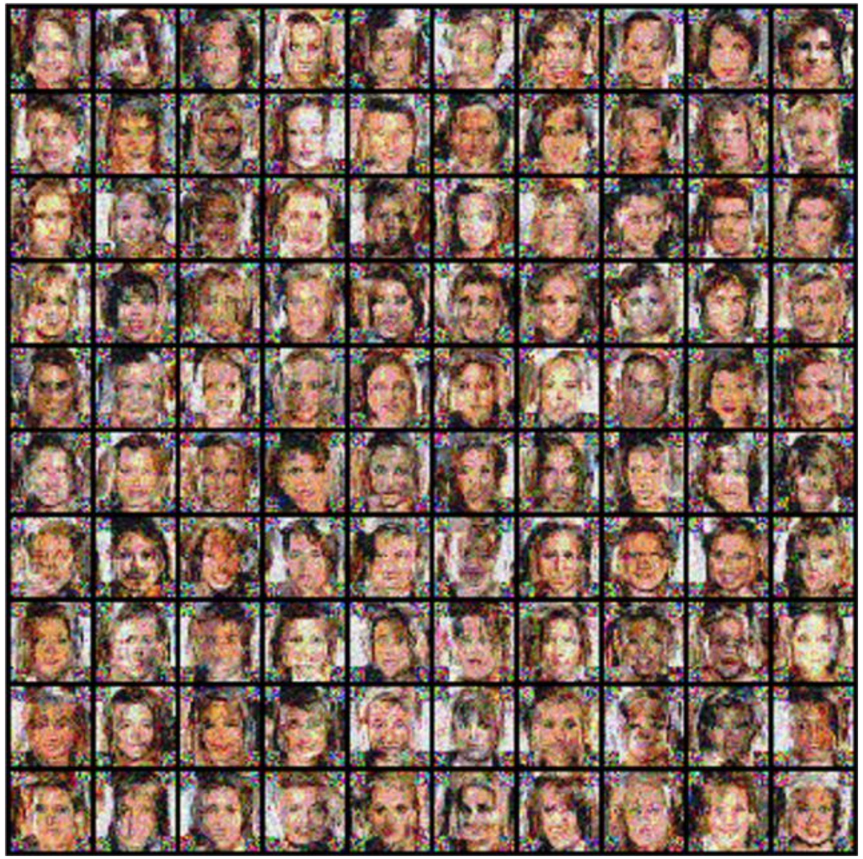
Input x: 32×32×c image

- Layer 1: (Checkerboard ×3, channel squeeze, channel ×3)
  - Split result to get $x_1$: 16×16×2c and $z_1$: 16×16×2c (fine-grained latents)
- Layer 2: (Checkerboard ×3, channel squeeze, channel ×3)
  - Split result to get $x_2$: 8×8×4c and $z_2$: 8×8×4c (coarser latents)
- Layer 3: (Checkerboard ×3, channel squeeze, channel ×3)
  - Get $z_3$: 4×4×16c (latents for highest-level details)

# Good vs Bad Partitioning

Checkerboard $\times 4$; channel squeeze; channel $\times 3$; channel unsqueeze; checkerboard $\times 3$

(Mask top half; mask bottom half; mask left half; mask right half) $\times 2$



# Lecture overview

- Foundations of Flows (1-D)
- 2-D Flows
- **N-D Flows**
  - Autoregressive Flows and Inverse Autoregressive Flows
  - RealNVP (like) architectures
  - **Glow, Flow++, FFJORD**
- Dequantization

# Choice of coupling transformation

- A Bayes net defines coupling dependency, but what invertible transformation f to use is a design question

$$\mathbf{x}_i = f_\theta(\mathbf{z}_i; \text{parent}(\mathbf{x}_i))$$

- Affine transformation is the most commonly used one (NICE, RealNVP, IAF-VAE, …)

$$\mathbf{x}_i = \mathbf{z}_i \cdot \mathbf{a}_\theta(\text{parent}(\mathbf{x}_i)) + \mathbf{b}_\theta(\text{parent}(\mathbf{x}_i))$$

- More complex, nonlinear transformations -> better performance
  - CDFs and inverse CDFs for Mixture of Gaussians or Logistics (Flow++)
  - Piecewise linear/quadratic functions (Neural Importance Sampling)

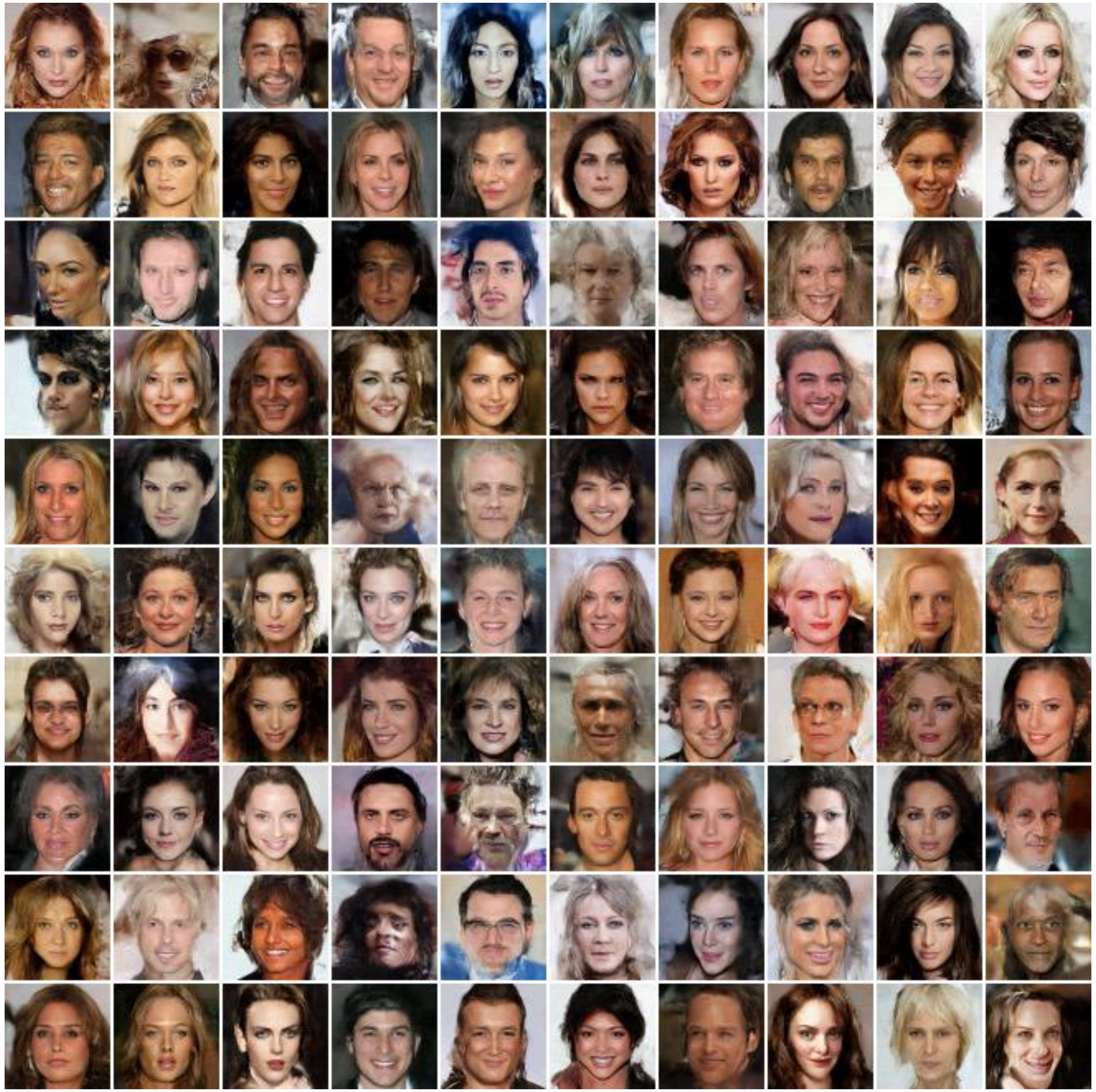
# NN architecture also matters

- Flow++ = MoL transformation + self-attention in NN
  - Bayes net (coupling dependency), transformation function class, NN architecture all play a role in a flow's performance.

*Table 2.* CIFAR10 ablation results after 400 epochs of training. Models not converged for the purposes of ablation study.

| Ablation | bits/dim | parameters |
|---|---|---|
| uniform dequantization | 3.292 | 32.3M |
| affine coupling | 3.200 | 32.0M |
| no self-attention | 3.193 | 31.4M |
| **Flow++ (not converged for ablation)** | **3.165** | **31.4M** |

# Flow++

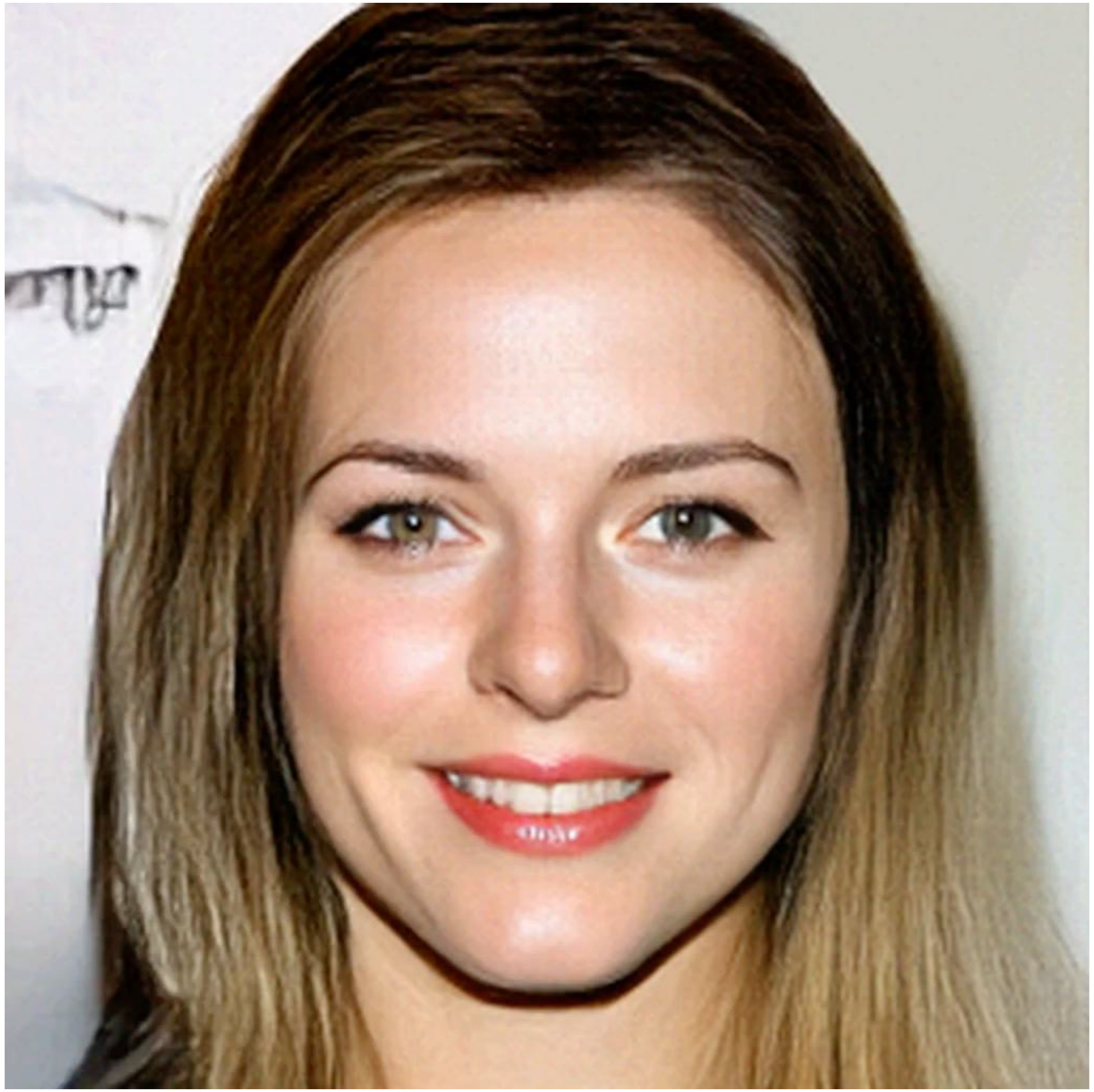


Samples from Flow++ trained on 64x64 CelebA

# Other classes of flows

- Glow (link)
  - Replacing permutation with 1x1 convolution (soft permutation)
  - Large-scale training

- Continuous time flows (FFJORD)
  - Allows for unrestricted architectures. Invertibility and fast log probability computation guaranteed.



# Glow: Interpolation

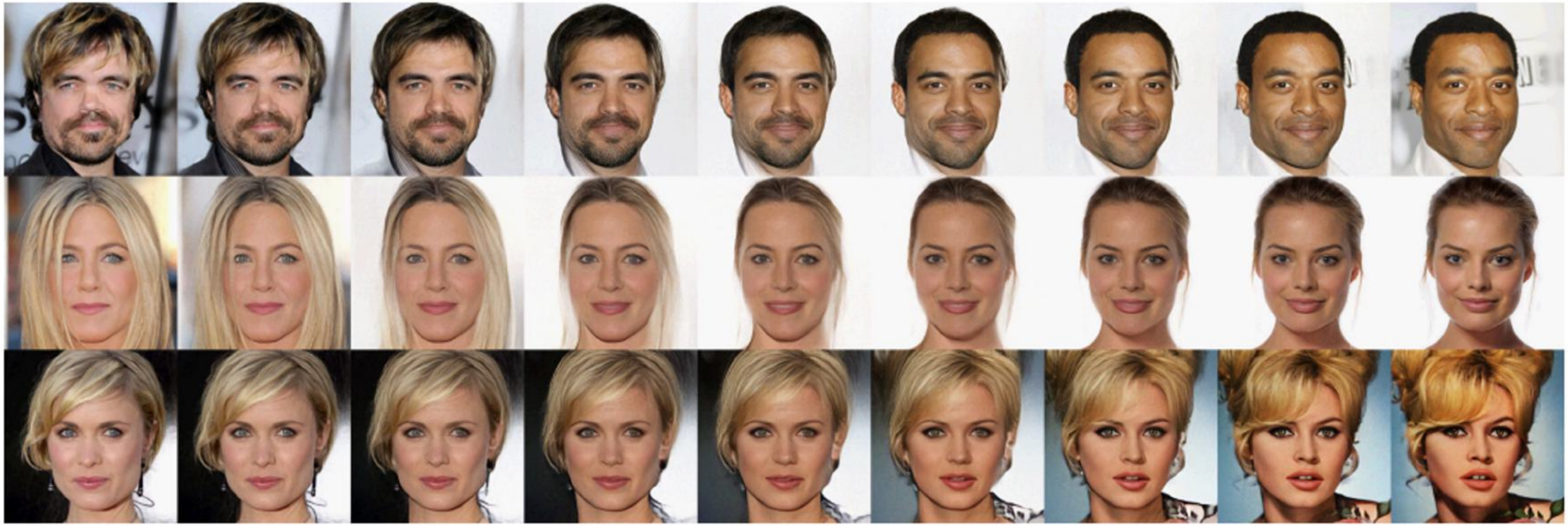


Figure 5: Linear interpolation in latent space between real images

# Glow: Attribute Control

(a) Smiling

(b) Pale Skin

(c) Blond Hair

(d) Narrow Eyes

(e) Young

(f) Male

# Architectural Taxonomy

**Sparse connection**

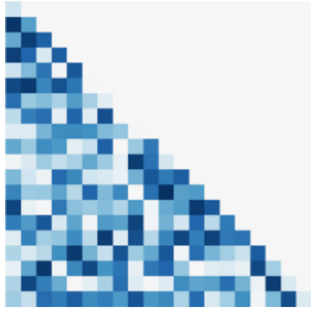
$$f(\boldsymbol{x})_t = g(\boldsymbol{x}_{1:t})$$

**Residual Connection**

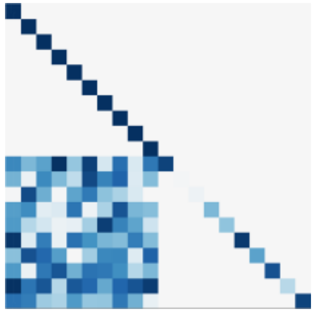
$$f(\boldsymbol{x}) = \boldsymbol{x} + g(\boldsymbol{x})$$

| **1. Autoregressive** | **2. Block coupling** | **3. Det identity** | **4. Stochastic estimation** |
|---|---|---|---|
| IAF/MAF/NAF<br>SOS polynomial<br>UMNN | NICE/RealNVP/Glow<br>Cubic Spline Flow<br>Neural Spline Flow | Planar/Sylvester flows<br>Radial flow | Residual Flow<br>FFJORD |

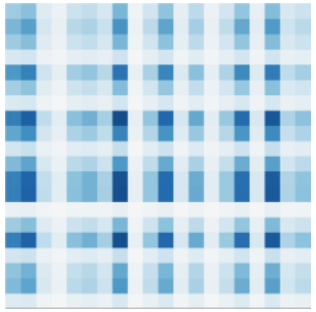
Jacobian



(Lower triangular)



(Lower triangular + structured)



(Low rank)

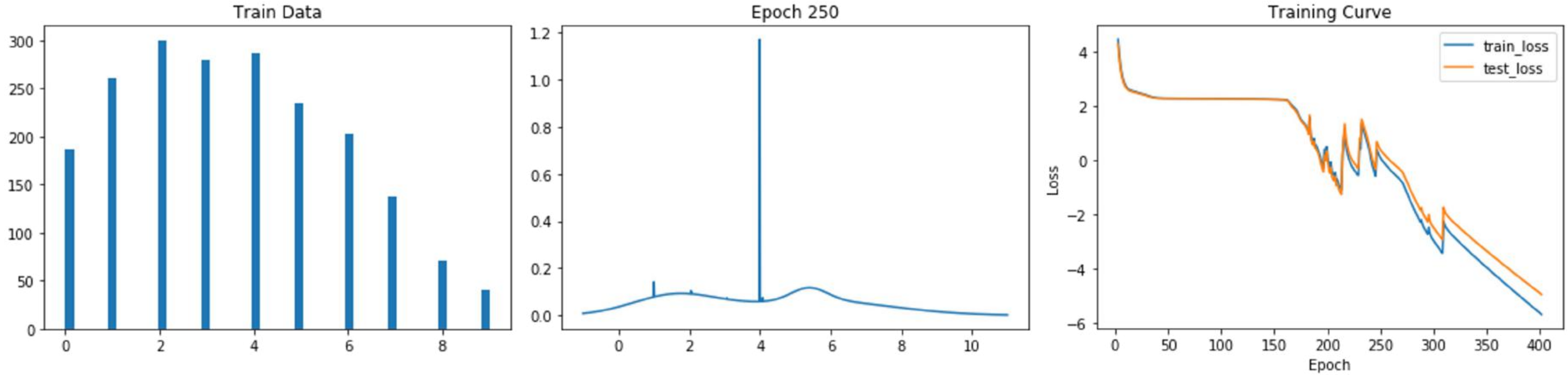
(Arbitrary)

Figures from Ricky Chen

# Lecture overview

- Foundations of Flows (1-D)
- 2-D Flows
- N-D Flows
- Dequantization

# Flow on Discrete Data Without Dequantization...



# Continuous flows for discrete data

- A problem arises when fitting continuous density models to discrete data: degeneracy
  - When the data are 3-bit pixel values, $\mathbf{x} \in \{0, 1, 2, \ldots, 255\}$
  - What density does a model assign to values between bins like 0.4, 0.42…?
- Correct semantics: we want the integral of probability density within a discrete interval to approximate discrete probability mass

$$P_{\text{model}}(\mathbf{x}) := \int_{[0,1)^D} p_{\text{model}}(\mathbf{x} + \mathbf{u})\, d\mathbf{u}$$

# Continuous flows for discrete data

- Solution: **Dequantization**. Add noise to data.

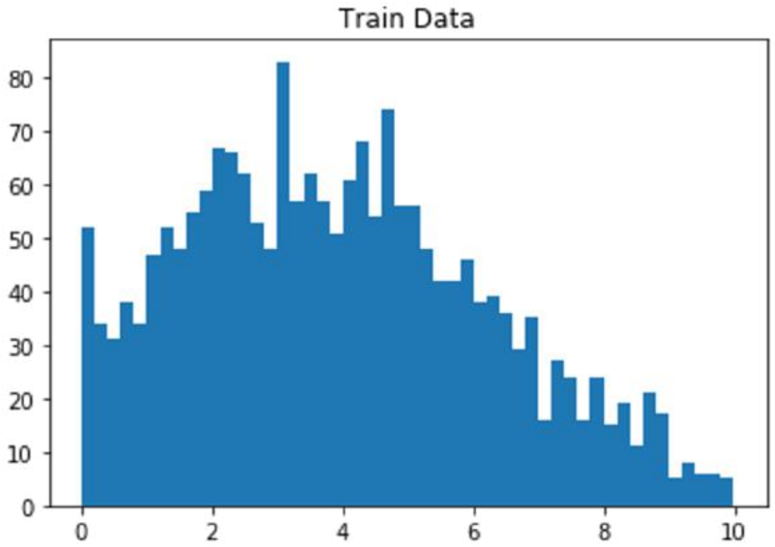
  $$\mathbf{x} \in \{0, 1, 2, \ldots, 255\}$$

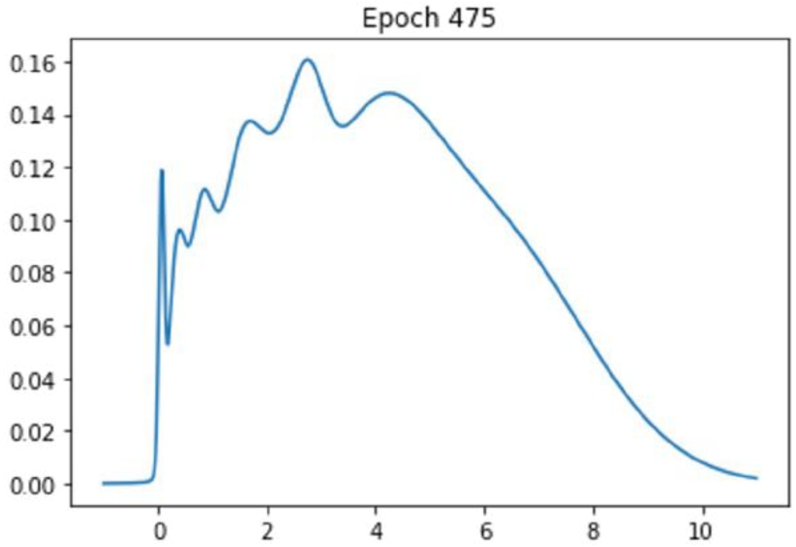
  – We draw noise u uniformly from $[0, 1)^D$

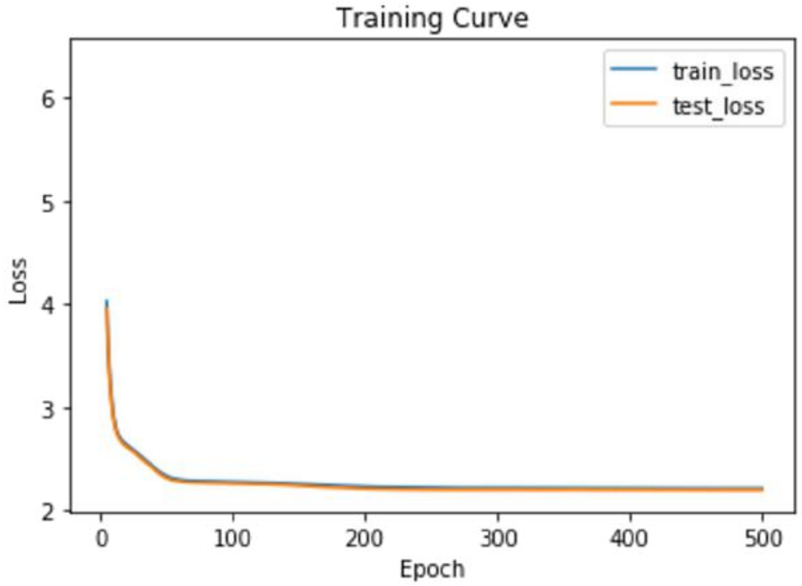
$$\begin{aligned}\mathbb{E}_{\mathbf{y}\sim p_{\text{data}}}\left[\log p_{\text{model}}(\mathbf{y})\right] &= \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \int_{[0,1)^D} \log p_{\text{model}}(\mathbf{x}+\mathbf{u})\, d\mathbf{u} \\ &\leq \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \log \int_{[0,1)^D} p_{\text{model}}(\mathbf{x}+\mathbf{u})\, d\mathbf{u} \\ &= \mathbb{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_{\text{model}}(\mathbf{x})\right]\end{aligned}$$

[Theis, Oord, Bethge, 2016]

# Flow on Discrete Data With Dequantization

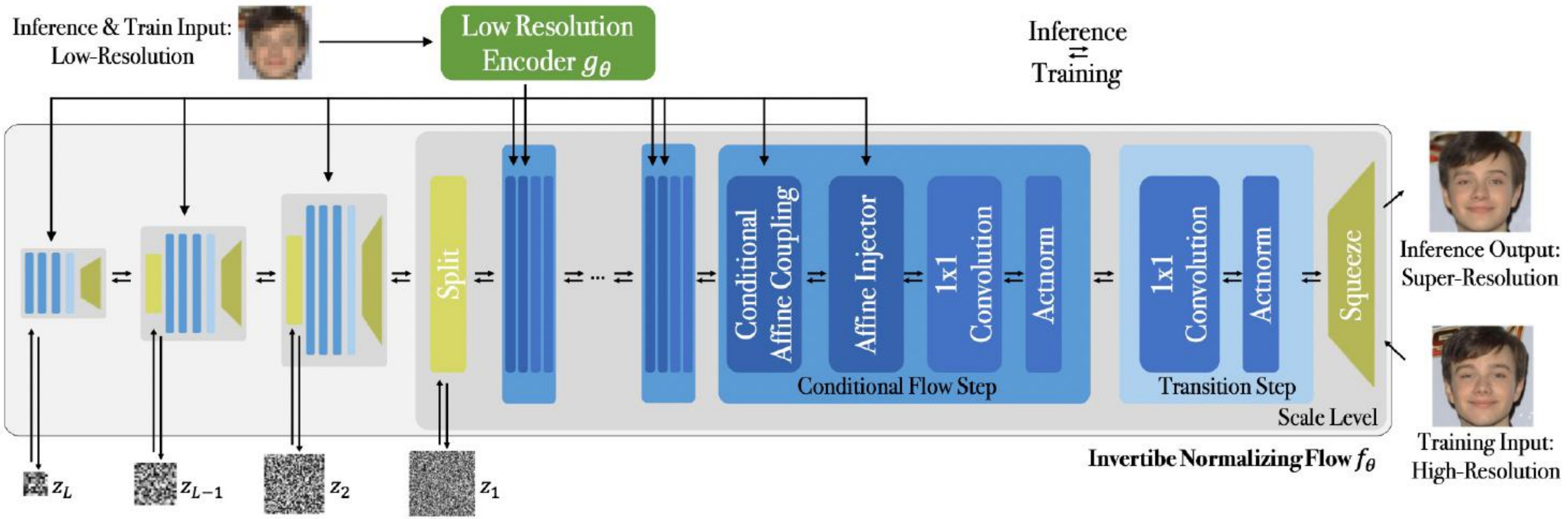


# Applications: Super-Resolution

- SRFlow
  - A normalizing flow based super-resolution method, allowing diversity
  - Outperforms state-of-the-art GAN-based approaches

# Application: Text Synthesis

- Language Flow
  - non-autoregressive and autoregressive flow-based models

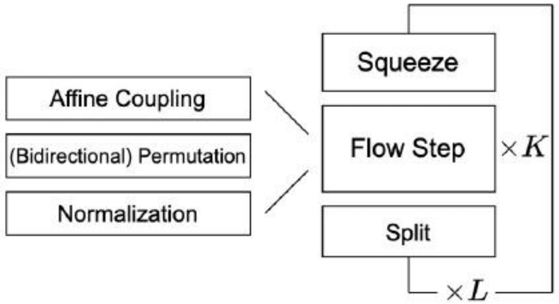



Figure 2: Non-autoregressive Language Flow model with Multi-Scale architecture.

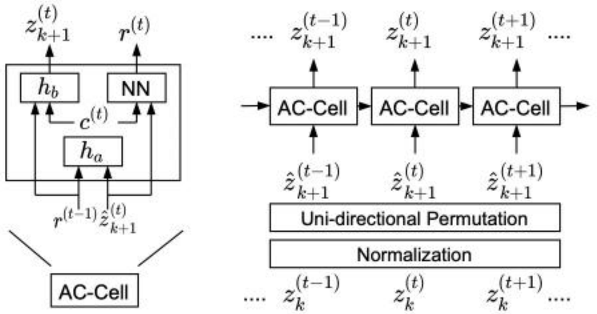



Figure 3: Autoregressive Language Generative Flow model. The whole autoregressive flow model contains multiple K steps. This figure illustrates one flow step from $z_k$ to $z_{k+1}$.

| **Non-Autoregressive Samples** | **Autoregressive Samples** |
|---|---|
| what does house way when when that little he when the even? | what does wilson probably do after drawing? |
| what did richard know when he she else there the | what did jamie want after charlie forget her immediately |
| what does nelson going when he she when he what that to? | what is brian aware |
| what did richard know when he she else there the | what did caleb say after he went out? |
| what does nelson going when he she when he what that to? | what does phoebe think? |

Table 1: Data samples generated by our flow models. We sample from a Gaussian distribution and generate questions by our non-autoregressive or autoregressive flow decoders. Models are trained on TVQA questions.

# Applications: Audio Synthesis

- FloWaveNet
  - A flow-based generative model for raw audio synthesis
  - Efficiently samples raw audio in real-time

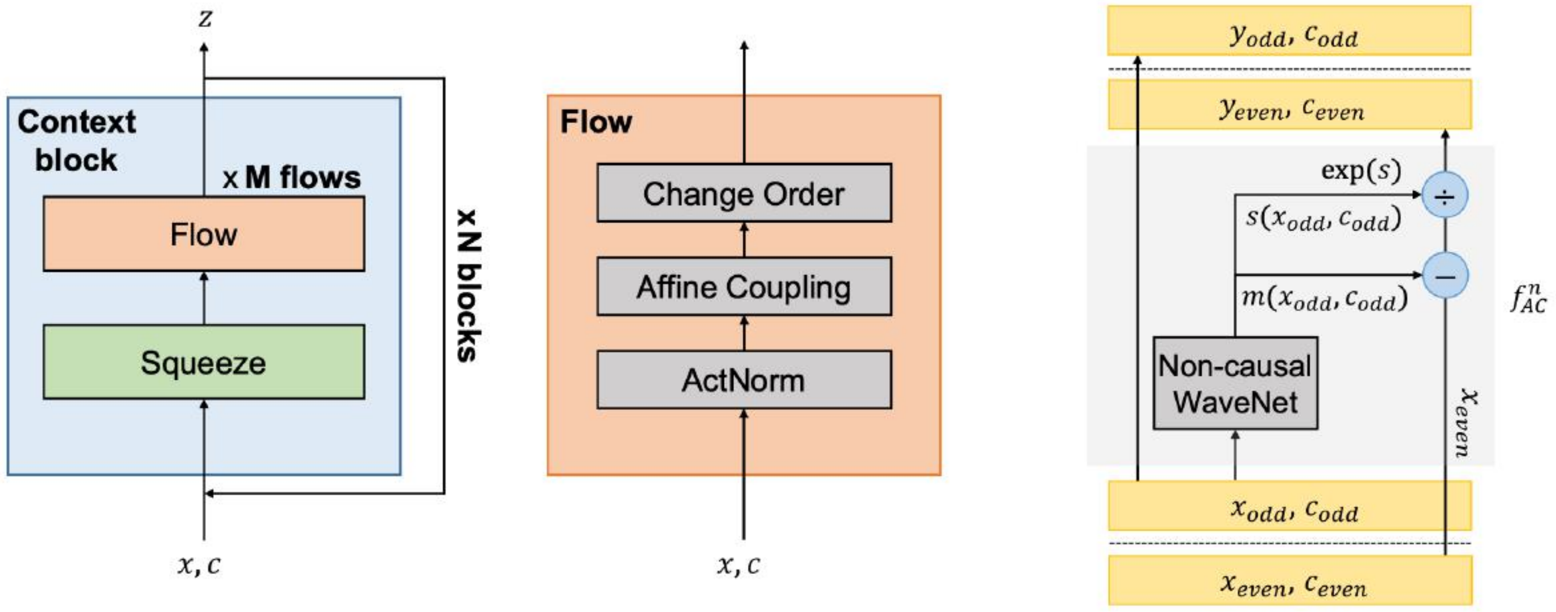
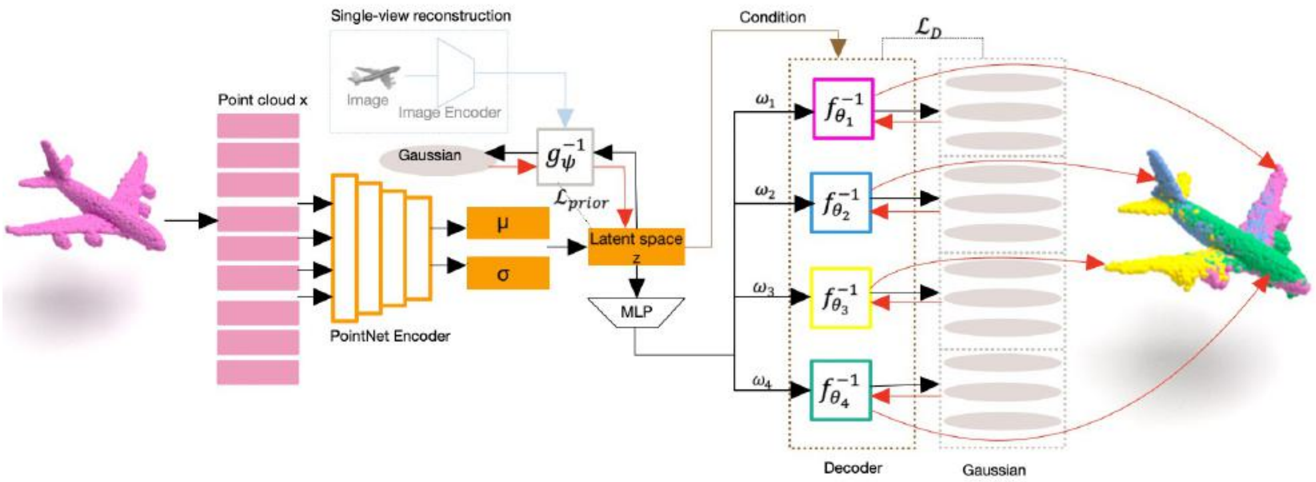
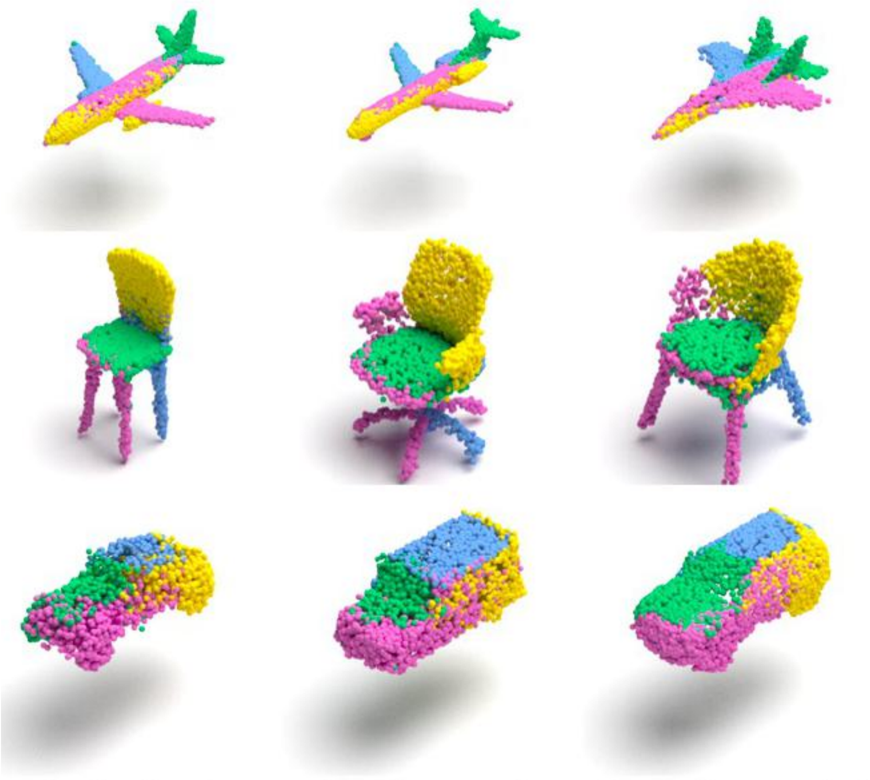



*Figure 1.* Schematic diagram of FloWaveNet. Left: an entire forward pass of the FloWaveNet consisting of N context blocks. Middle: an abstract diagram of the flow operation. Right: a detailed version of the affine coupling operation.

# Applications: Point Cloud Generation

- Mixture of Normalizing Flows for modeling 3D point clouds
- Each mixture component learns to specialize in a distinct subregion in an unsupervised fashion.



# Future directions

- The ultimate goal: a likelihood-based model with
  - fast sampling
  - fast inference
  - fast training
  - good samples
  - good compression
- Flows seem to let us achieve some of these criteria.
- But how exactly do we design and compose flows for great performance? That’s an open question.
- Some requirements that might pose permanent challenges:
  - Dimensionality preserving
  - Invertibility
  - Cheap determinant

**Next lecture:**
Variational Autoencoders