

# COMP547

## DEEP UNSUPERVISED LEARNING

### Lecture #6 – Normalizing Flow Models



**KOÇ**  
**UNIVERSITY**

Aykut Erdem // Koç University // Spring 2021



# Previously on COMP547

- Motivation
- Simple generative models: histograms
- Parameterized distributions and maximum likelihood
- Autoregressive Models
  - Recurrent Neural Nets
  - Masking-based 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  $p_{\theta}(x)$
  - And, ideally, a latent representation that's meaningful

# Our Goal Today

- How to fit a density model  $p_{\theta}(x)$  with **continuous**  $x \in \mathbb{R}^n$
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  - For new  $x$ , ability to evaluate  $p_{\theta}(x)$
  - Ability to sample from  $p_{\theta}(x)$
  - And, ideally, **a latent representation** that's meaningful
- **Differences from Autoregressive Models from last lecture**

# Lecture overview

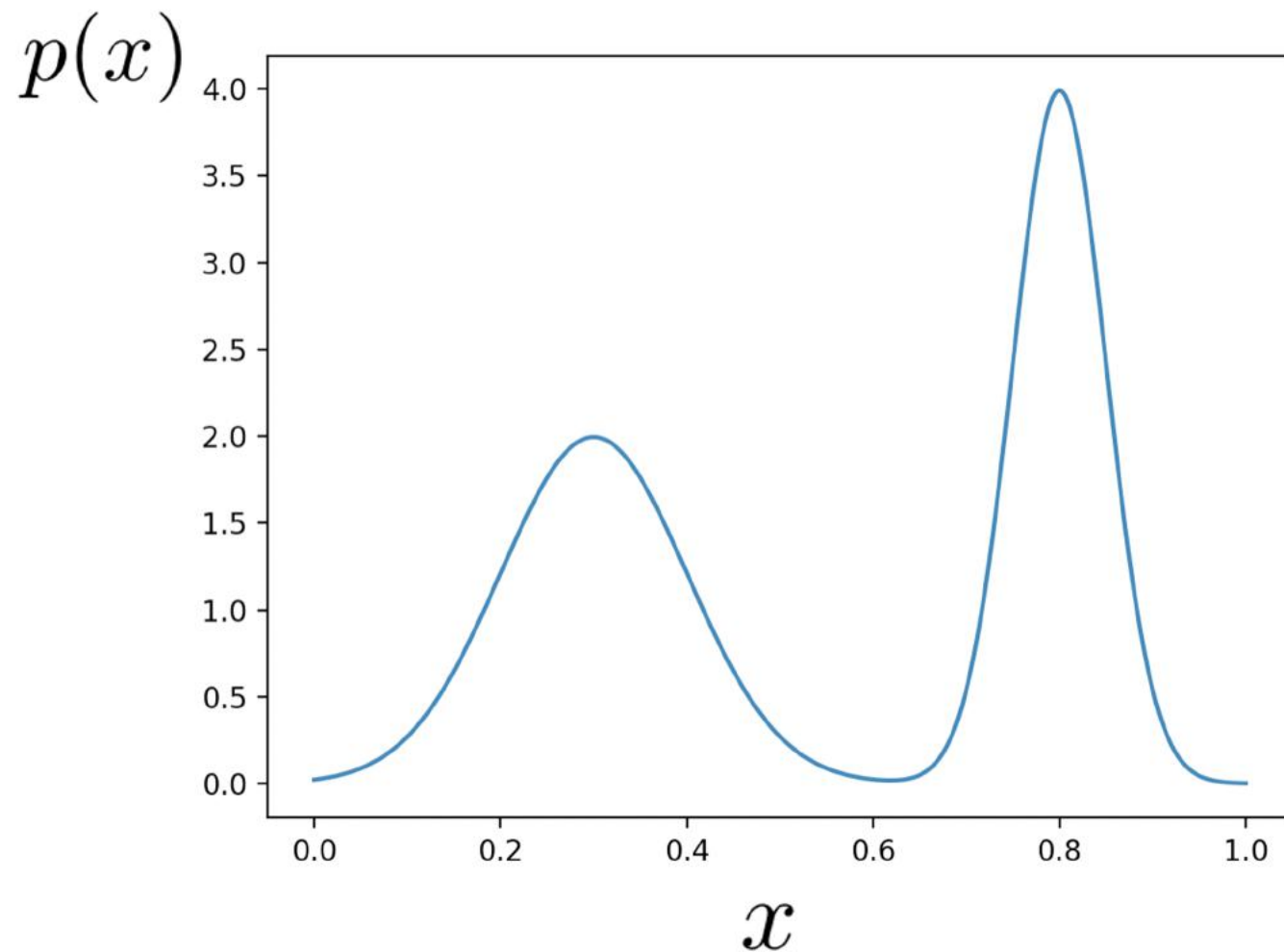
- Foundations of Flows (1-D)
- 2-D Flows
- N-D Flows
- Dequantization

**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:

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

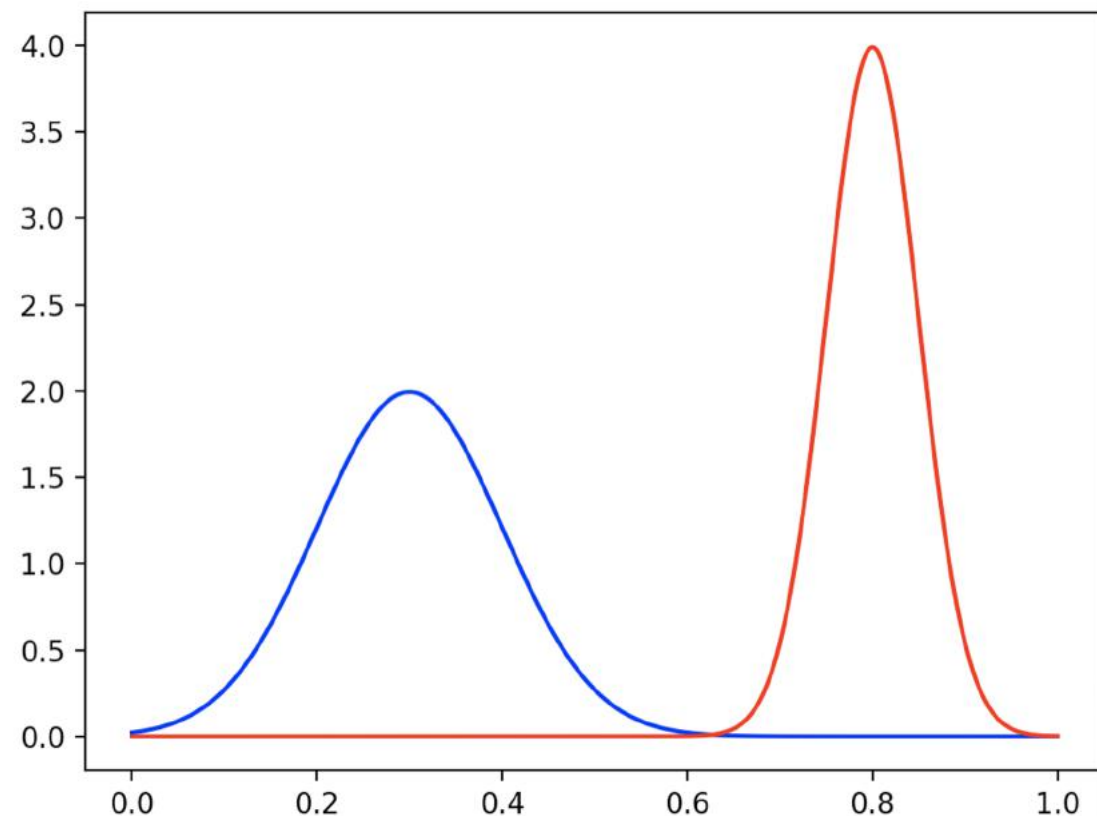


# Example Density Model: Mixtures of Gaussians

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

Parameters: means and variances of components, mixture weights

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



# Aside on Mixtures of Gaussians

Do mixtures of Gaussians work for high-dimensional data?

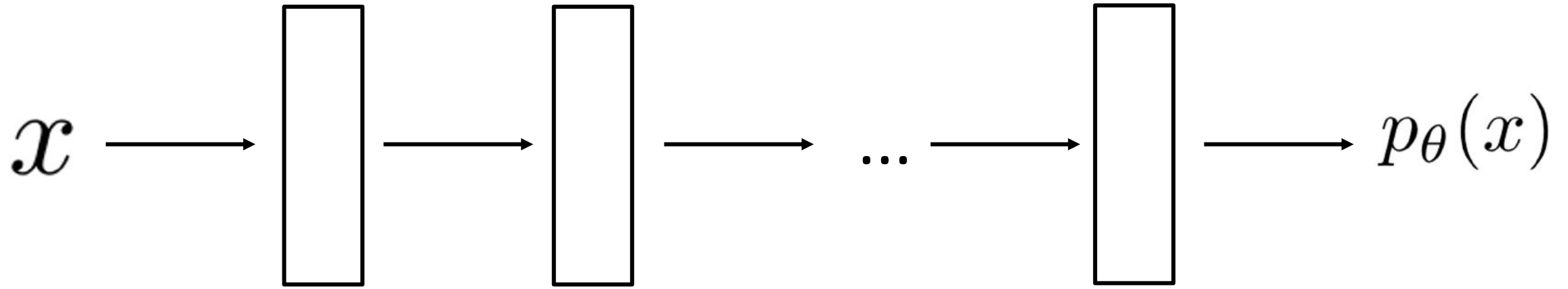
Not really. The sampling process is:

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?



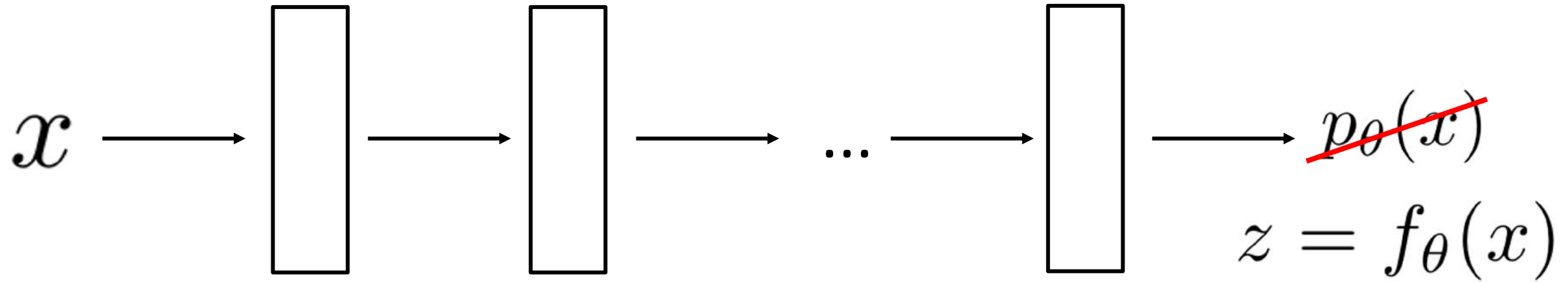
- How to ensure proper distribution?

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

- How to sample?
- Latent representation?

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

# Flows: Main Idea



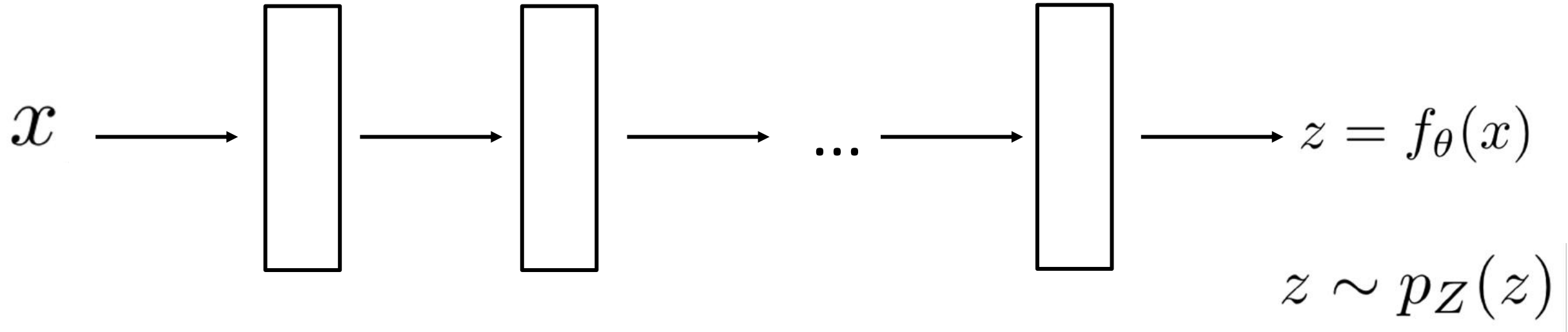
Generally:  $z \sim p_Z(z)$

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

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



# Flows: Training



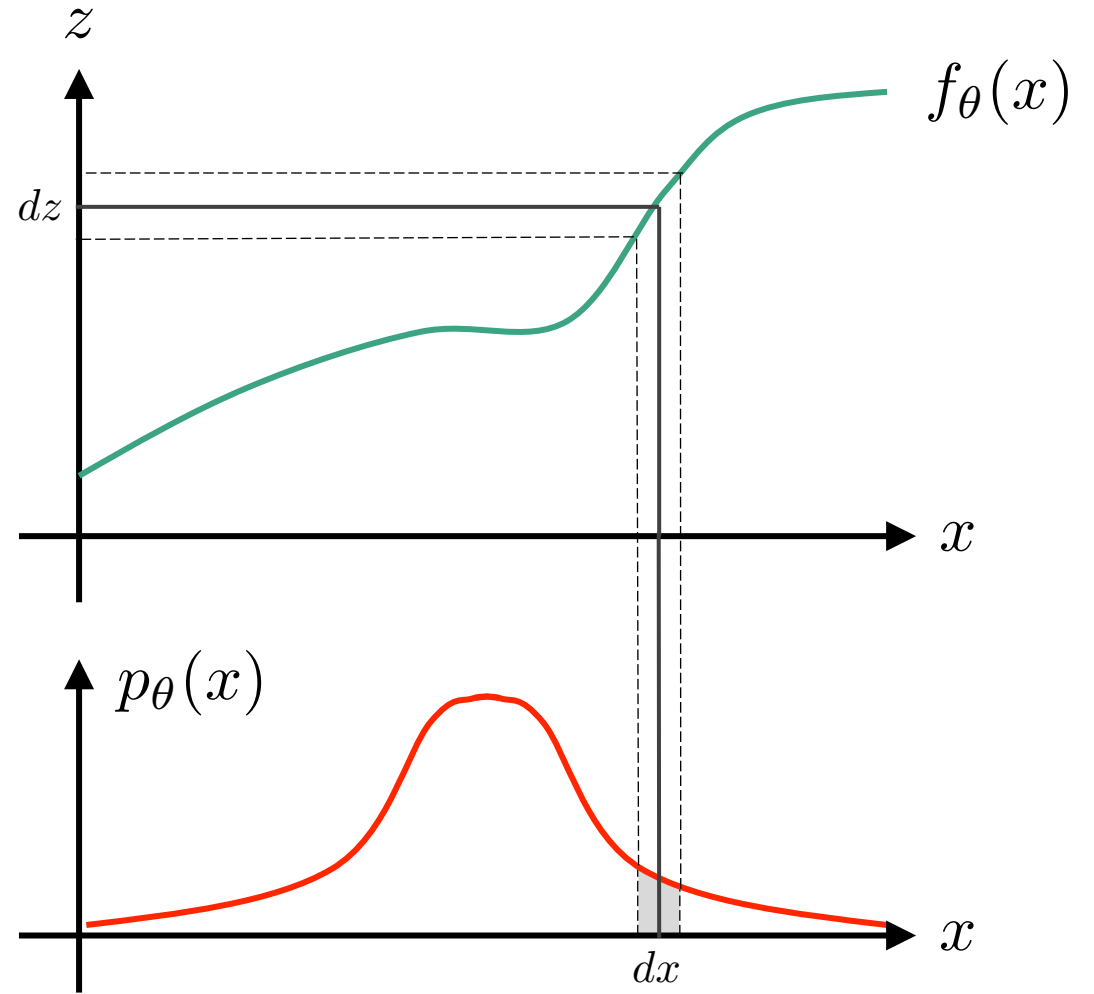
$$\max_{\theta} \sum_i \log p_{\theta}(x^{(i)})$$

# Change of Variables

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

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

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

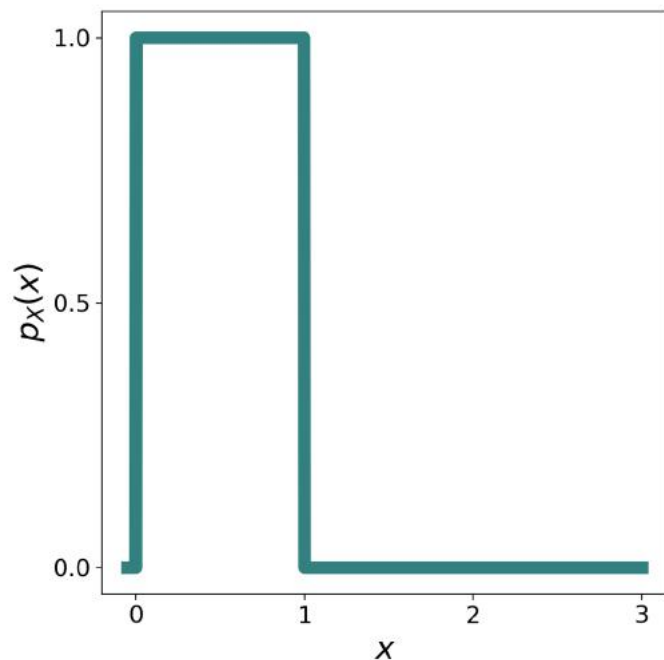


**Note:** requires  $f_{\theta}$  invertible & differentiable

# Change of Variable Density Needs to Be Normalized

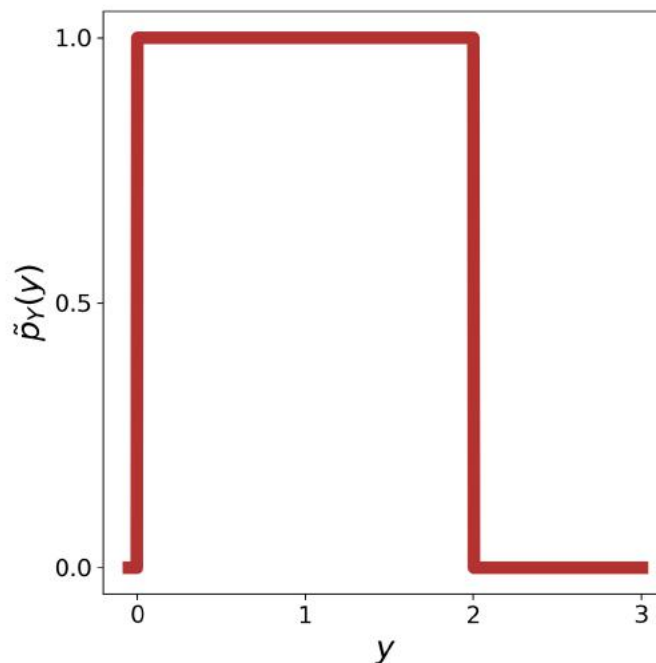
$$X \sim p_X$$

$$p_X(x) = \begin{cases} 1 & \text{for } 0 \leq x \leq 1 \\ 0 & \text{else} \end{cases}$$

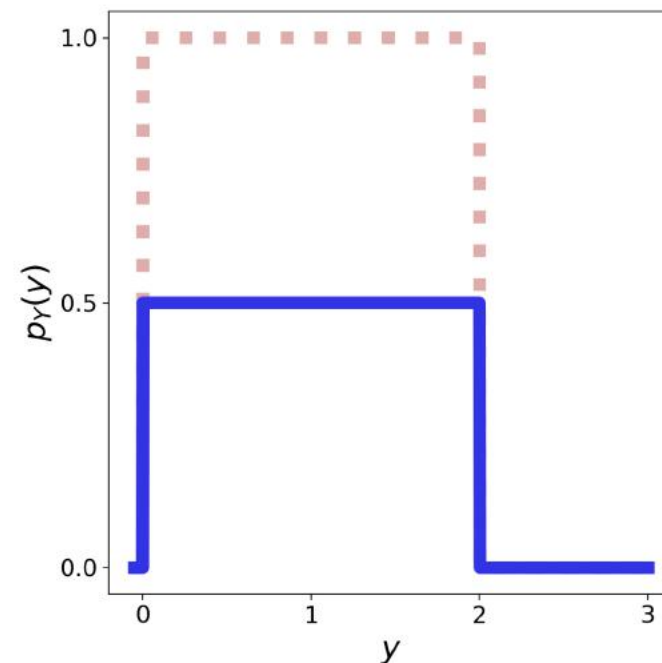


$$Y := 2X$$

$$\tilde{p}_Y(y) = p_X(y/2)$$



$$p_Y(y) = p_X(y/2)/2$$



# Flows: Training

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

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

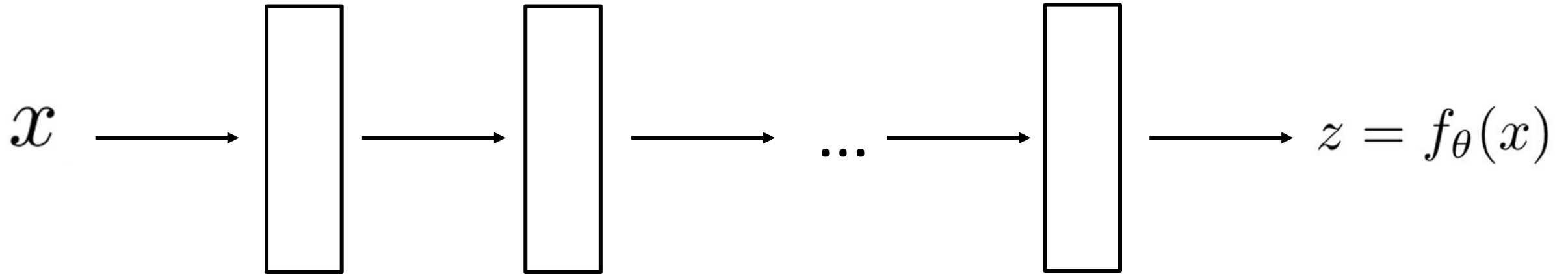
$$\begin{aligned} p_{\theta}(x^{(i)}) &= p_Z(z^{(i)}) \left| \frac{\partial z}{\partial x}(x^{(i)}) \right| \\ &= p_Z(f_{\theta}(x^{(i)})) \left| \frac{\partial f_{\theta}}{\partial x}(x^{(i)}) \right| \end{aligned}$$

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

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



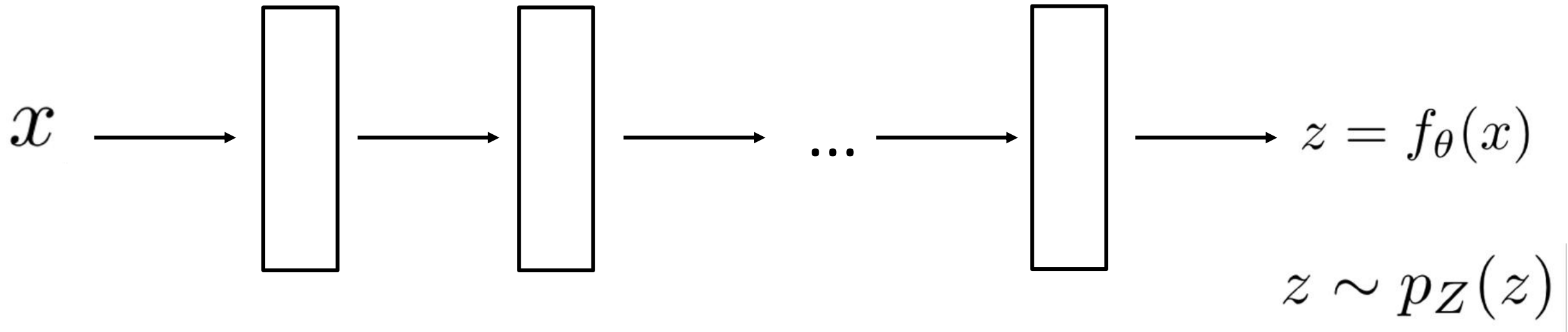
# Flows: Sampling



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

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

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

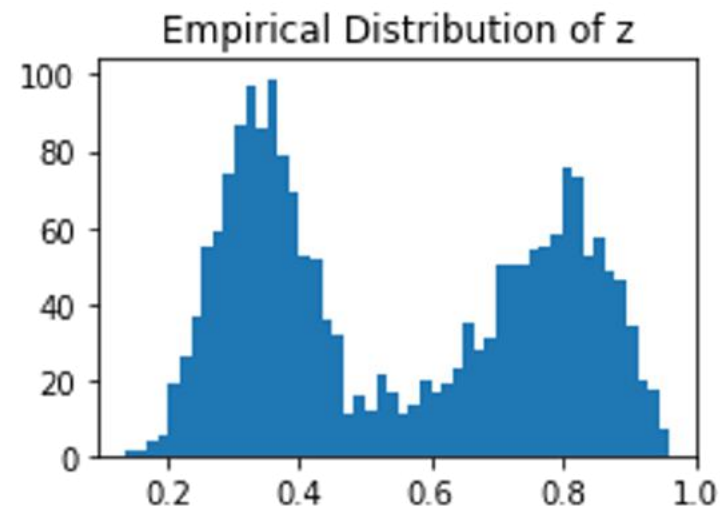
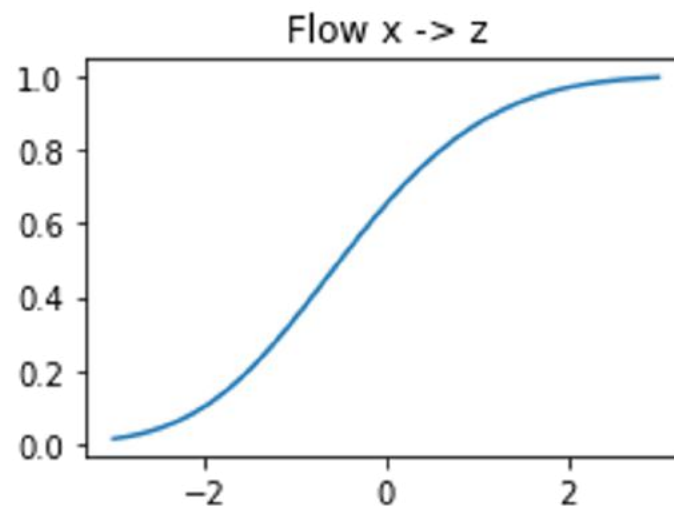
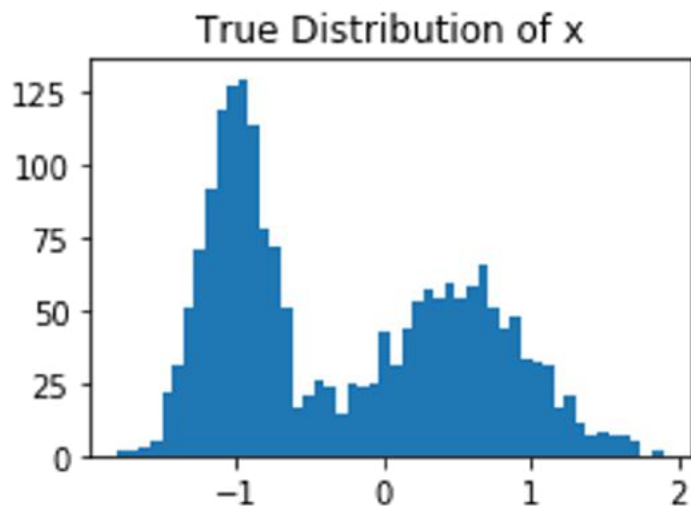


Recall, change of variable formula requires

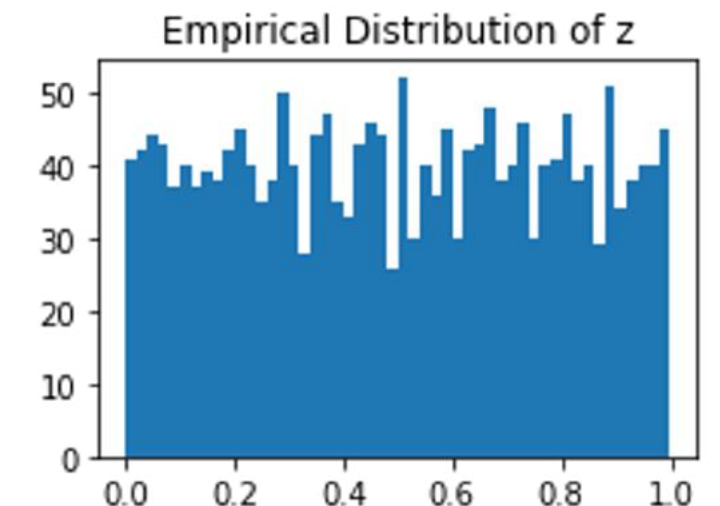
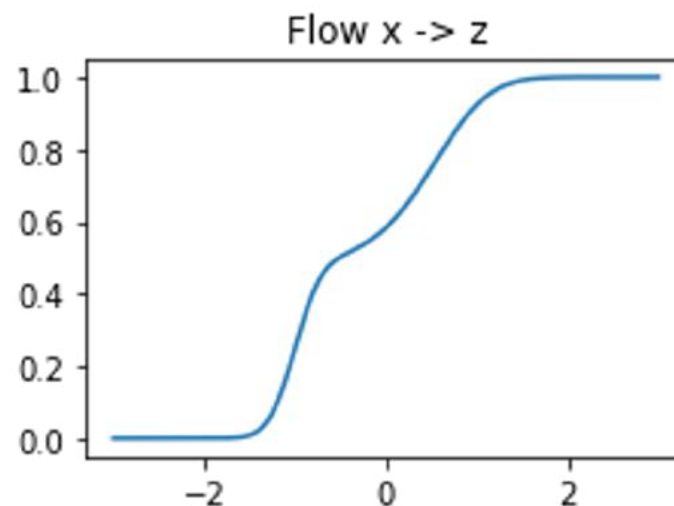
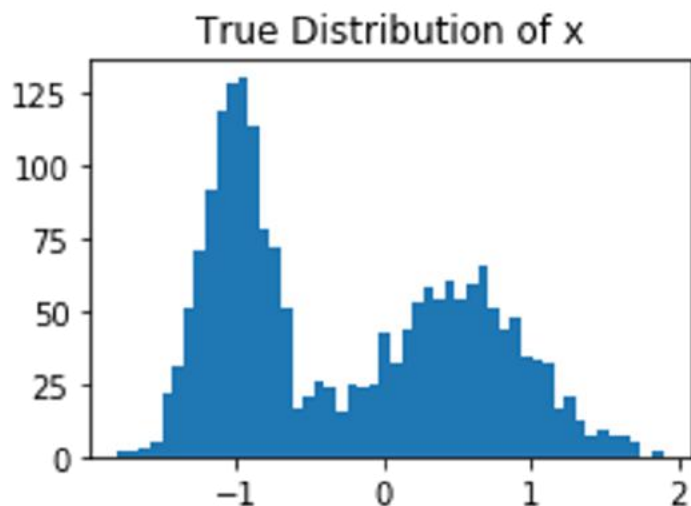
- $f_{\theta}$  Invertible & differentiable

# Example: Flow to Uniform z

Before training



After training



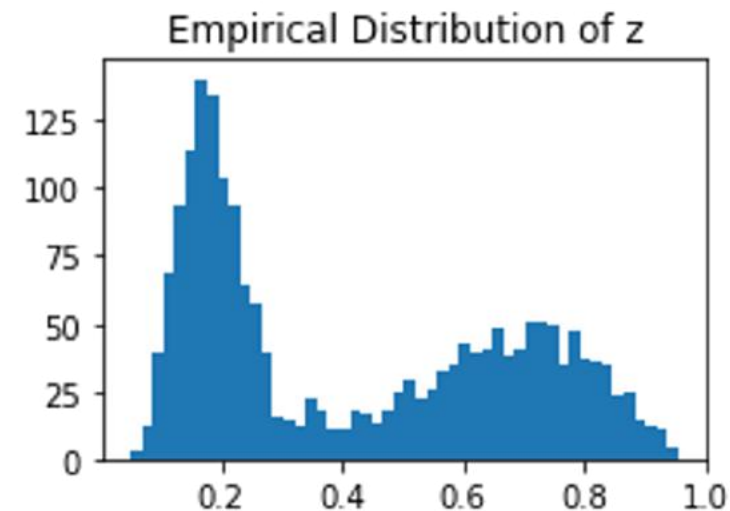
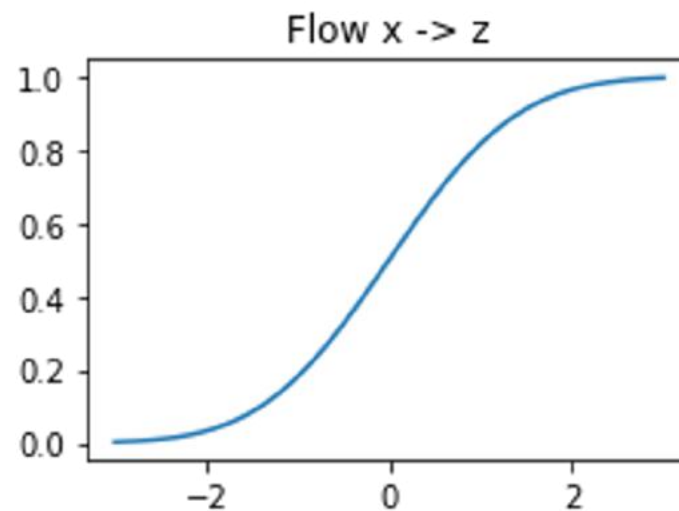
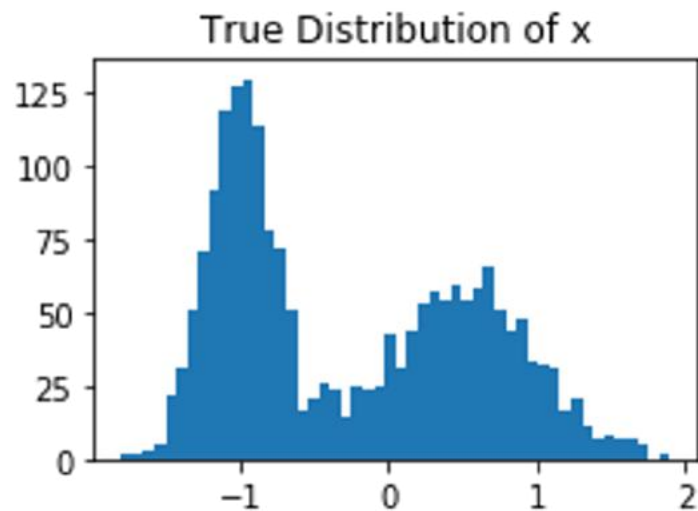
True distribution of x

Flow  $x \rightarrow z$

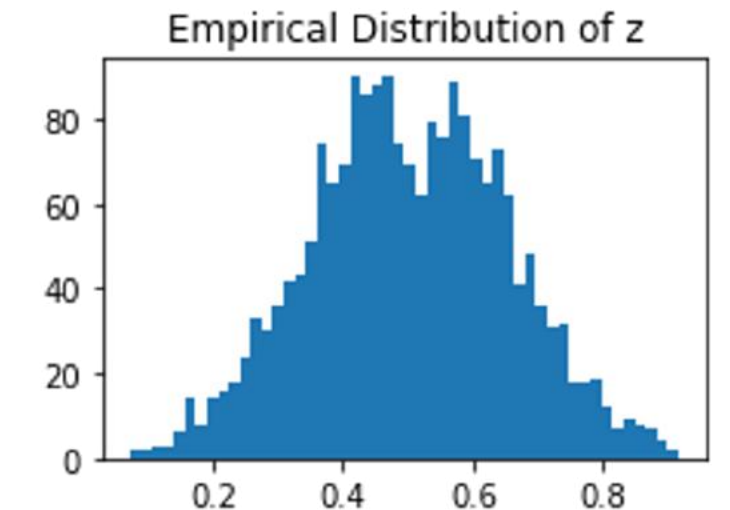
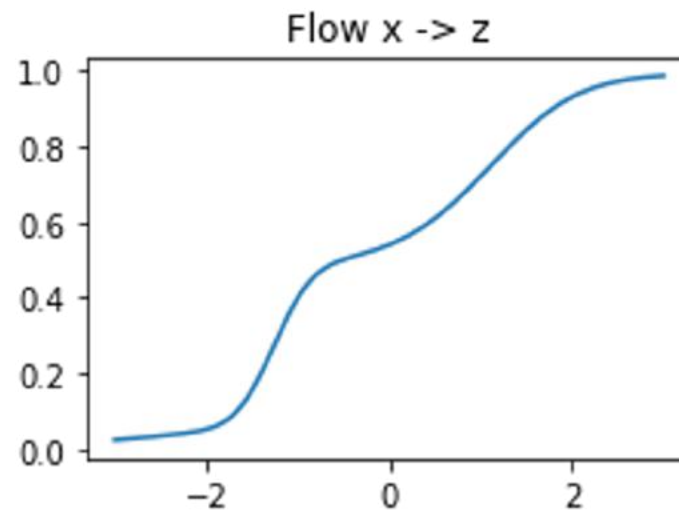
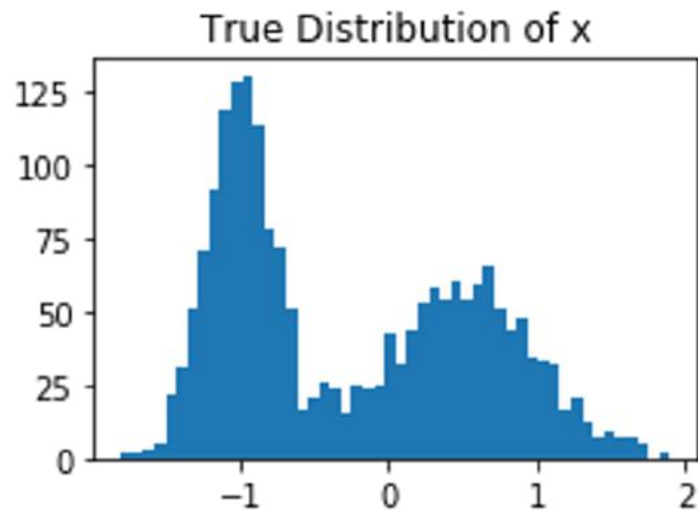
Empirical distribution of z

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

Before training



After training



True distribution of x

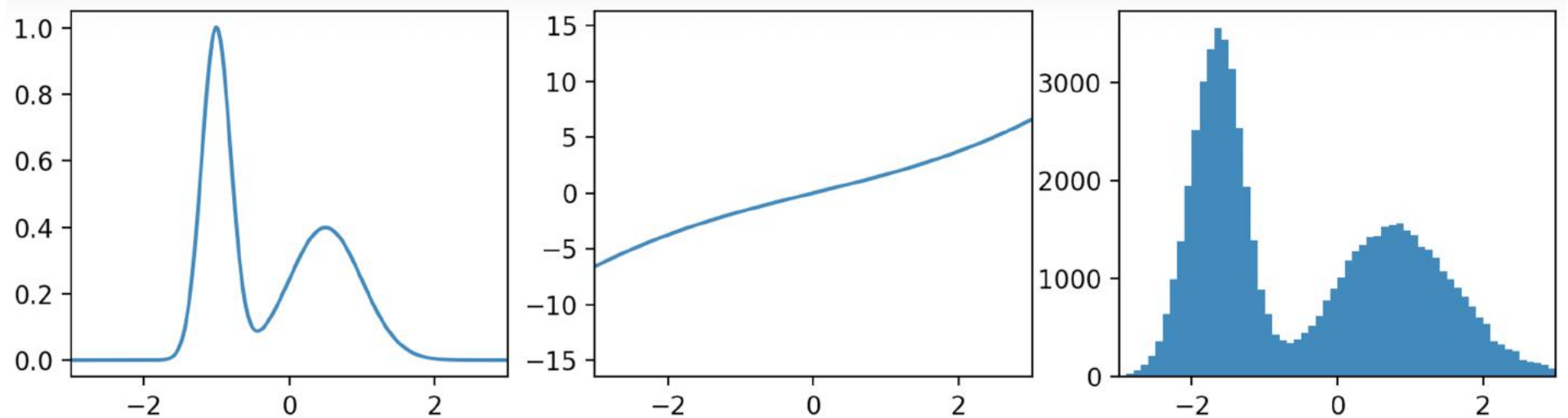
Flow x  $\rightarrow$  z

Empirical distribution of z

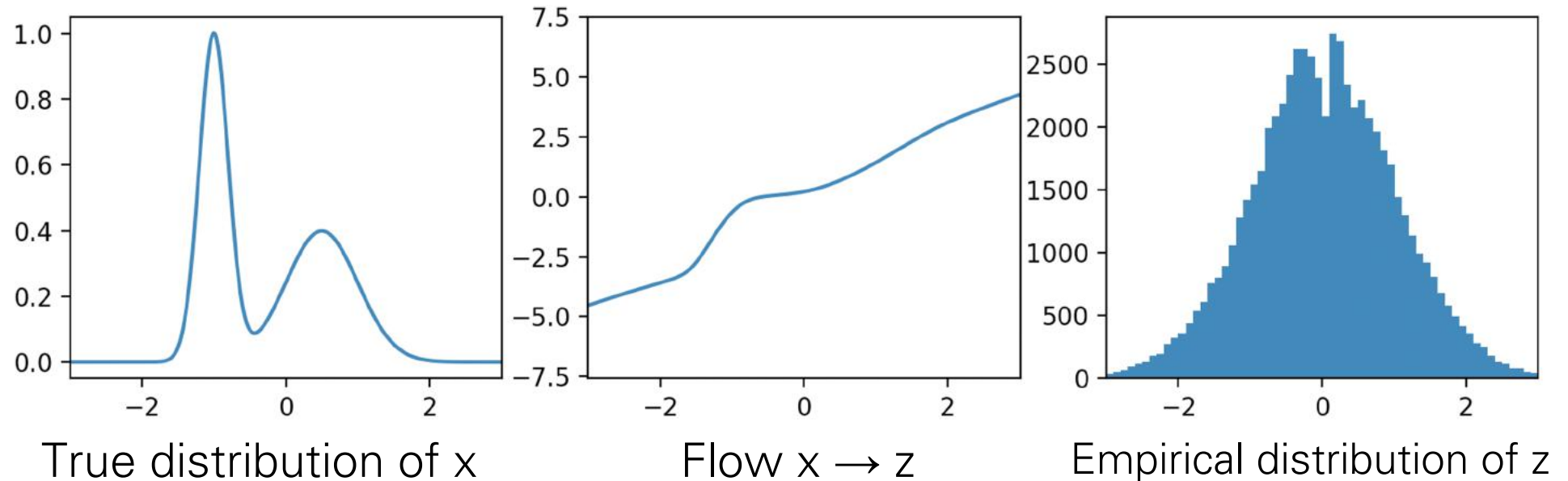


# Example: Flow to Gaussian z

Before training



After training



# Practical Parameterizations of Flows

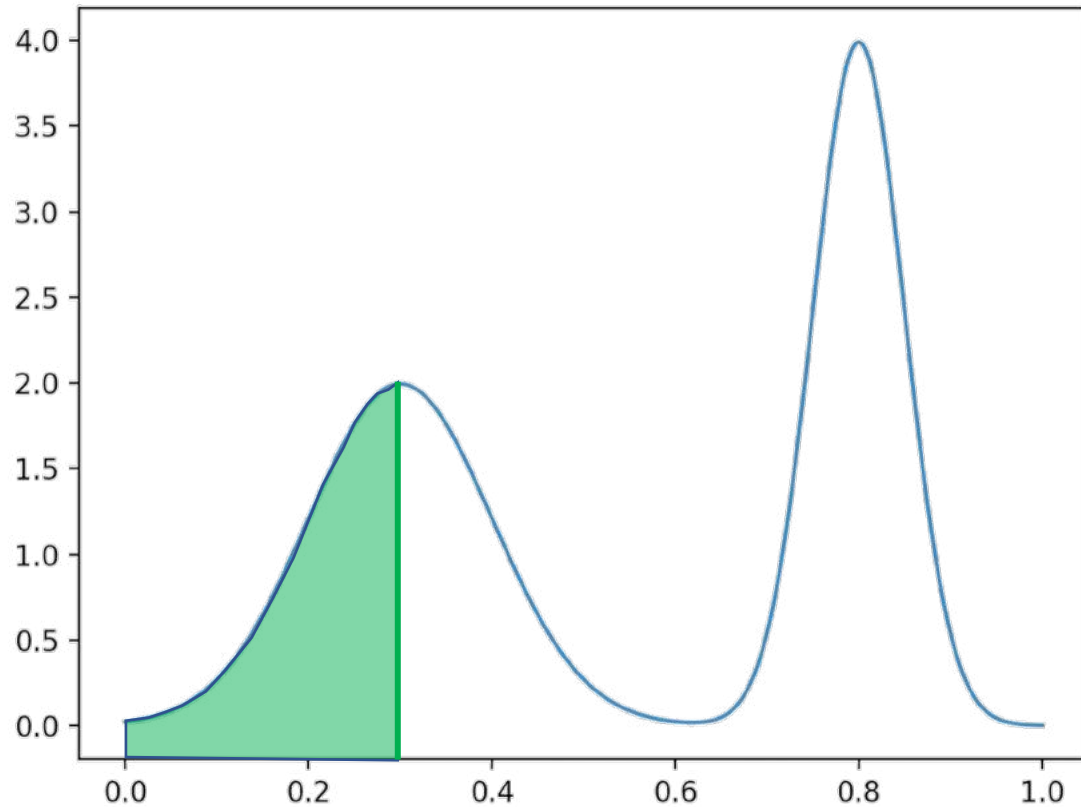
**Requirement:** Invertible and Differentiable

- 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?

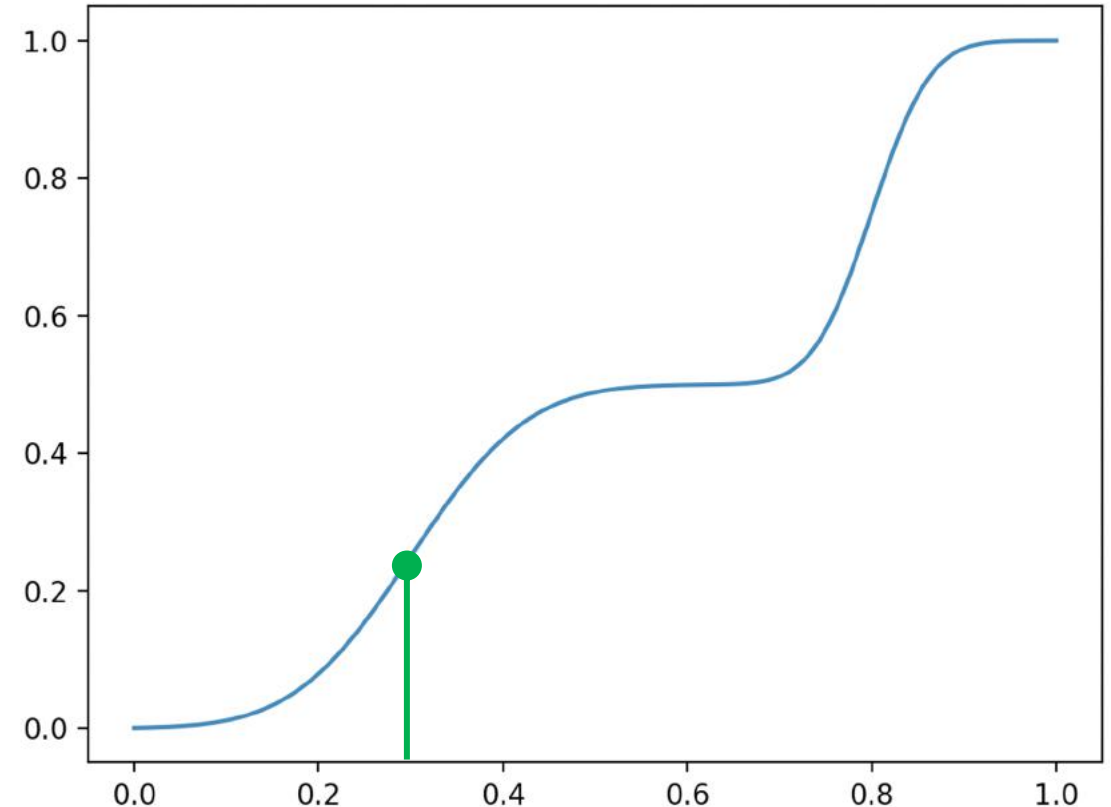
# How general are flows?

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

# Refresher: Cumulative Density Function (CDF)



$p_{\theta}(x)$



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

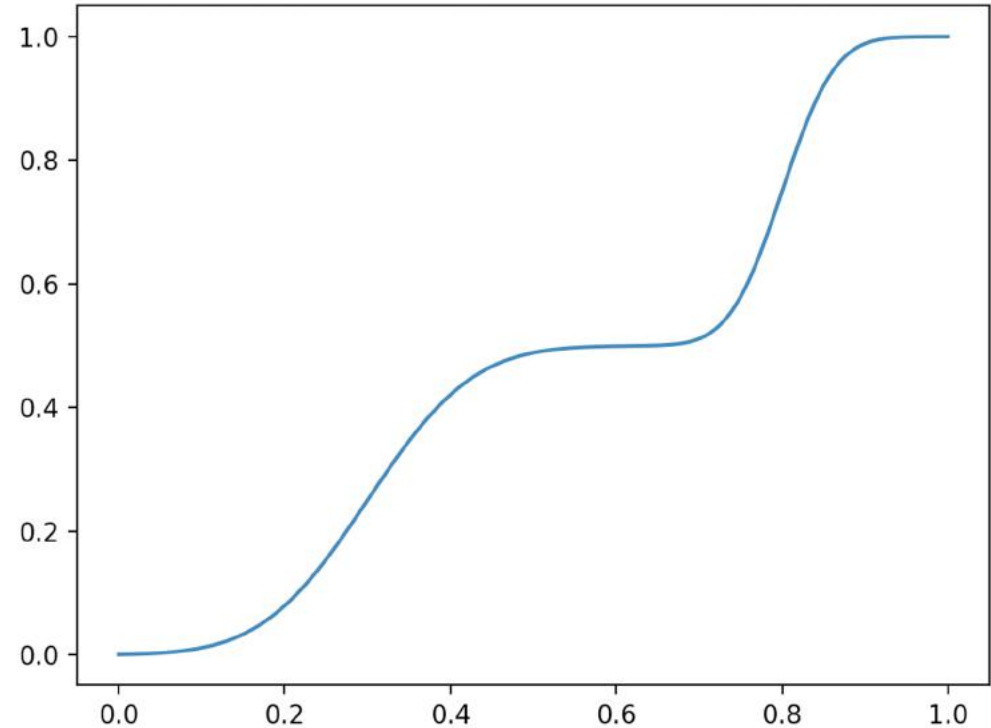
# Sampling via inverse CDF

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

$$x \xrightarrow{\text{CDF}} u$$

$$z \xrightarrow{\text{CDF}} u$$

$$x \xrightarrow{\text{CDF}} u \xrightarrow{\text{CDF}} z$$

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



# Lecture overview

- Foundations of Flows (1-D)
- **2-D Flows**
- N-D Flows
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# 2-D Autoregressive Flow

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

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

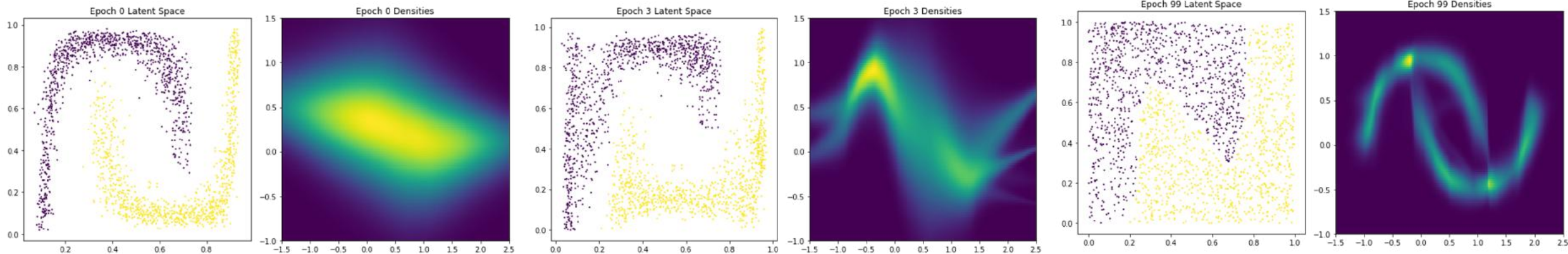
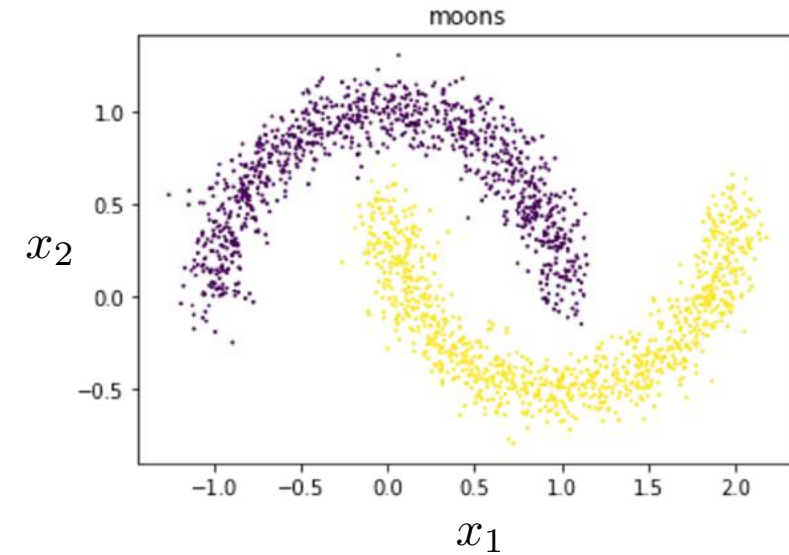
$$\max_{\theta, \phi} \sum_i \log p_{z_1}(f_\theta(x_1)) + \log \left| \frac{dz_1}{dx_1} \right| + \log p_{z_2}(f_\phi(x_1, x_2)) + \log \left| \frac{dz_2}{dx_2} \right|$$

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

# 2-D Autoregressive Flow: Two Moons

## Architecture:

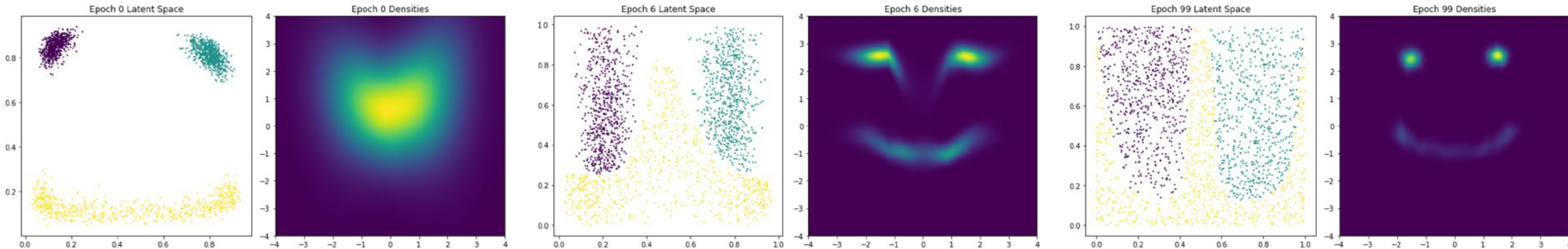
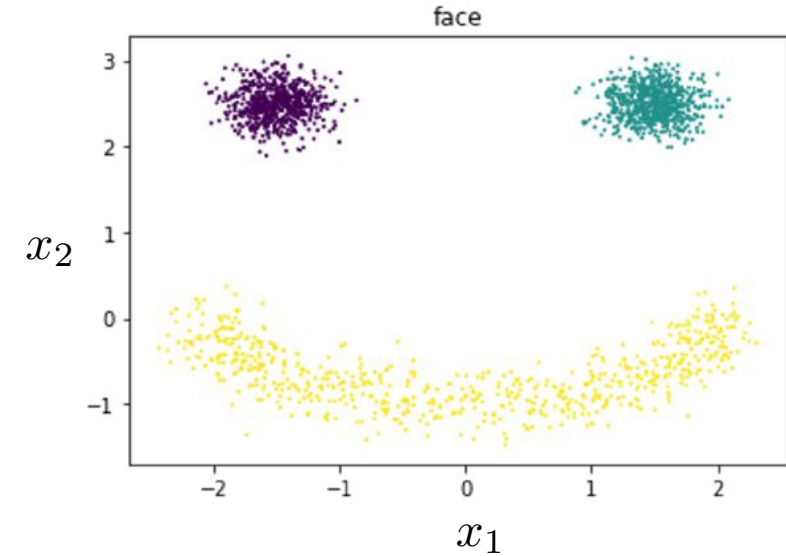
- Base distribution:  $\text{Uniform}[0,1]^2$
- $x_1$ : mixture of 5 Gaussians
- $x_2$ : mixture of 5 Gaussians, conditioned on  $x_1$



# 2-D Autoregressive Flow: Face

## Architecture:

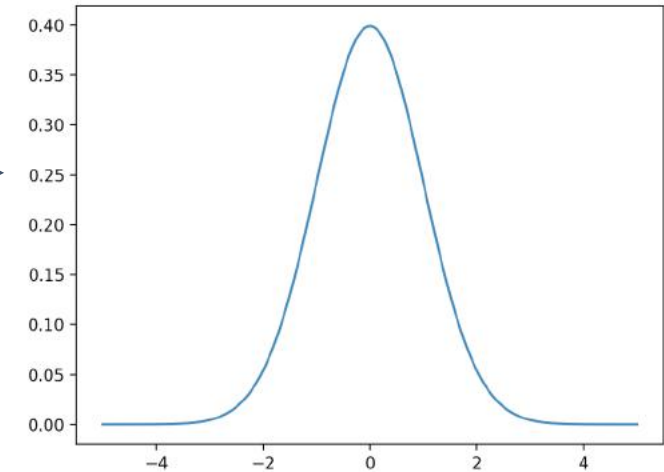
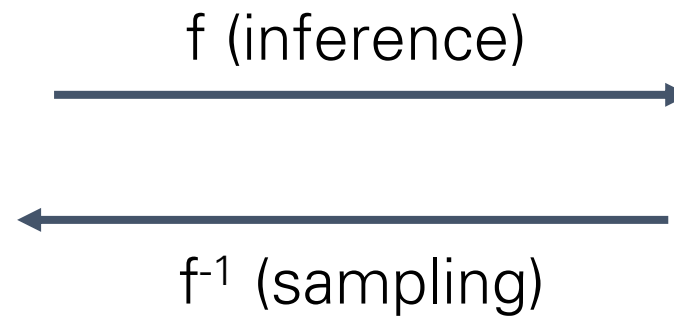
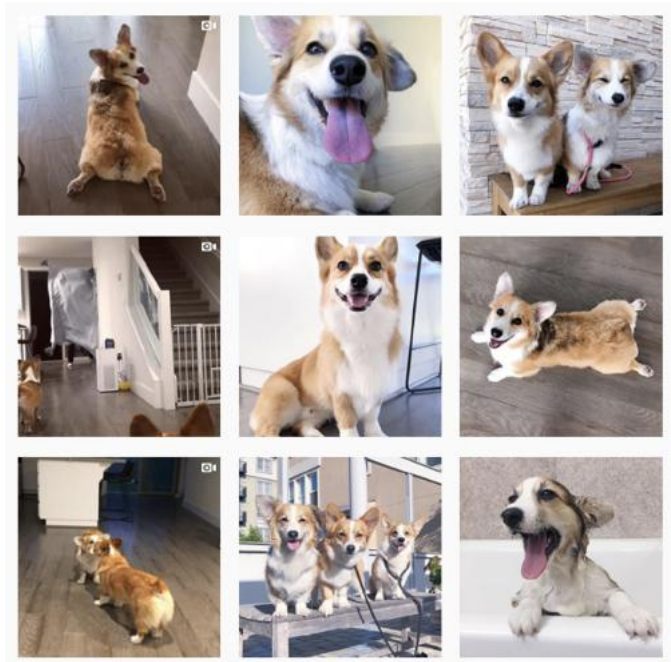
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- 2-D Flows
- **N-D Flows**
- Dequantization

# High-dimensional data



$x$  and  $z$  must have the same dimension



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

# Pathways to Designing a Normalizing Flow

1. Require an invertible architecture.
  - Coupling layers, autoregressive, etc.
2. Require efficient computation of a change of variables equation.

$$\log p(x) = \log p(f(x)) + \log \left| \det \frac{df(x)}{dx} \right|$$

Model distribution      Base distribution

(or a continuous version)  $\log p(x(t_N)) = \log p(x(t_0)) + \int_{t_0}^{t_N} \text{tr} \left( \frac{\partial f(x(t), t)}{\partial x(t)} \right) dt$

$\mathcal{O}(m^3)$

# 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  $\mathbf{x}$  to  $\mathbf{z}$
- Fully parallelizable

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

- Notice

- $\mathbf{x} \rightarrow \mathbf{z}$  has the same structure as the **log likelihood** computation of an autoregressive model
- $\mathbf{z} \rightarrow \mathbf{x}$  has the same structure as the **sampling** procedure of an autoregressive model

$$z_1 = f_{\theta}(x_1)$$

$$z_2 = f_{\theta}(x_2; x_1)$$

$$z_3 = f_{\theta}(x_3; x_1, x_2)$$

$$x_1 = f_{\theta}^{-1}(z_1)$$

$$x_2 = f_{\theta}^{-1}(z_2; x_1)$$

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

# 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**

$$z_1 = f_{\theta}^{-1}(x_1)$$

$$x_1 = f_{\theta}(z_1)$$

$$z_2 = f_{\theta}^{-1}(x_2; z_1)$$

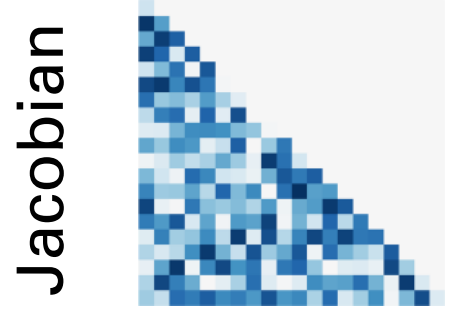
$$x_2 = f_{\theta}(z_2; z_1)$$

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

$$x_3 = f_{\theta}(z_3; z_1, z_2)$$

# AF vs IAF

- 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



(Lower triangular)



# AF and IAF

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

- E.g. 1MP image  $\rightarrow$  1M layers...

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

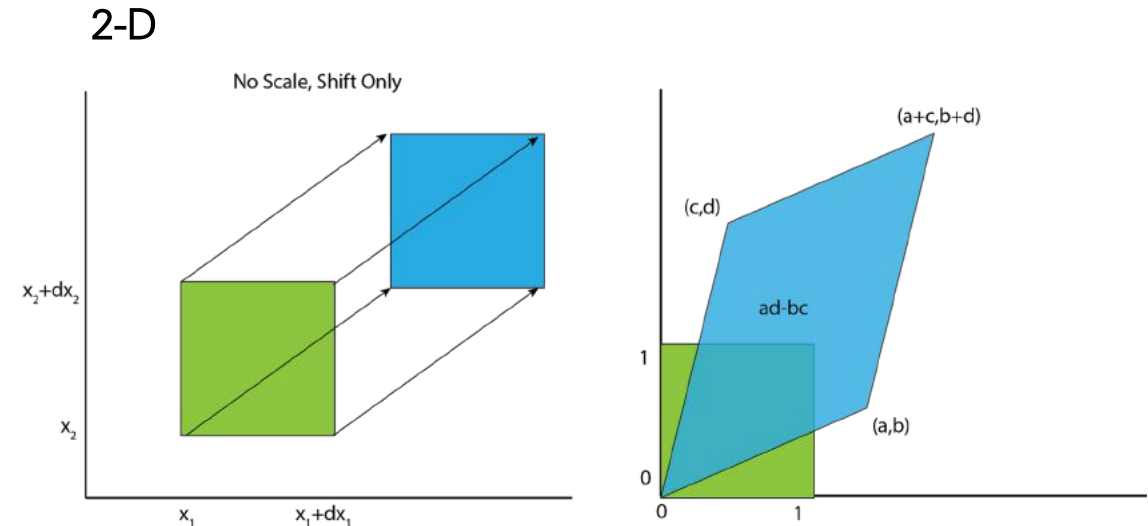
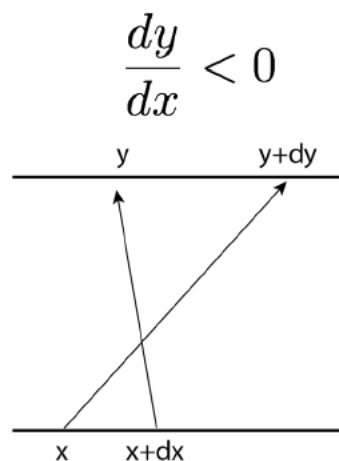
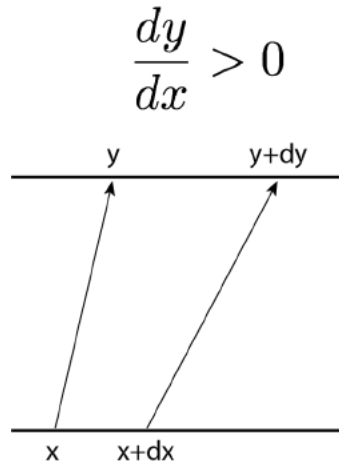
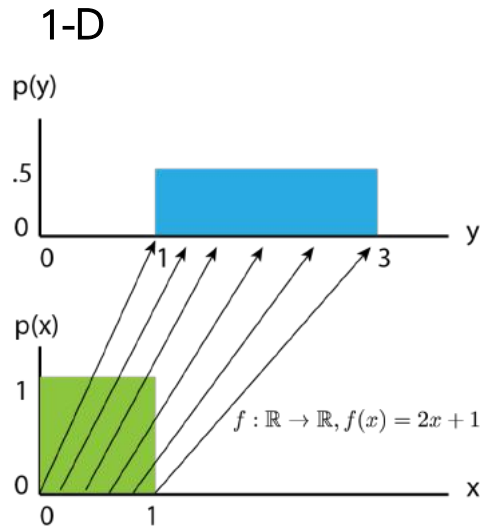
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# Change of MANY variables

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

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



# Change of MANY variables

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

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

**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  $\mathbf{x}$ :

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

Train with maximum likelihood:

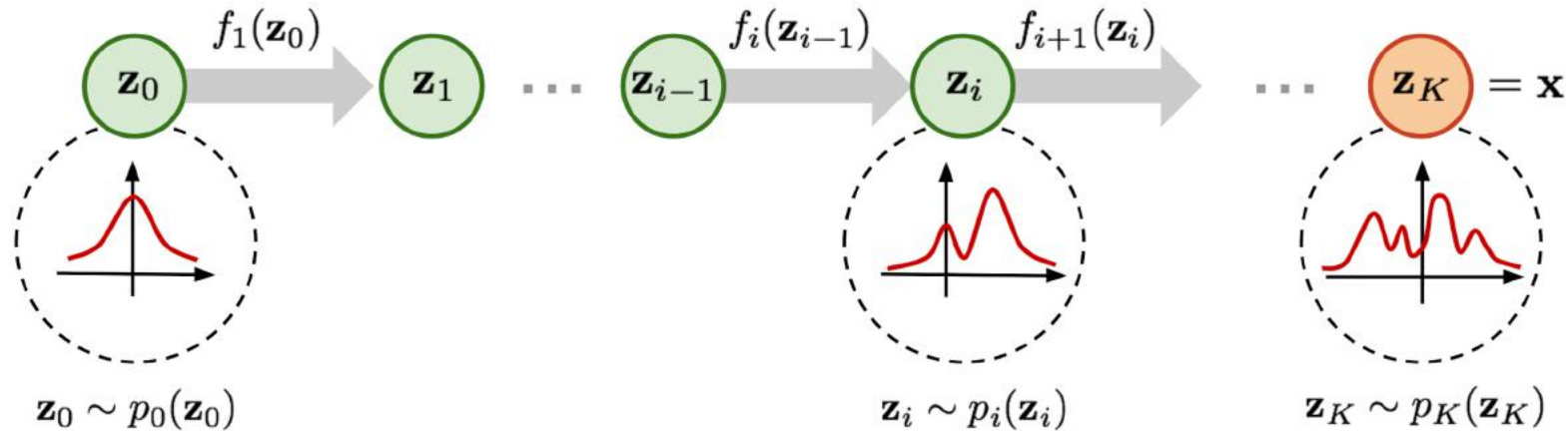
$$\arg \min_{\theta} \mathbb{E}_{\mathbf{x}} [-\log p_{\theta}(\mathbf{x})] = \mathbb{E}_{\mathbf{x}} \left[ -\log p(f_{\theta}(\mathbf{x})) - \log \det \left| \frac{\partial f_{\theta}(\mathbf{x})}{\partial \mathbf{x}} \right| \right]$$

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

# Chaining Invertible Mappings

$$f = f_S \circ \cdots \circ f_2 \circ f_1$$

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



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

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



# Constructing flows: composition

- Flows can be composed

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

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

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

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

- 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

$$f_{\theta}((x_1, \dots, x_d)) = (f_{\theta}(x_1), \dots, f_{\theta}(x_d))$$

- 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.

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

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

# NICE/RealNVP

Affine coupling layer

- Split variables in half:  $\mathbf{x}_{1:d/2}$ ,  $\mathbf{x}_{d/2+1:d}$

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

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

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

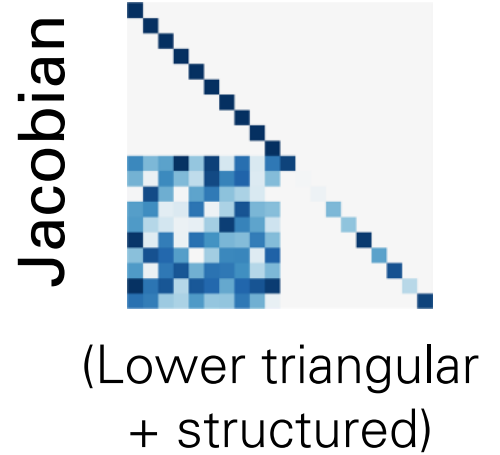
# NICE/RealNVP

- It also has a tractable Jacobian determinant

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

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

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



- 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 Architecture

Input  $x$ :  $32 \times 32 \times c$  image

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

Can be better??

# RealNVP: How to partition variables?

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

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

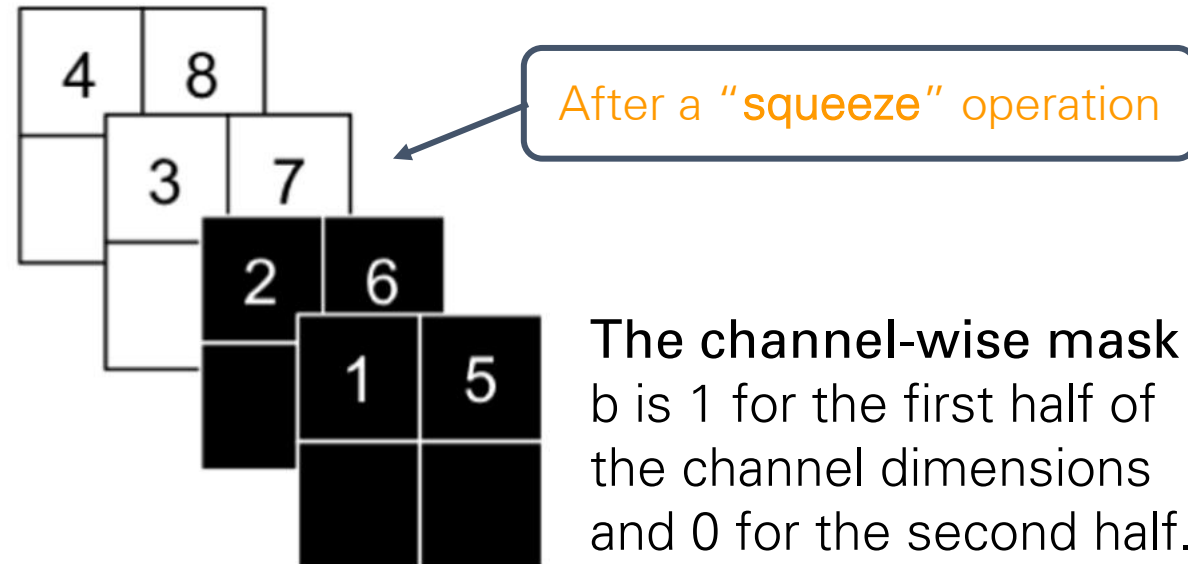


# RealNVP: How to partition variables?

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.

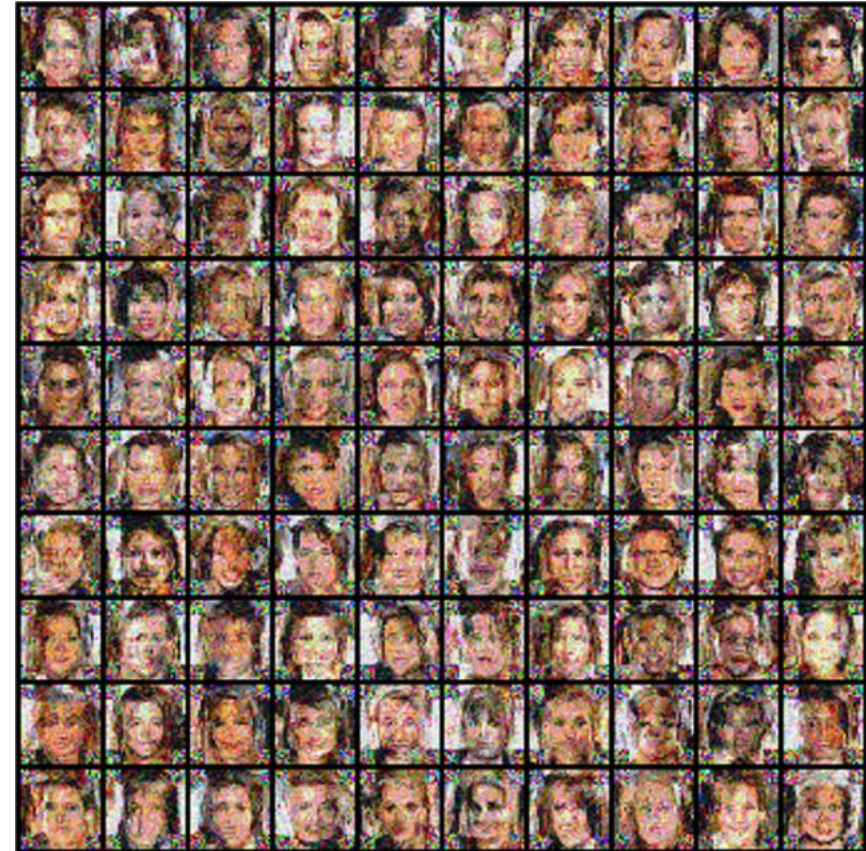


# Good vs Bad Partitioning

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)



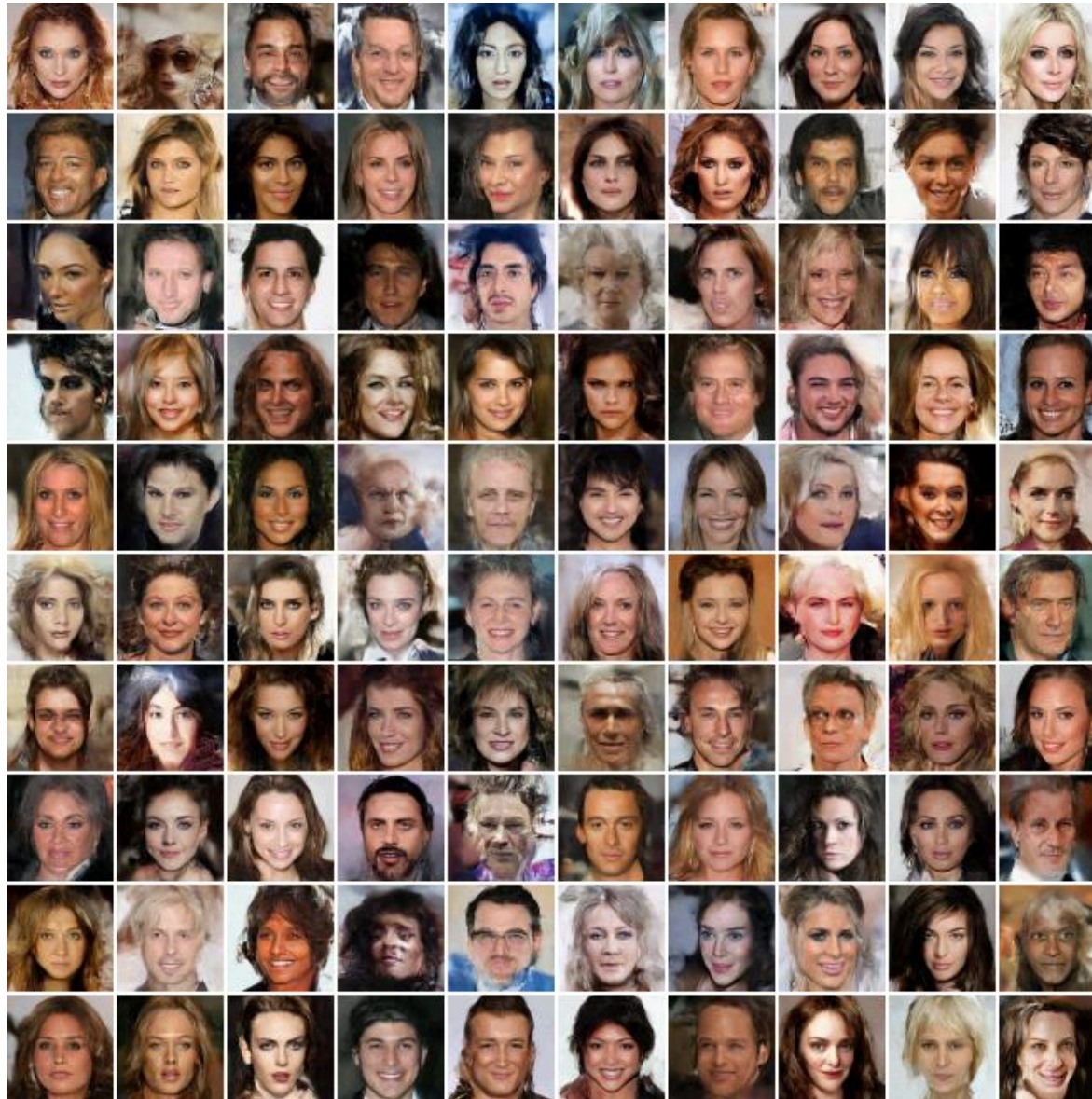
# NN architecture also matters

- 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.*

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

# Flow++

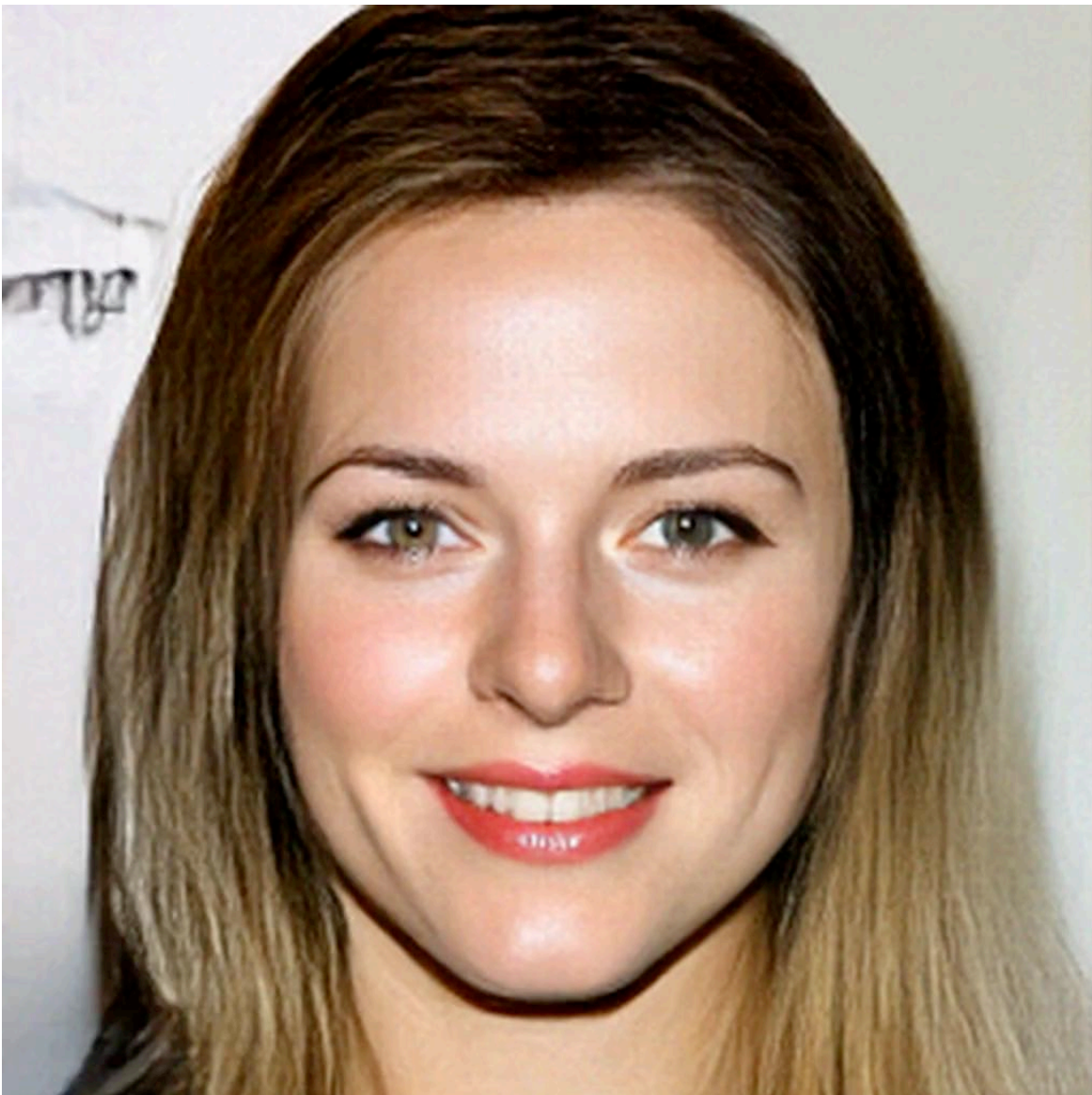


Samples from Flow++  
trained on 64x64 CelebA



# Other classes of flows

- Glow ([link](#))
  - Replacing permutation with  $1 \times 1$  convolution (soft permutation)
  - Large-scale training
- Continuous time flows (FFJORD)
  - Allows for unrestricted architectures. Invertibility and fast log probability computation guaranteed.



# Architectural Taxonomy

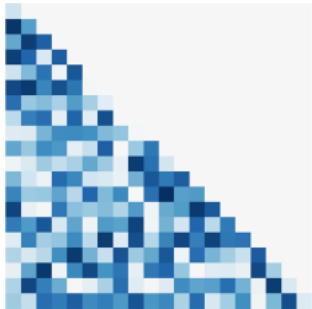
## Sparse connection

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

### 1. Autoregressive

IAF/MAF/NAF  
SOS polynomial  
UMNN

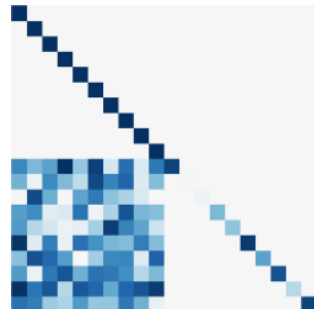
Jacobian



(Lower triangular)

### 2. Block coupling

NICE/RealNVP/Glow  
Cubic Spline Flow  
Neural Spline Flow



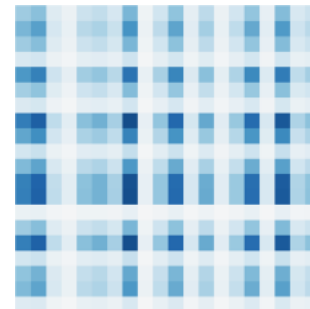
(Lower triangular +  
structured)

## Residual Connection

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

### 3. Det identity

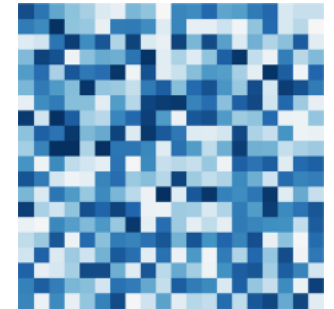
Planar/Sylvester  
flows  
Radial flow



(Low rank)

### 4. Stochastic estimation

Residual  
Flow  
FFJORD



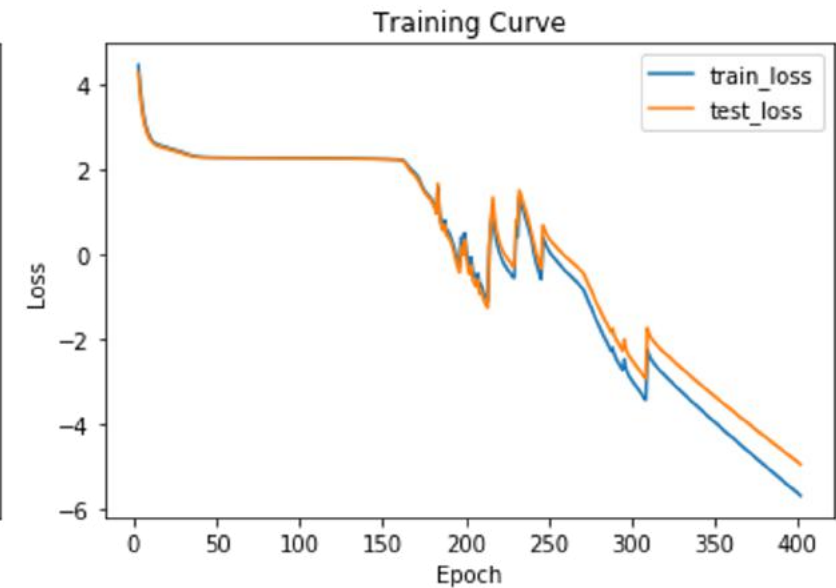
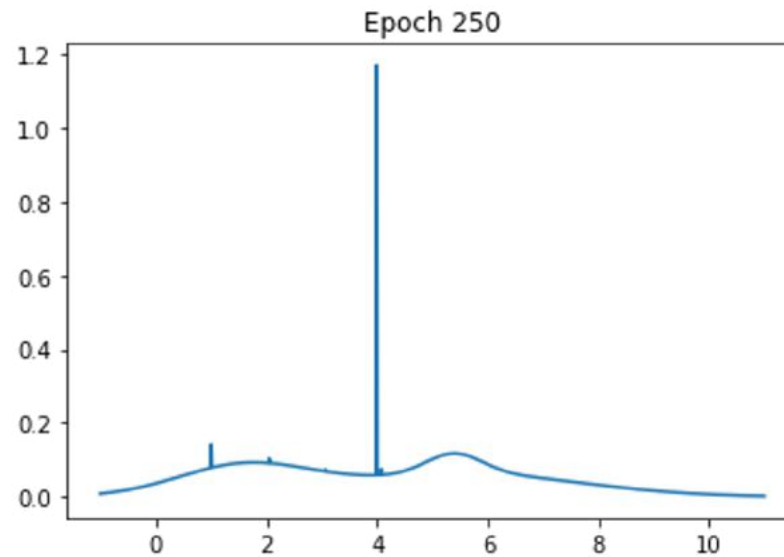
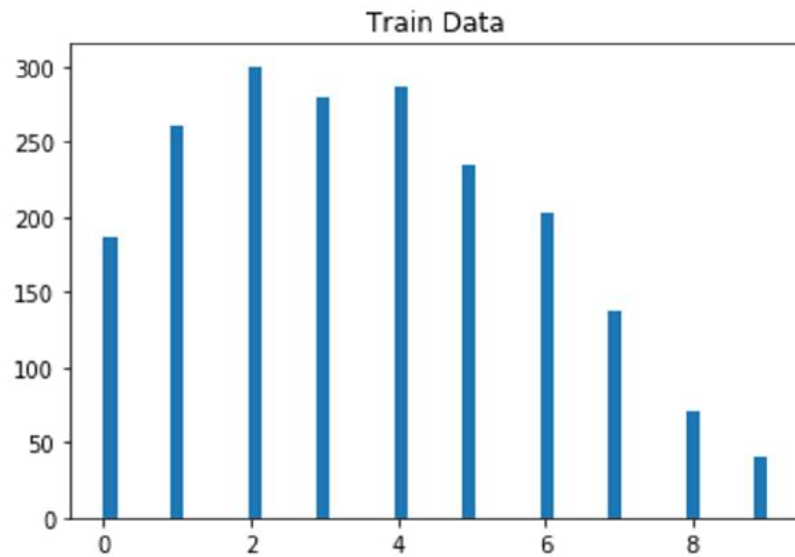
(Arbitrary)



# 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,  $\mathbf{x} \in \{0, 1, 2, \dots, 255\}$
  - 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

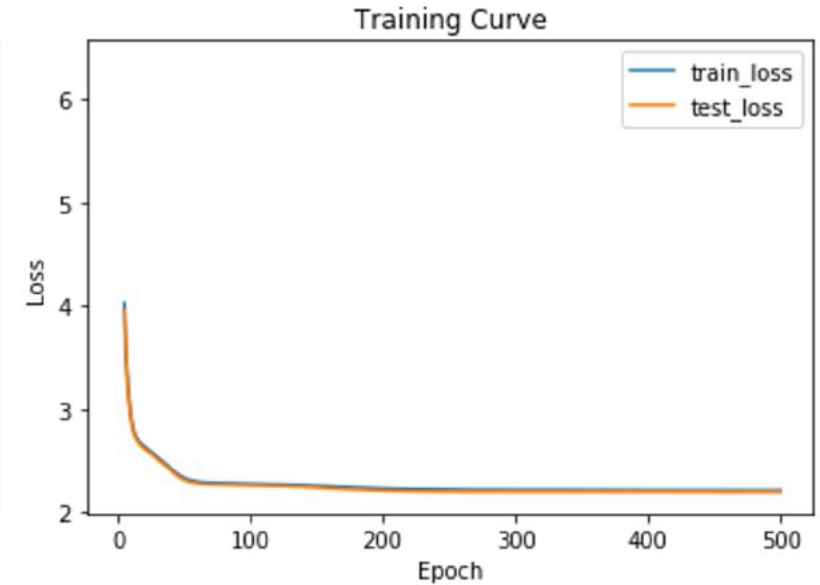
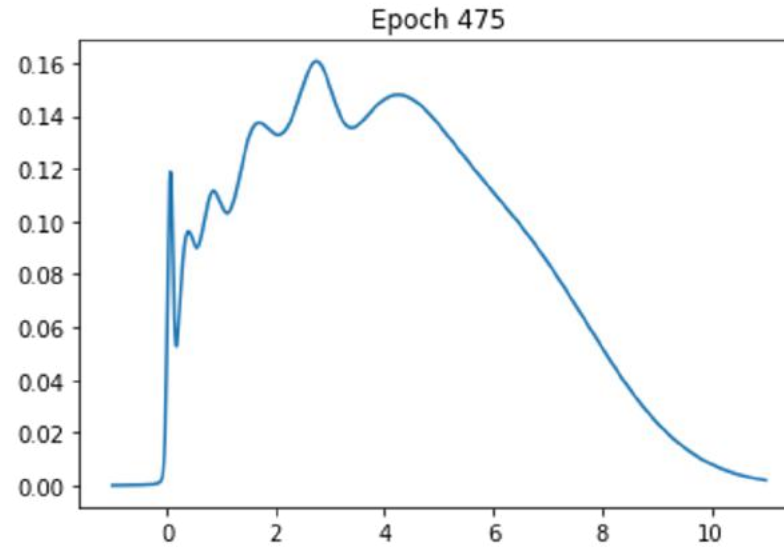
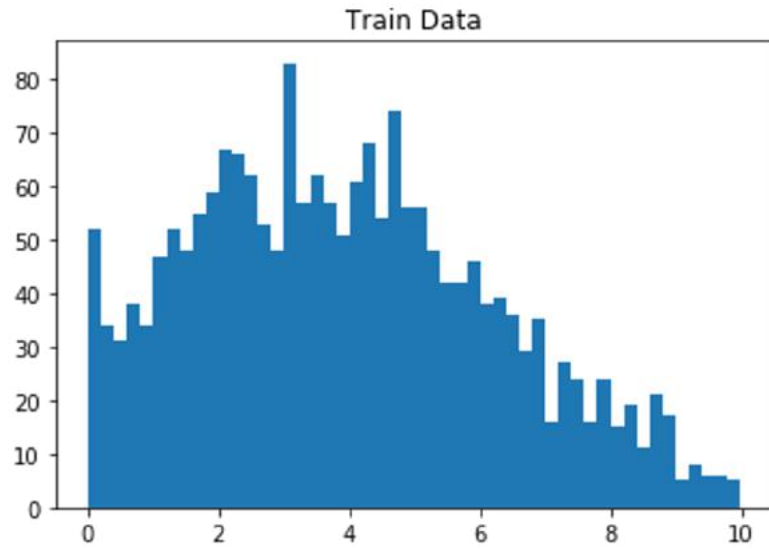
- Solution: **Dequantization**. Add noise to data.

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

- We draw noise  $\mathbf{u}$  uniformly from  $[0, 1)^D$

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

# Flow on Discrete Data With Dequantization



# Applications

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

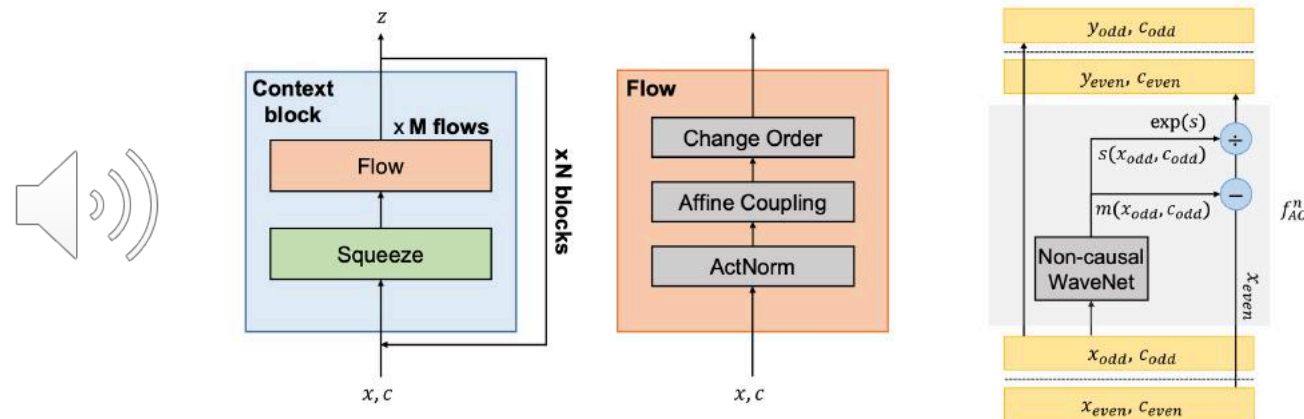


Figure 1. Schematic diagram of FloWaveNet. Left: an entire forward pass of the FloWaveNet consisting of  $N$  context blocks. Middle: an abstract diagram of the flow operation. Right: a detailed version of the affine coupling operation.

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



Output: SR Image Distribution

# 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.

# **Next lecture: Variational Autoencoders**