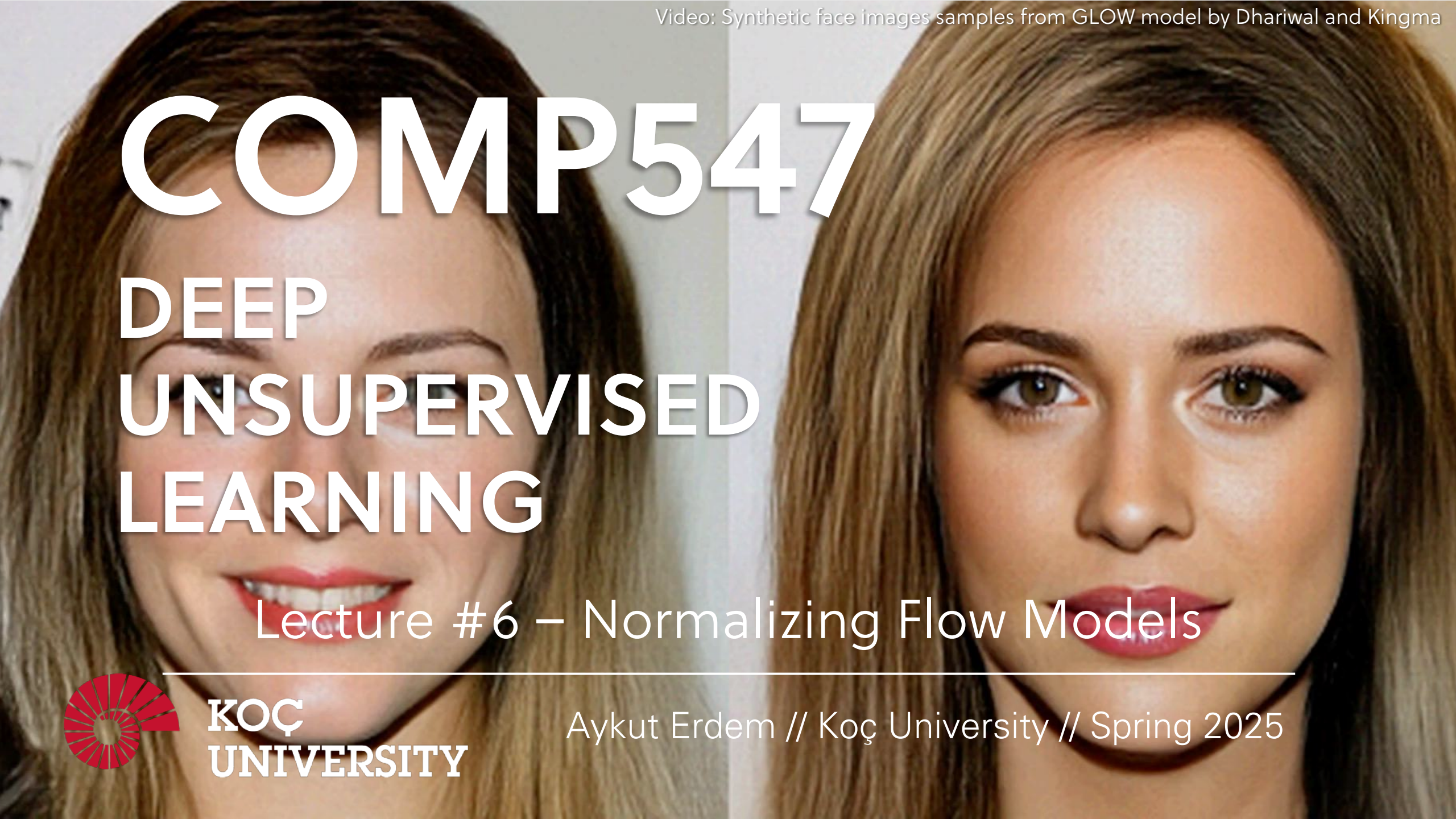

COMP547

DEEP UNSUPERVISED LEARNING

Lecture #6 – Normalizing Flow Models

KOÇ UNIVERSITY

Aykut Erdem // Koç University // Spring 2025

Good news, everyone!

- Assignment 1 is out (due Mar 23, 23:59)!

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 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!)
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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

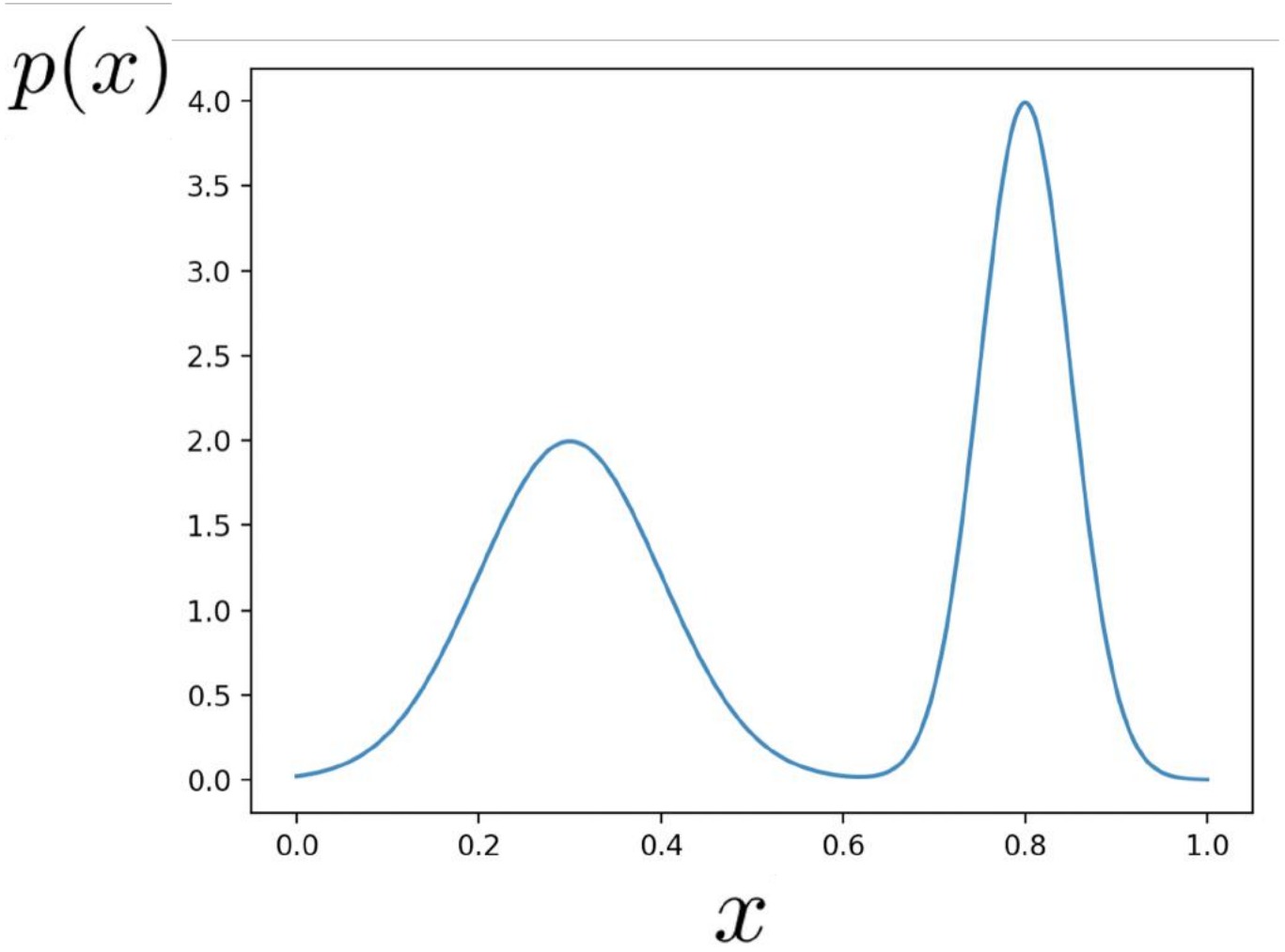
—Beidi Chen and Xun Huang's CMU 18-789 class

—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:

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

One possibility(not this lecture): quantize to discrete

Continuous data

0.22159854, 0.84525919, 0.09121633, 0.364252 , 0.30738086,

0.32240615, 0.24371194, 0.22400792, 0.39181847, 0.16407012,

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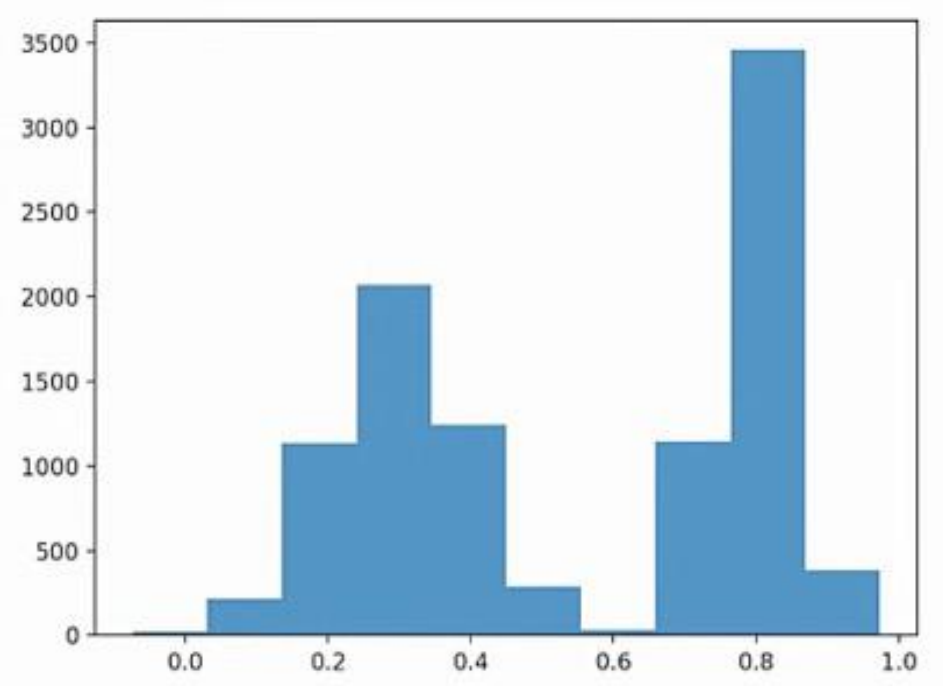
One modeling approach:

quantize and fit a discrete model

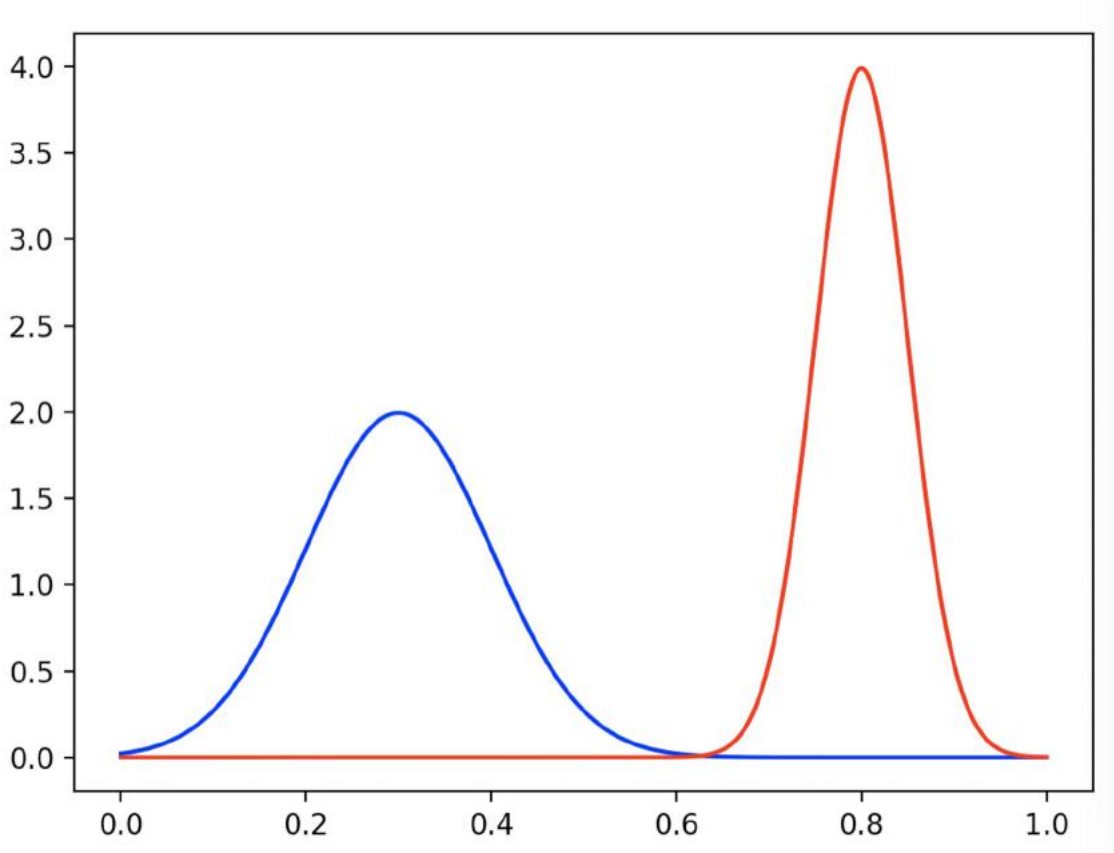


Example Density Model: Mixtures of Gaussians

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

Parameters: means and variances of components, mixture weights

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



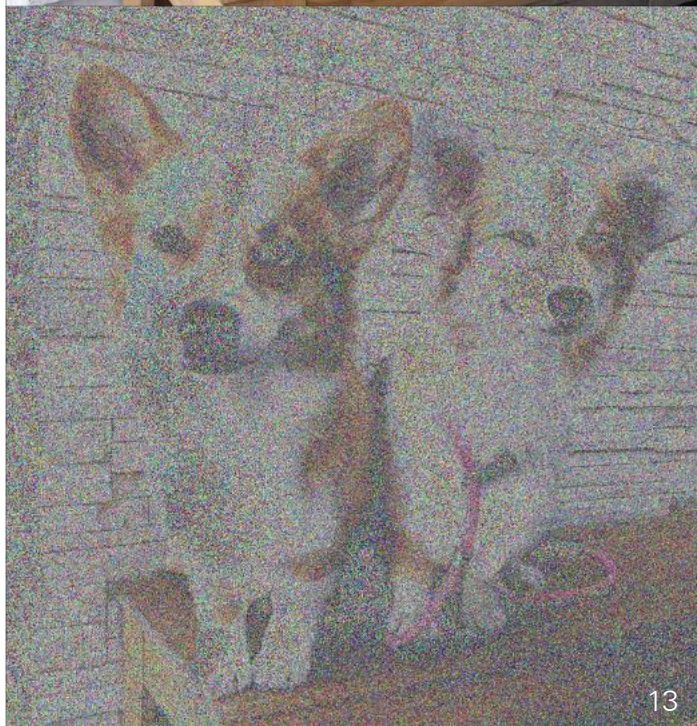
Aside on Mixtures of Gaussians

Do mixtures of Gaussians work for high-dimensional data?

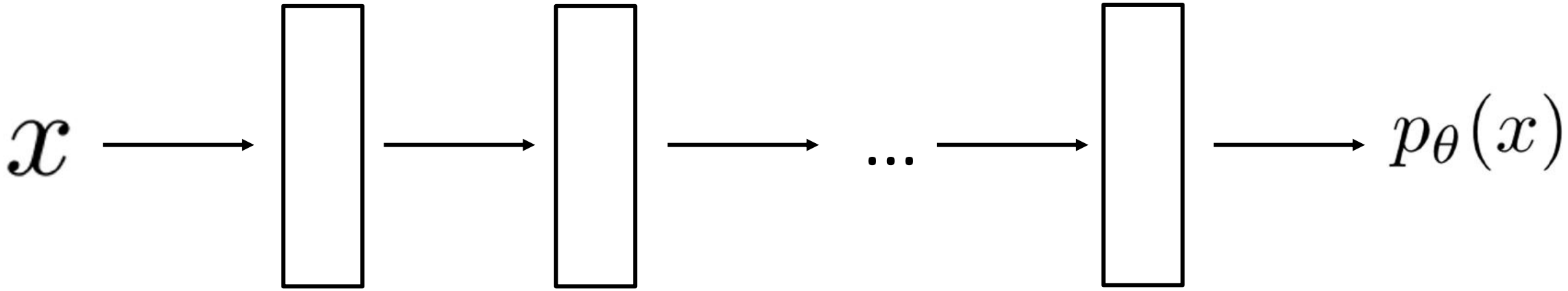
Not really. The sampling process is:

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?

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

$$p_\theta(x) \geq 0 \quad \forall x$$

Easily achieved for discrete data, using softmax

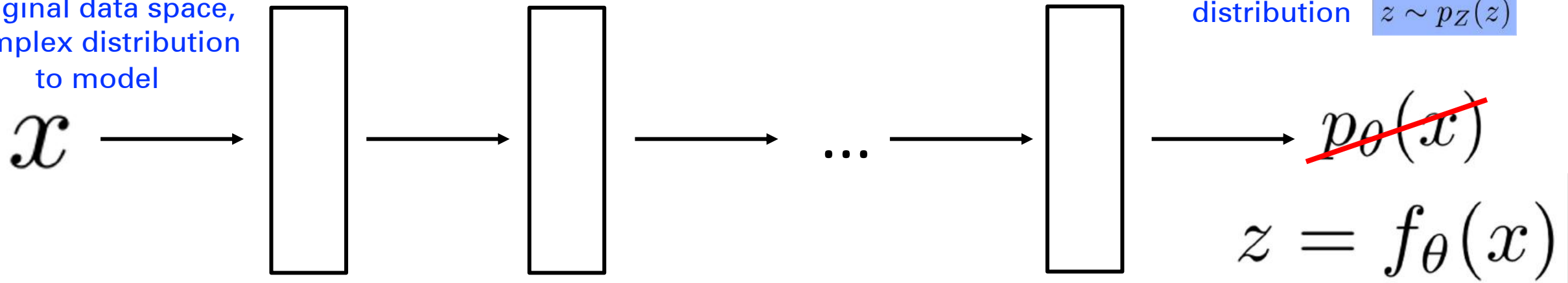
What about continuous data?

- How to sample?
- Latent representation?

Flows: Main Idea

Original data space, complex distribution to model

Embedding space, we enforce a simpler distribution $z \sim p_Z(z)$

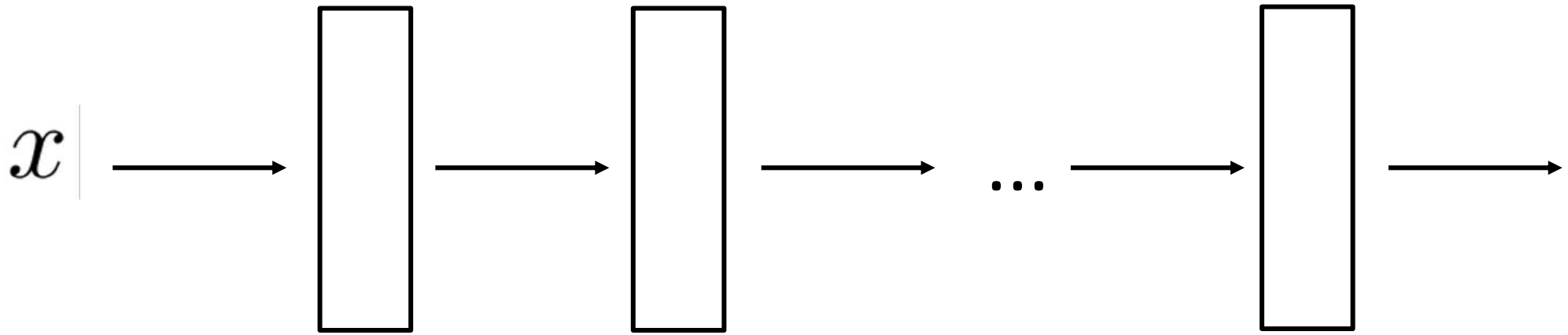


Generally: $z \sim p_Z(z)$

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

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

Flows: Training



$$z \sim p_Z(z)$$

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

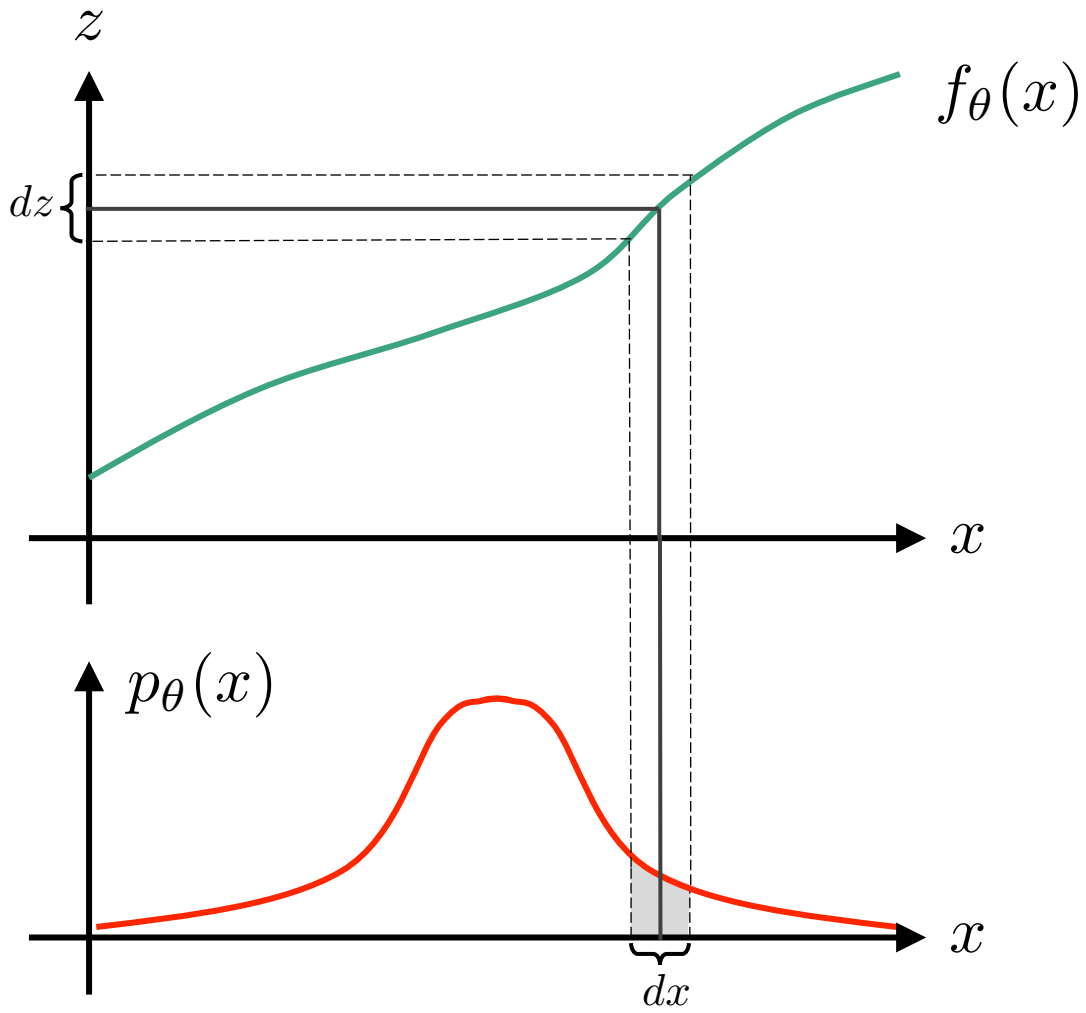
Change of Variables

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

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

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

$$= \frac{dz}{dx}$$



Note: requires f_θ invertible & differentiable

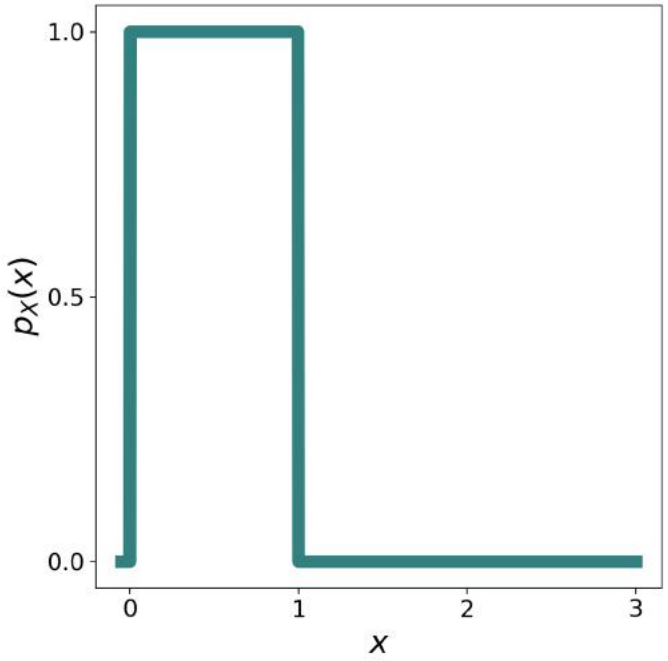
Change of Variable Density Needs to Be Normalized

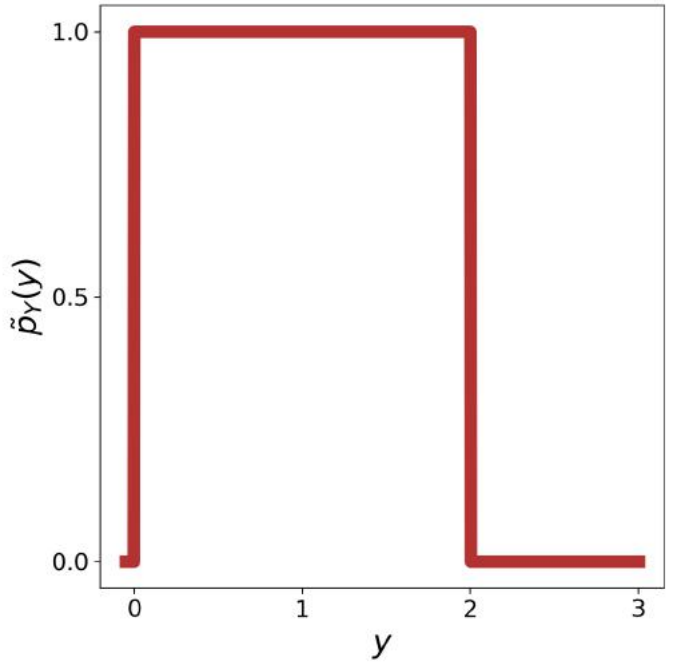
$$X \sim p_X \qquad Y := 2X$$

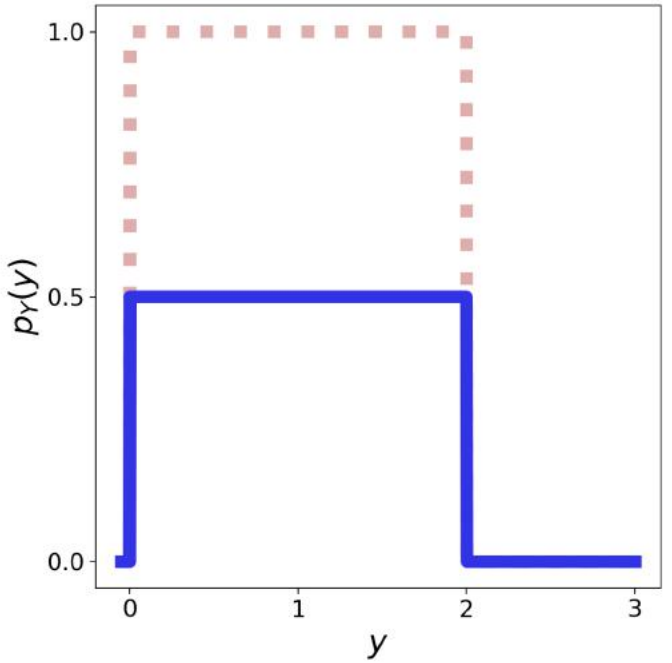
$$p_X(x) = \begin{cases} 1 & \text{for } 0 \leq x \leq 1 \\ 0 & \text{else} \end{cases}$$

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

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







Flows: Training

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

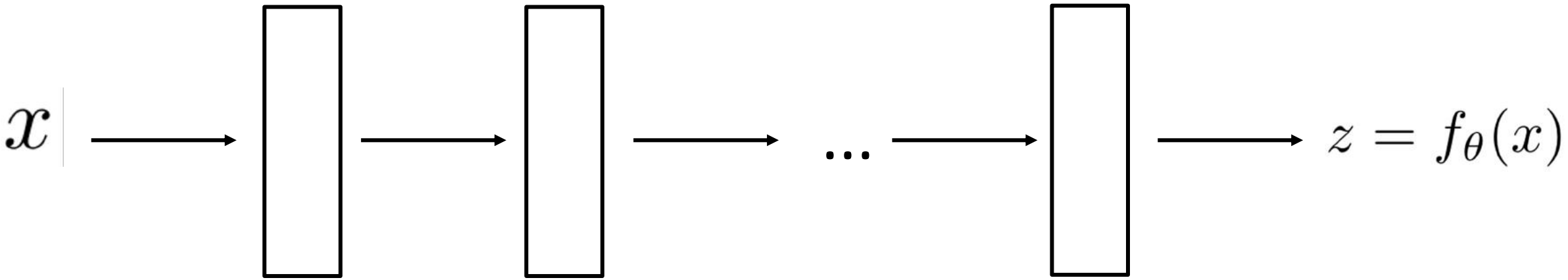
$$z^{(i)} = f_\theta(x^{(i)})$$

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

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

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

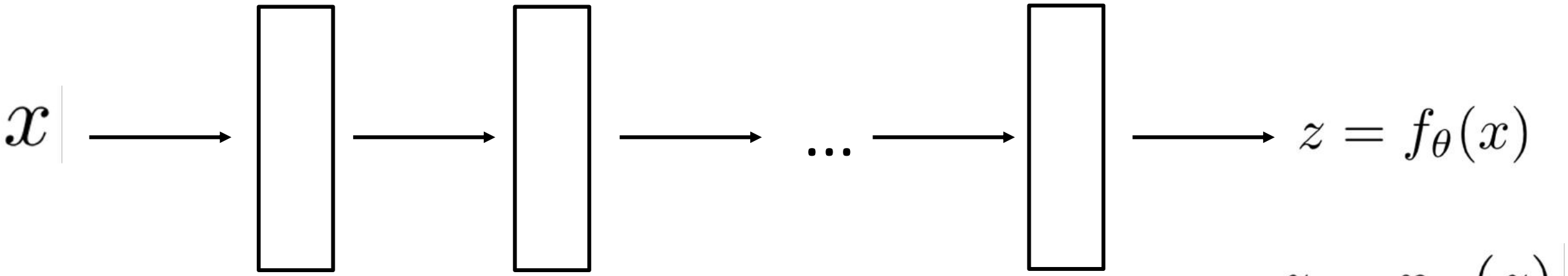
Flows: Sampling



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

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

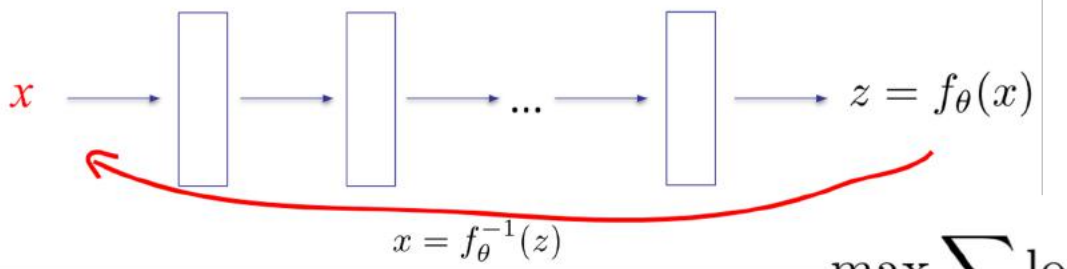
What do we need to keep in mind for f?



Recall, change of variable formula requires

- f_θ Invertible & differentiable

Flow Models: Examples



$$z \sim p_Z(z)$$

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

Two choices to make:

Invertible function class $z = f_\theta(x)$

i.e., in 1-D this is any monotonically increasing (or decreasing) function

E.g.:
- a x + b (for positive a)
- polynomials with positive coefficients and only odd powers
- exp (theta x)
- sigmoid (a x + b)
- cumulative density functions, e.g. CDF of mixture of Gaussians or weighted sum of logistics
- composition of flows = flow

Embedding space density $z \sim p_Z(z)$

Ideally an easy distribution to sample from

E.g.:

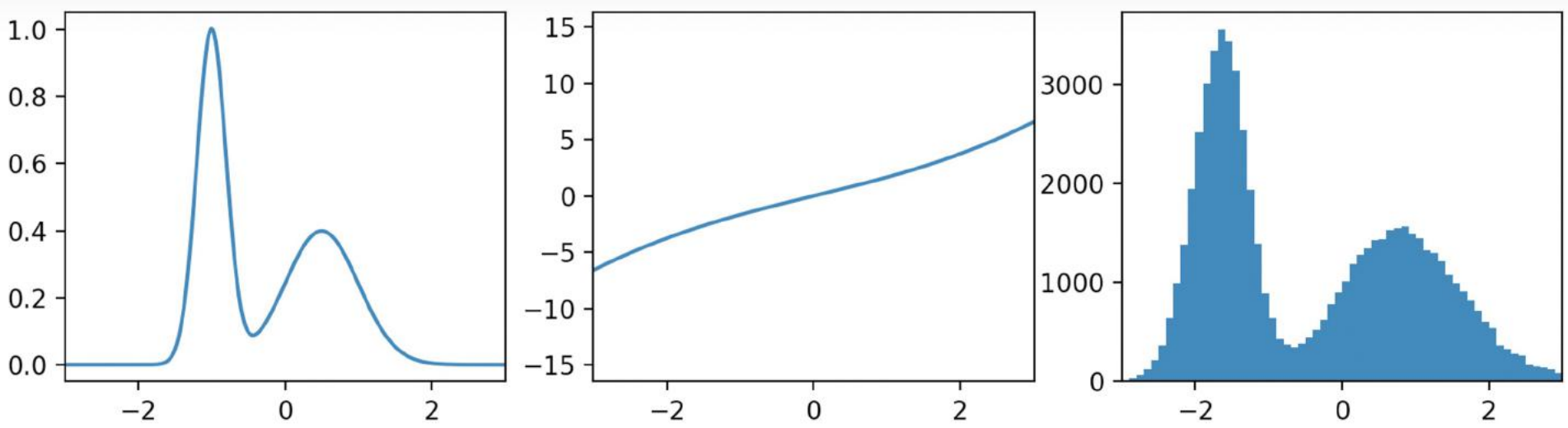
$z \sim \mathcal{N}(0, 1)$ "normalizing flow"

$z \sim \sum_k \pi_k \mathcal{N}(z; \mu_k, \sigma_k^2)$ mixture of Gaussians

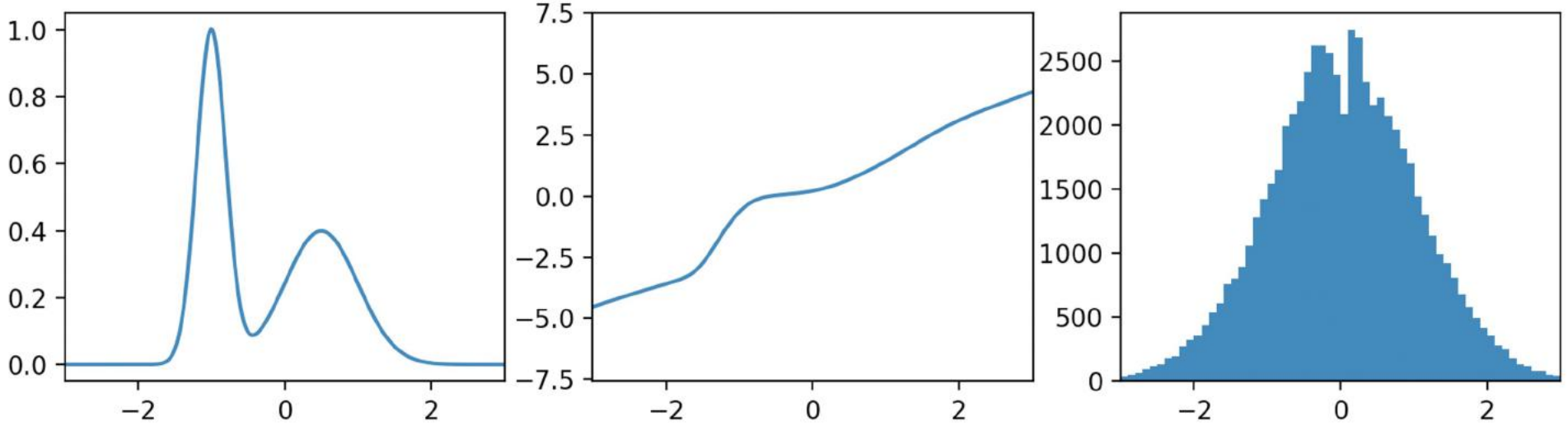
$z \sim \text{Uniform}([0, 1])$ → make sure f_θ maps to [0,1]

Example: Flow to Gaussian z

Before training



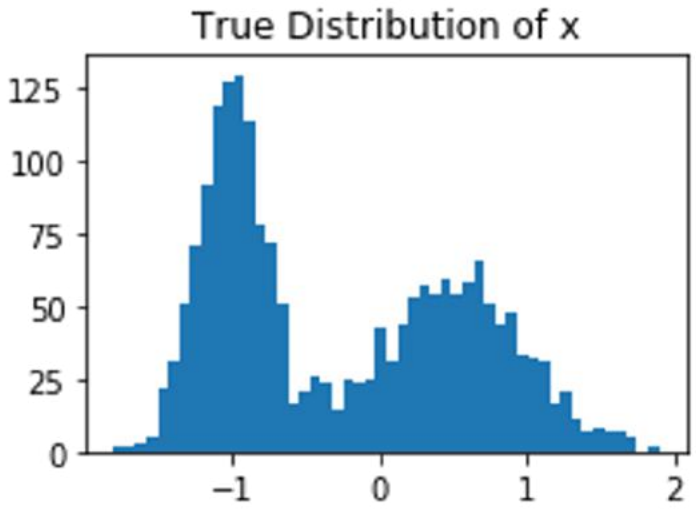
After training

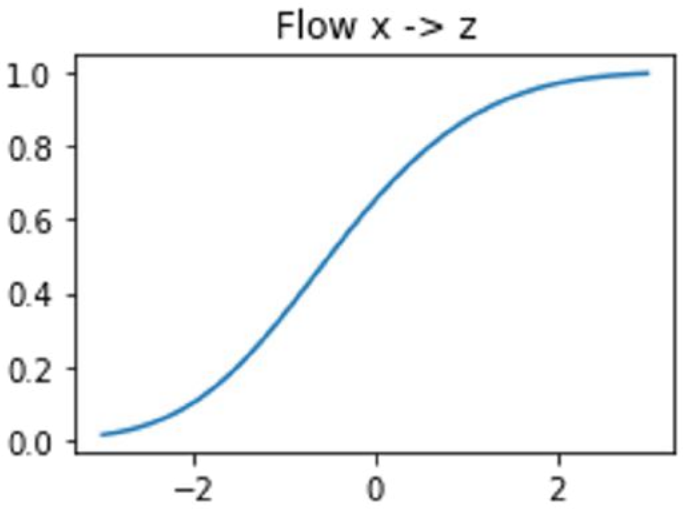


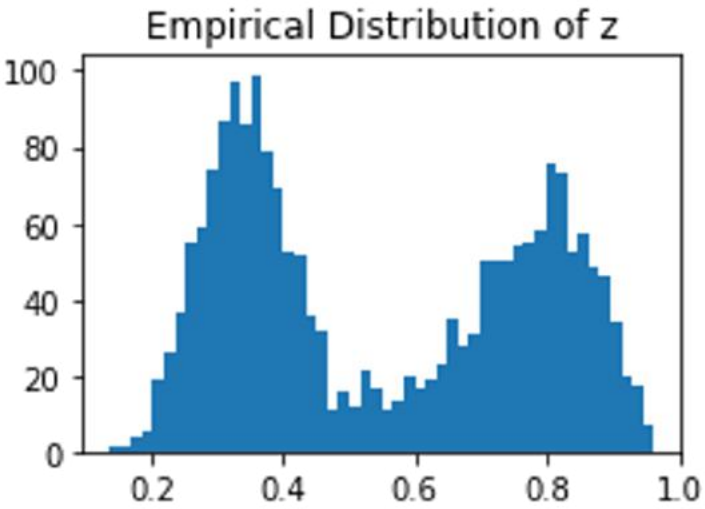
True distribution of x | Flow x → z | Empirical distribution of z

Example: Flow to Uniform z

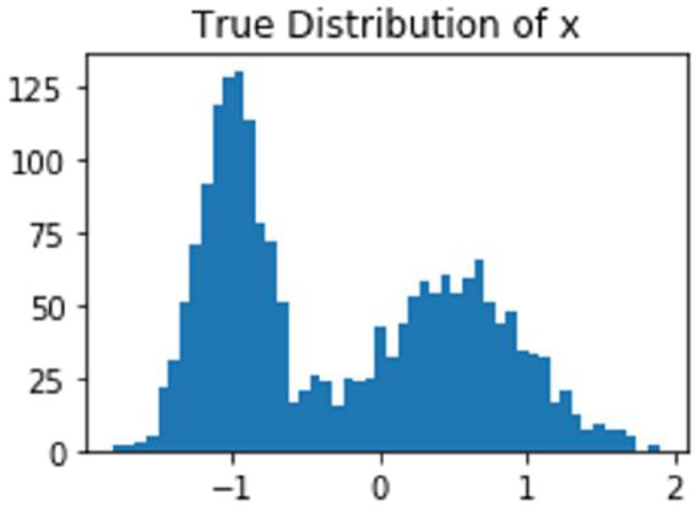
Before training

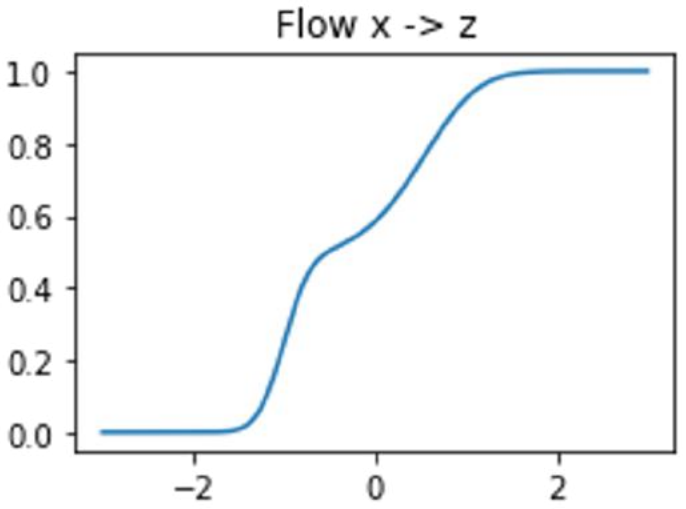


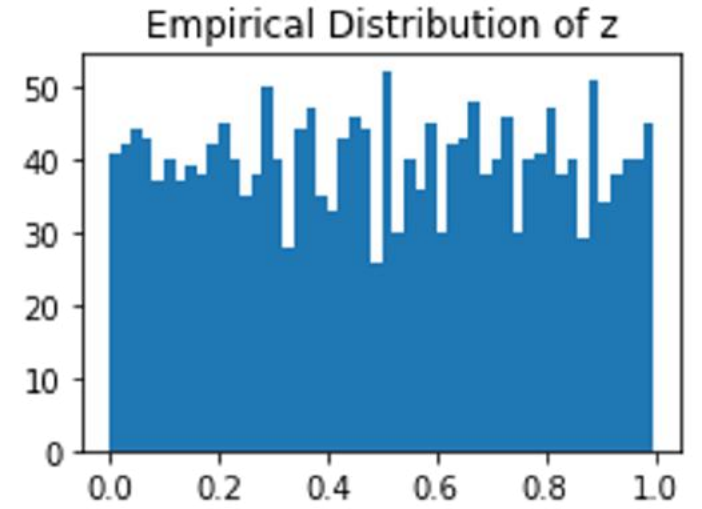




After training



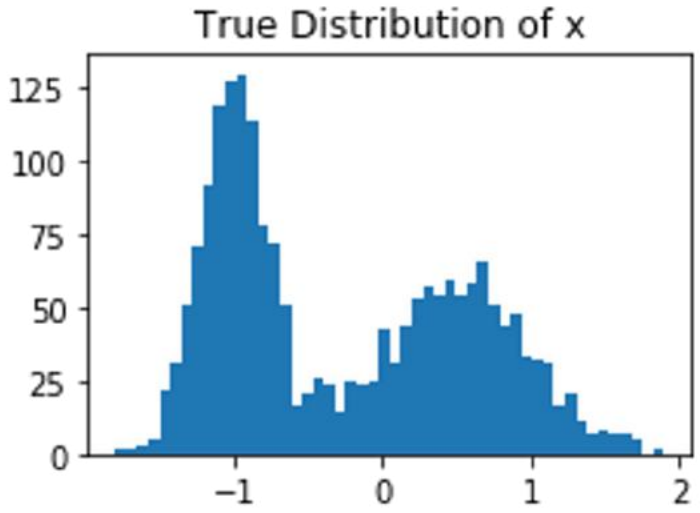


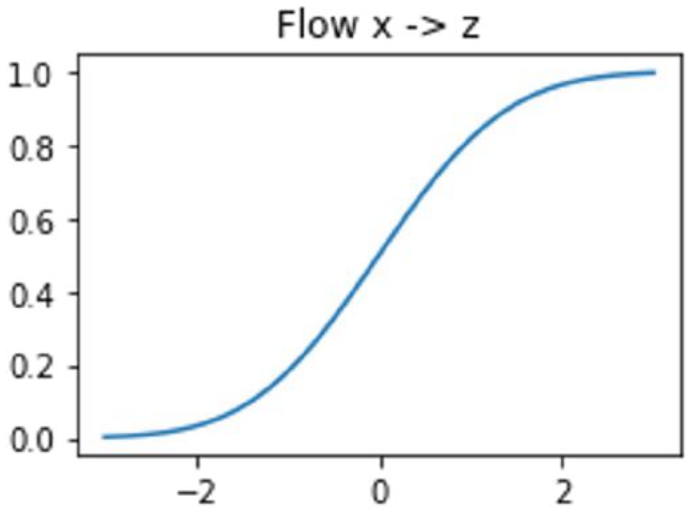


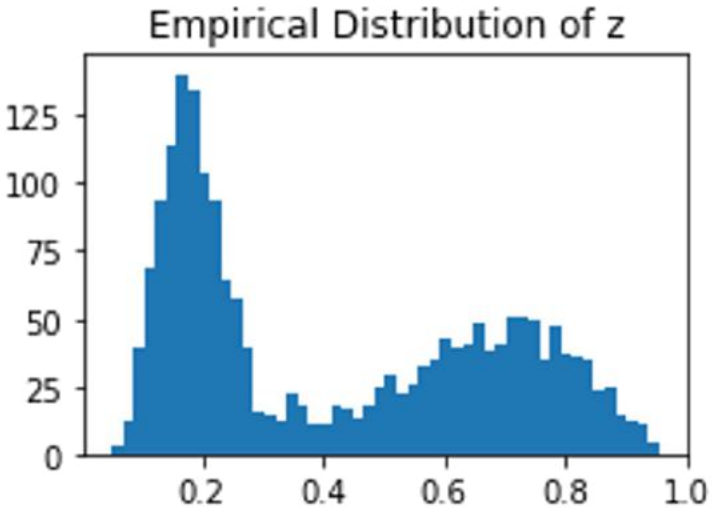
True distribution of x → Flow x → z → Empirical distribution of z

Example: Flow to Beta(5,5) z

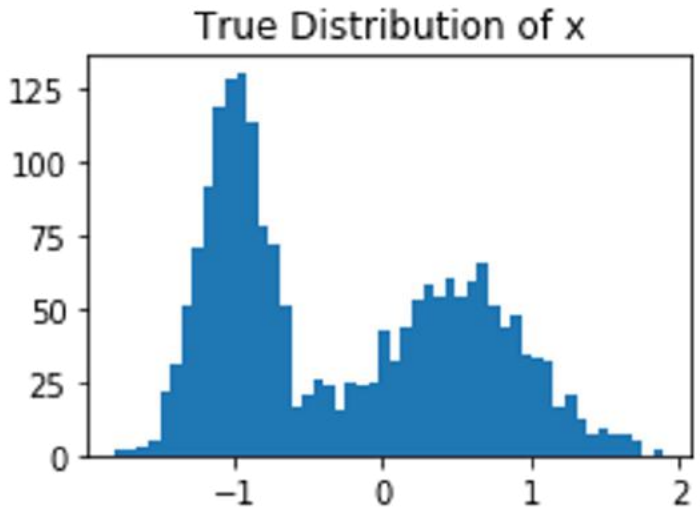
Before training

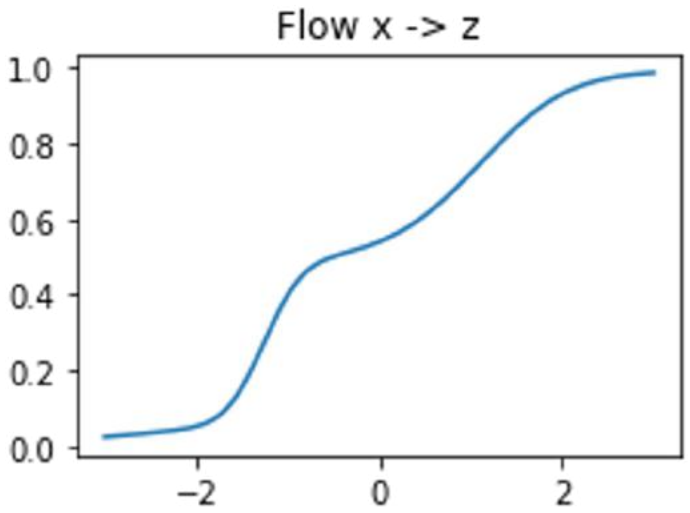


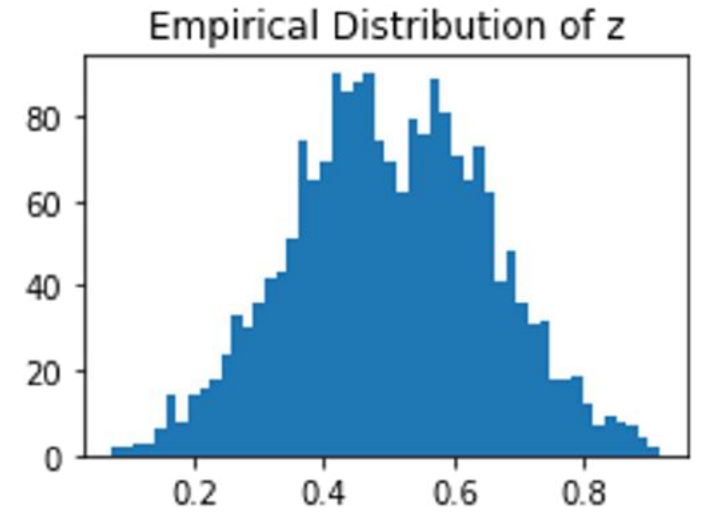




After training







True distribution of x

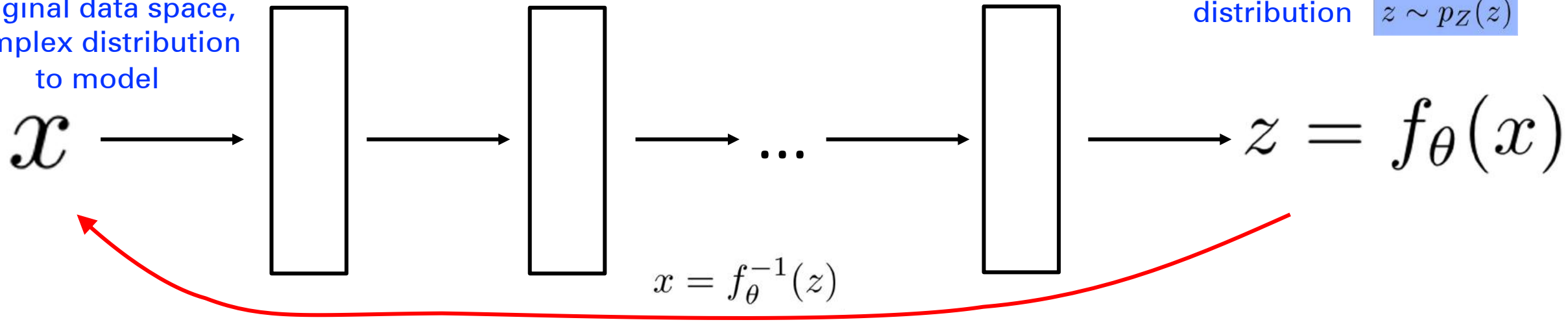
Flow x → z

Empirical distribution of z

1-D Flow Models Summary

Original data space, complex distribution to model

Embedding space, we enforce a simpler distribution $z \sim p_Z(z)$

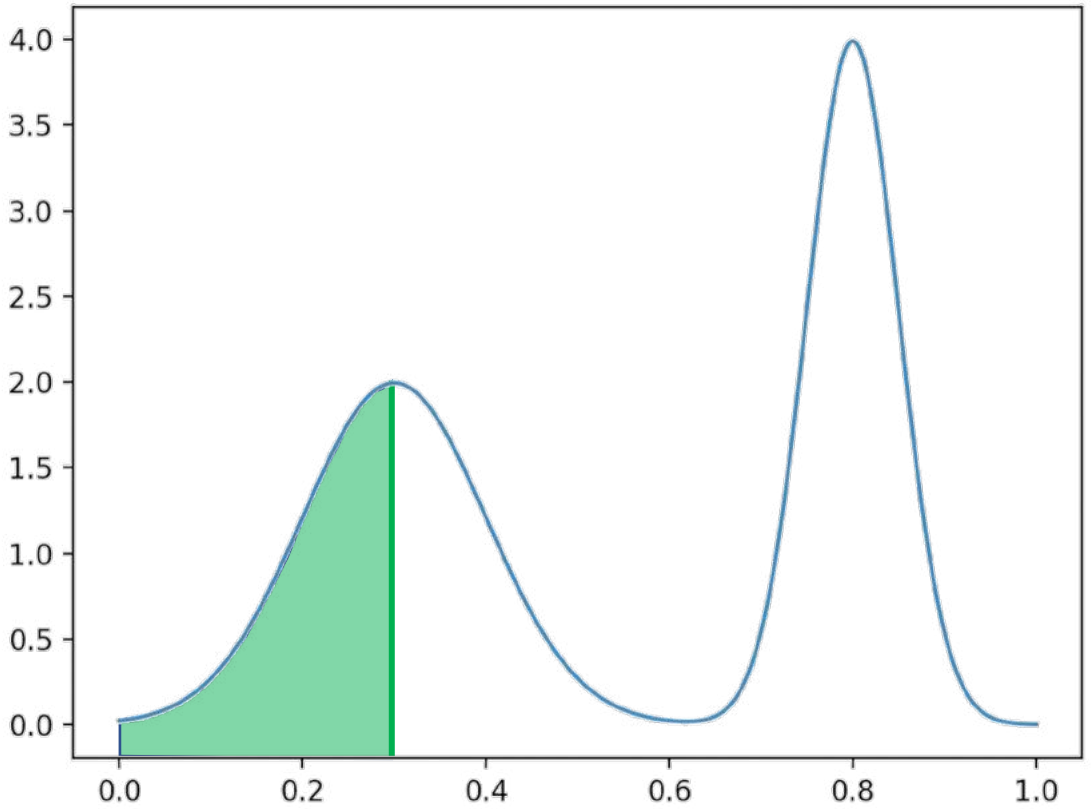


Training: $\max_\theta \sum_i \log p_\theta(x^{(i)}) = \max_\theta \sum_i \log p_Z(f_\theta(x^{(i)})) + \log \left| \frac{\partial f_\theta}{\partial x}(x^{(i)}) \right|$

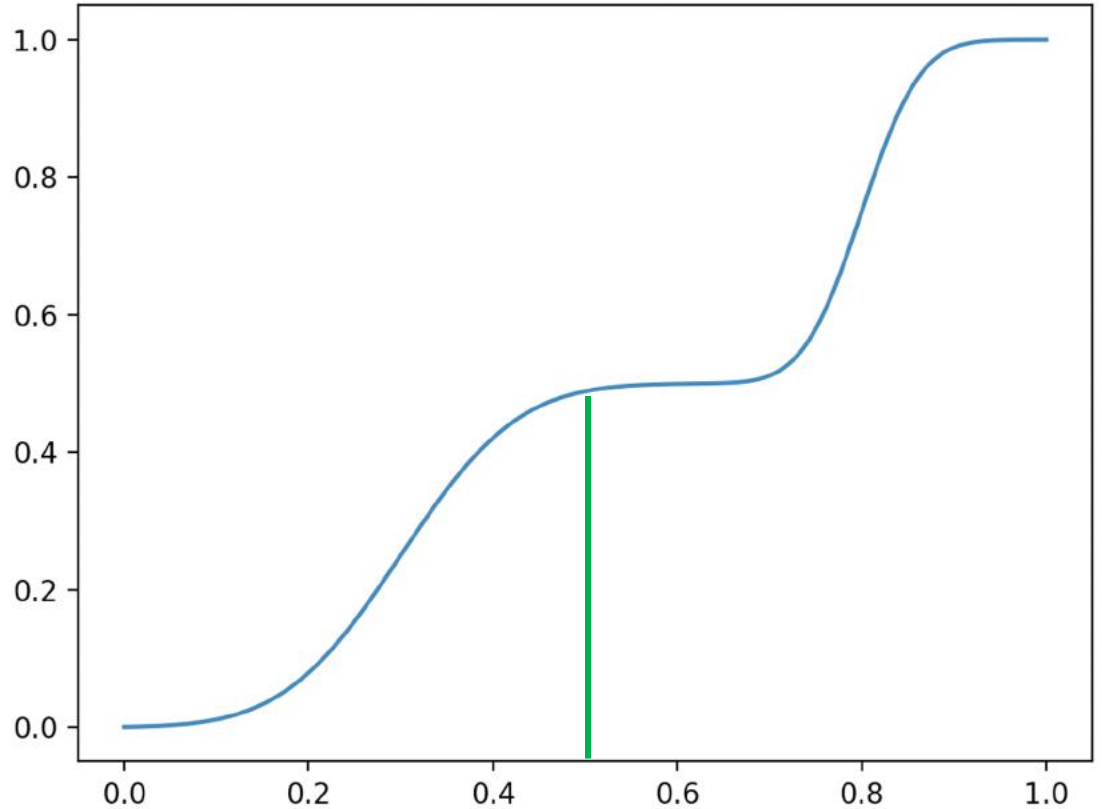
Inference: evaluate training objective

Sampling: first sample z from $z \sim p_Z(z)$ then compute $x = f_\theta^{-1}(z)$

Refresher: Cumulative Density Function (CDF)



$$p_\theta(x)$$



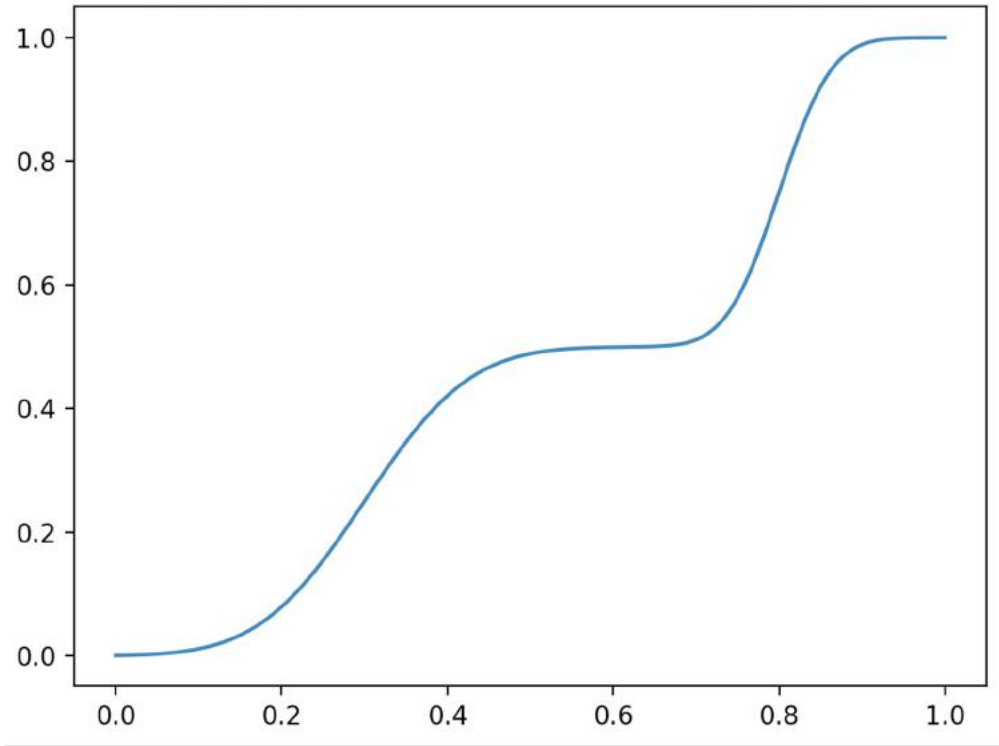
$$f_\theta(x) = \int_{-\infty}^{x} p_\theta(t)\, dt$$

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]



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

CDF Flows: special case of $z = f_\theta(x)$ a CDF and p(z) U[0,1]

- If we use a flow defined as a parameterized CDF, we recover the original objective for fitting the corresponding parameterized PDF.

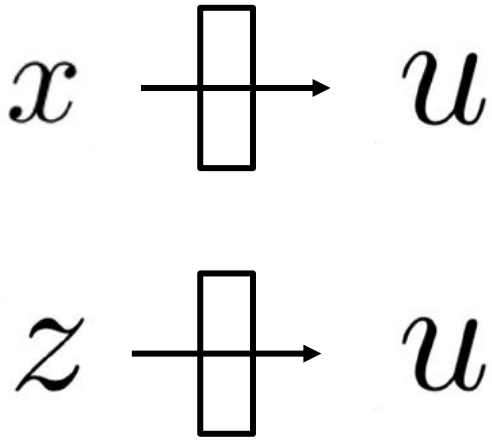
$$\max_\theta \sum_i \log p_\theta(x^{(i)}) = \max_\theta \sum_i \log p_Z(f_\theta(x^{(i)})) + \log \left| \frac{\partial f_\theta}{\partial x}(x^{(i)}) \right|$$

this term constant per p(z) uniform

cdf'(x) = pdf(x)

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)

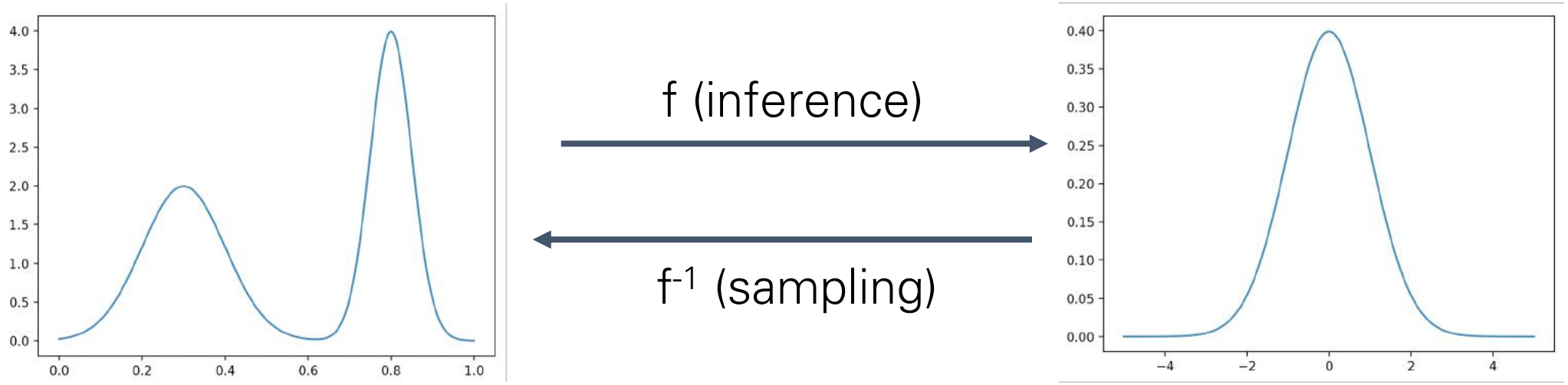
Recap of Flow Models in 1D

Flow: a differentiable, invertible mapping from x (data) to z (noise)

- Train so that it turns the data distribution into a **base distribution p(z)**
  - Common choices: uniform, standard normal

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

- This way, mapping **z ~ p(z)** through the flow's **inverse** will yield good samples



Lecture overview

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

2-D Autoregressive Flow

$$
\begin{aligned}
x_1 \to z_1 &= f_{\theta_1}(x_1) \\
x_2 \to z_2 &= f_{\theta_2}(x_1, x_2)
\end{aligned}
$$

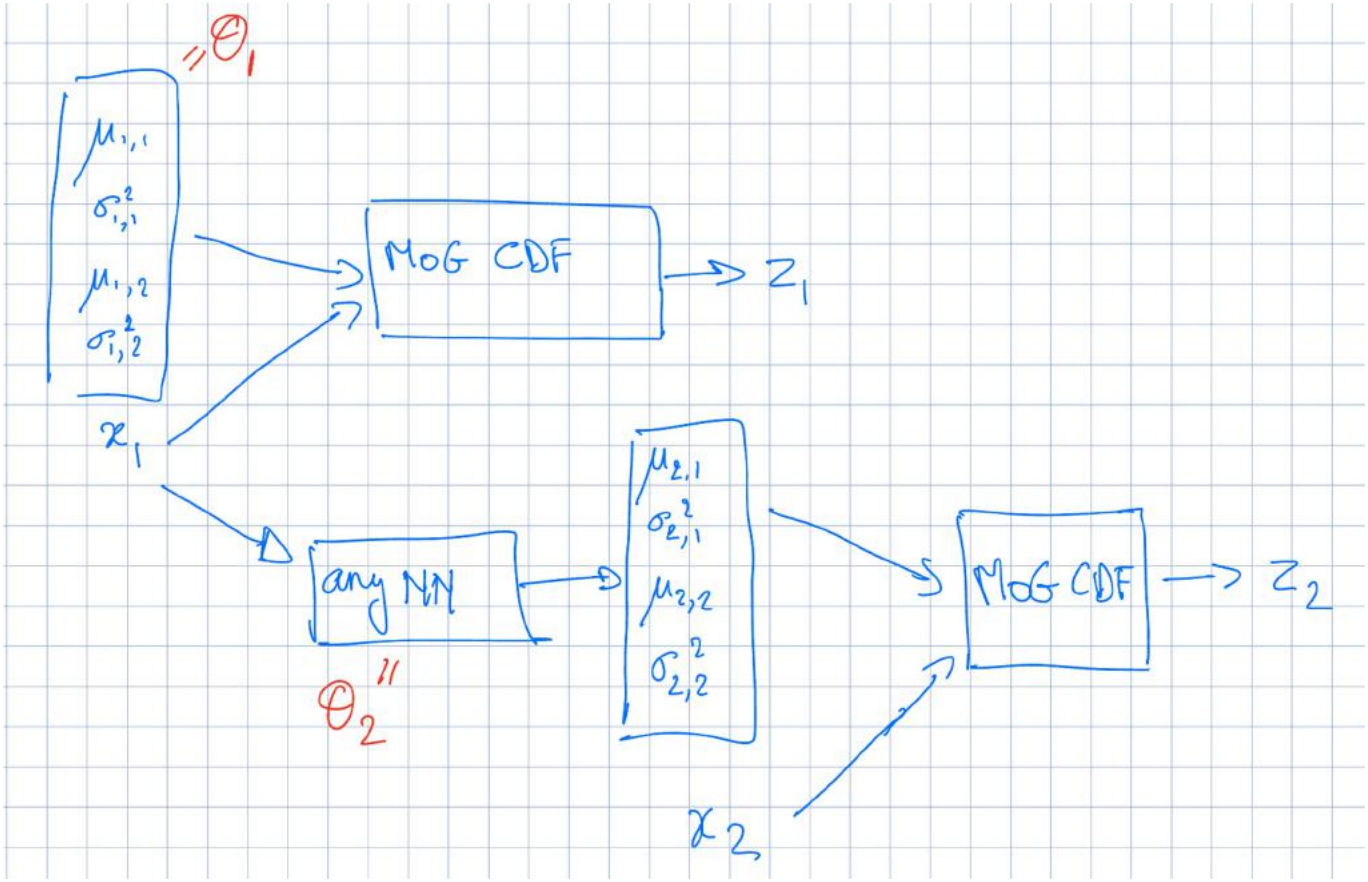
$$
\begin{aligned}
z_1 \to x_1 &= f_{\theta_1}^{-1}(x_1) \\
z_2, x_1 \to x_2 &= f_{\theta_2}^{-1}(x_1, z_2)
\end{aligned}
$$

- Note that the dependence on x1 in f_theta2 can be arbitrarily complex (including any neural net), no invertibility requirements

- Why?
  - x1 is also given when inverting from z2 to x2

Example 2-D Autoregressive Flow

$$
\begin{aligned}
x_1 \to z_1 &= f_{\theta_1}(x_1) \\
x_2 \to z_2 &= f_{\theta_2}(x_1, x_2)
\end{aligned}
$$



2-D Autoregressive Flow

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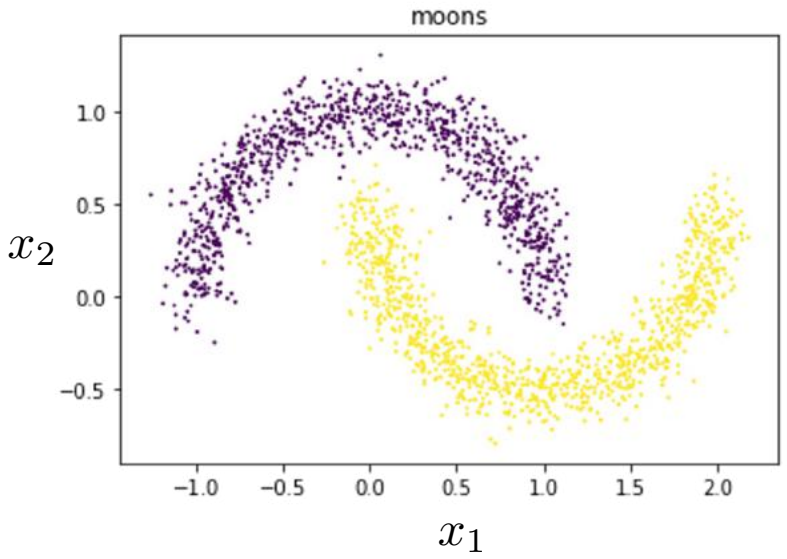
\begin{aligned}
x_1 \to z_1 &= f_{\theta_1}(x_1) \\
x_2 \to z_2 &= f_{\theta_2}(x_1, x_2)
\end{aligned}
$$

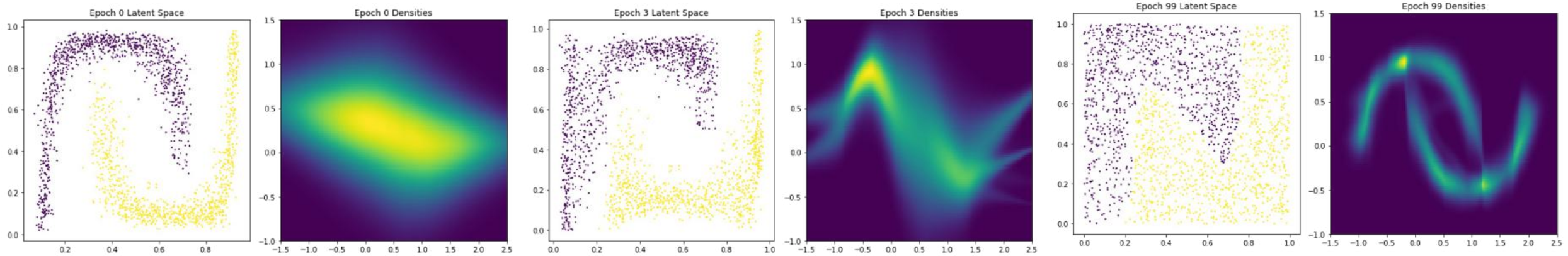
$$
\begin{aligned}
\log p_\theta(x_1, x_2) = & \log p_{Z_1}(z_1) + \log \left| \frac{\partial z_1(x_1)}{\partial x_1} \right| \\
& + \log p_{Z_2}(z_2) + \log \left| \frac{\partial z_2(x_1, x_2)}{\partial x_2} \right| \\
= & \log p_{Z_1}(f_{\theta_1}(x_1)) + \log \left| \frac{\partial f_{\theta_1}(x_1)}{\partial x_1} \right| \\
& + \log p_{Z_2}(f_{\theta_2}(x_1, x_2)) + \log \left| \frac{\partial f_{\theta_2}(x_1, x_2)}{\partial x_2} \right|
\end{aligned}
$$

2-D Autoregressive Flow: Two Moons

Architecture:

- Base distribution: Uniform$[0,1]^2$
- x_1: mixture of 5 Gaussians
  - i.e. z1 = cdf of Mo5G
- x_2: mixture of 5 Gaussians, conditioned on x_1
  - i.e. z2 = cdf of Mo5G with mixture weights w, means mu, variances sigma conditioned on x1. i.e. arbitrary NN can be trained to map from x1 to w, mu, sigma

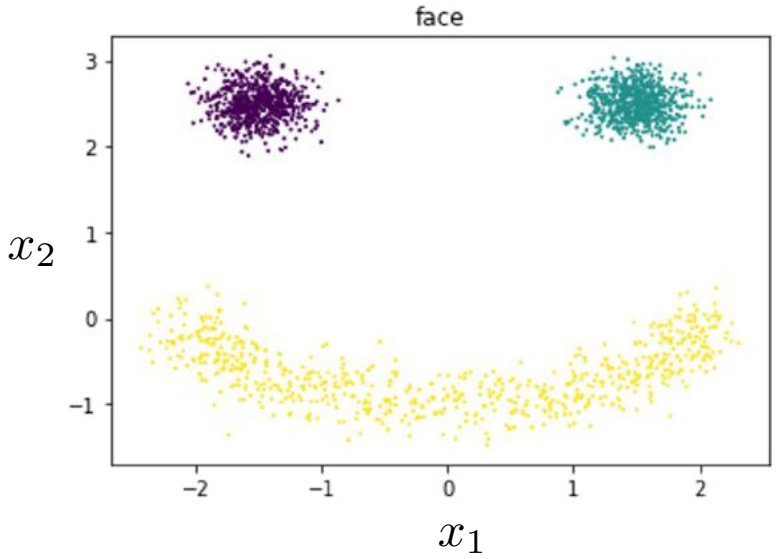


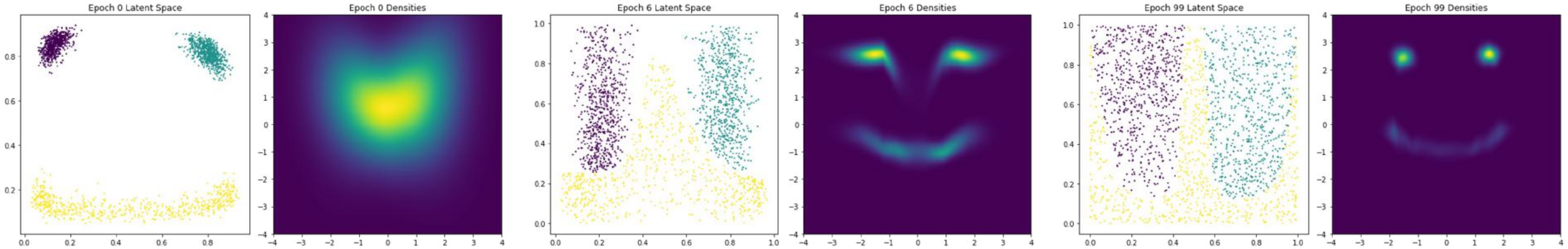


2-D Autoregressive Flow: Face

Architecture:

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





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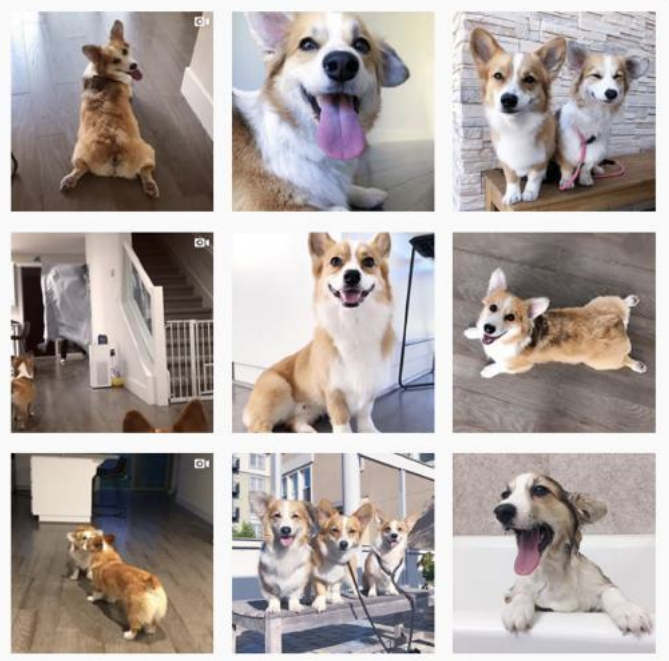
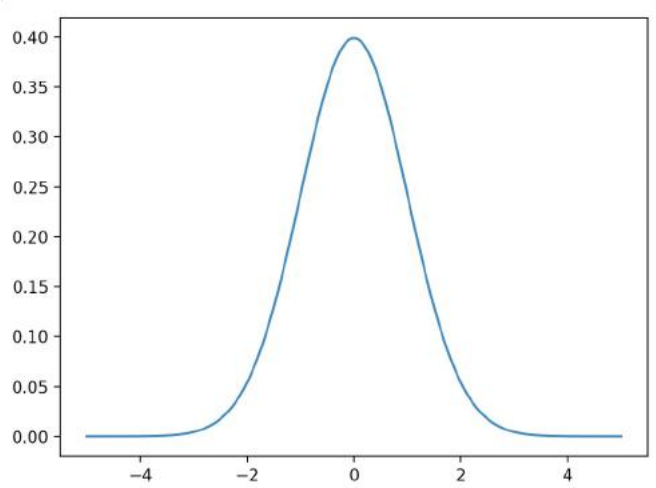
- **N-D Flows**
- Dequantization

High-dimensional data



f (inference)

f^{-1} (sampling)



x and z must have the same dimension

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**

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

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

Autoregressive flows

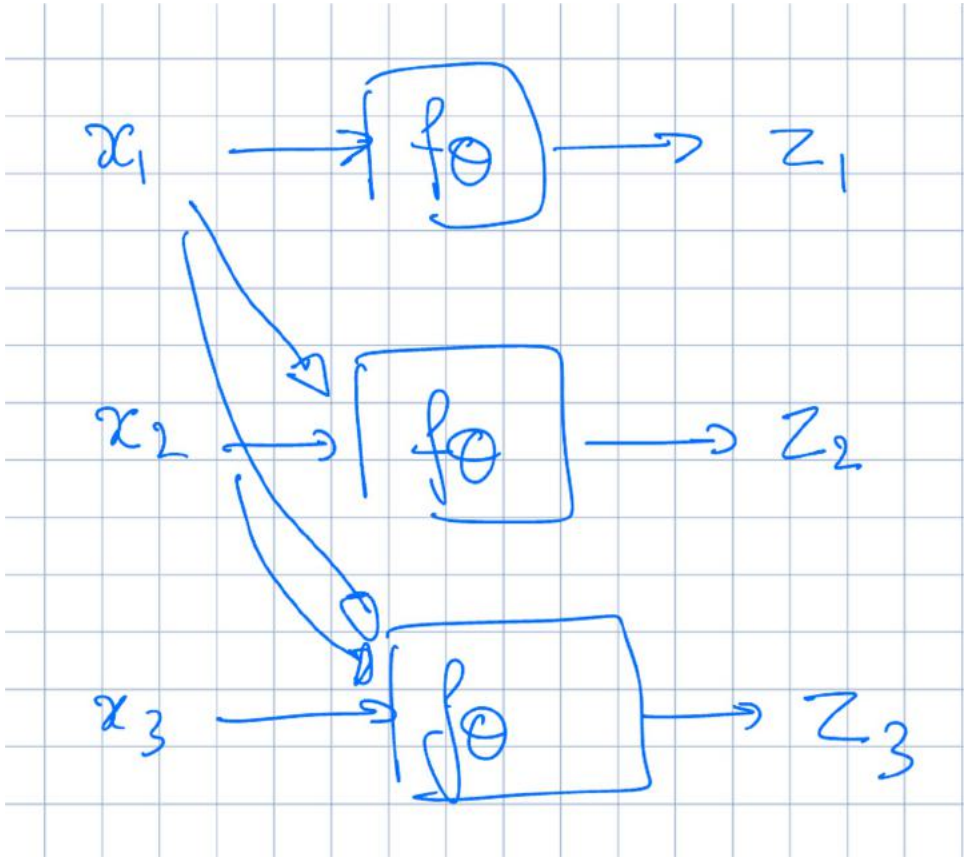
- How to fit autoregressive flows?
  - Map **x** to **z**
  - Fully parallelizable

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

- 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

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

Autoregressive flows

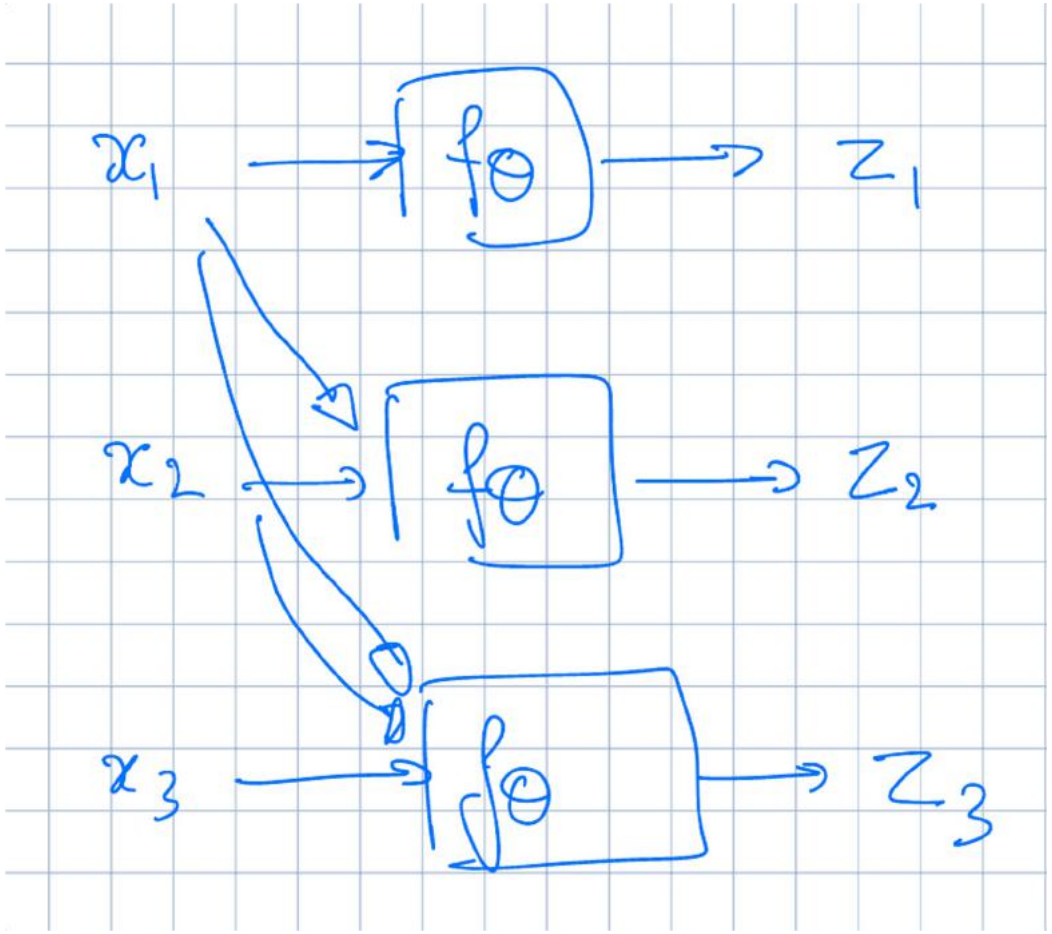


Inverse autoregressive flows

- 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**

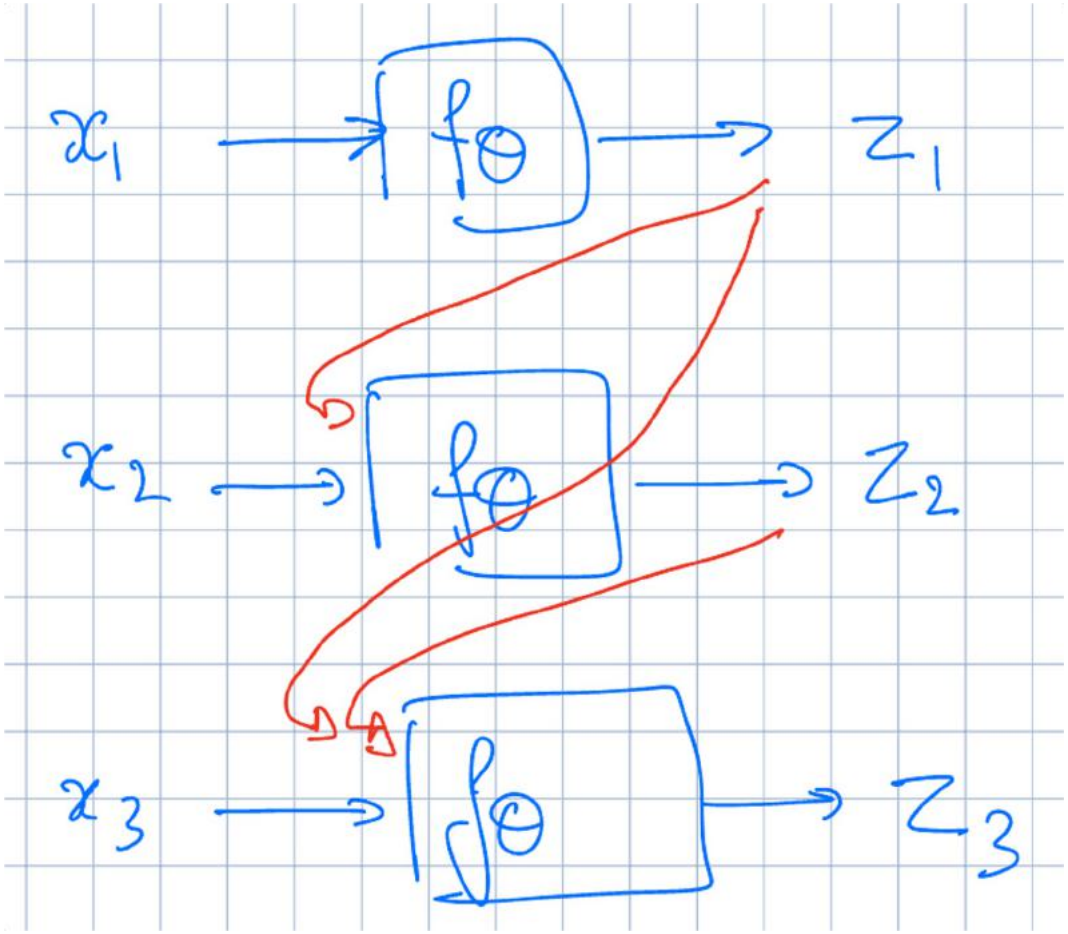
$$z_1 = f_\theta^{-1}(x_1) \qquad x_1 = f_\theta(z_1)$$
$$z_2 = f_\theta^{-1}(x_2; z_1) \qquad x_2 = f_\theta(z_2; z_1)$$
$$z_3 = f_\theta^{-1}(x_3; z_1, z_2) \qquad x_3 = f_\theta(z_3; z_1, z_2)$$

AF



Training: parallel / fast
Sampling: long serial chain

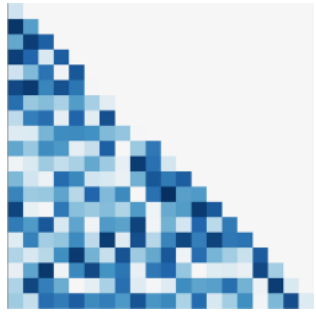
IAF



Training: long serial chain
Sampling: parallel / fast

AF vs IAF

Jacobian



(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]

Lecture overview

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

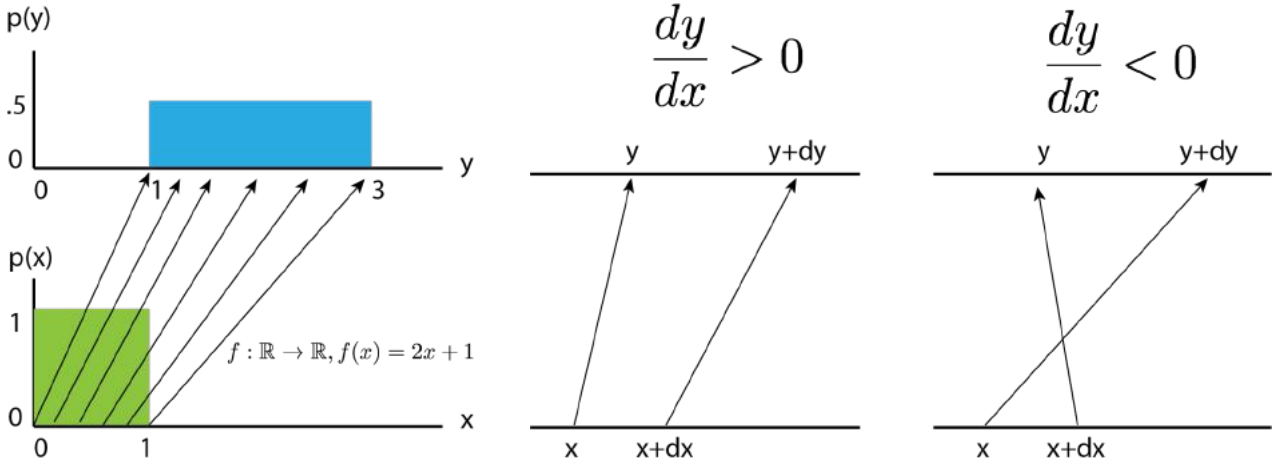
Refresher: Change of MANY variables

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

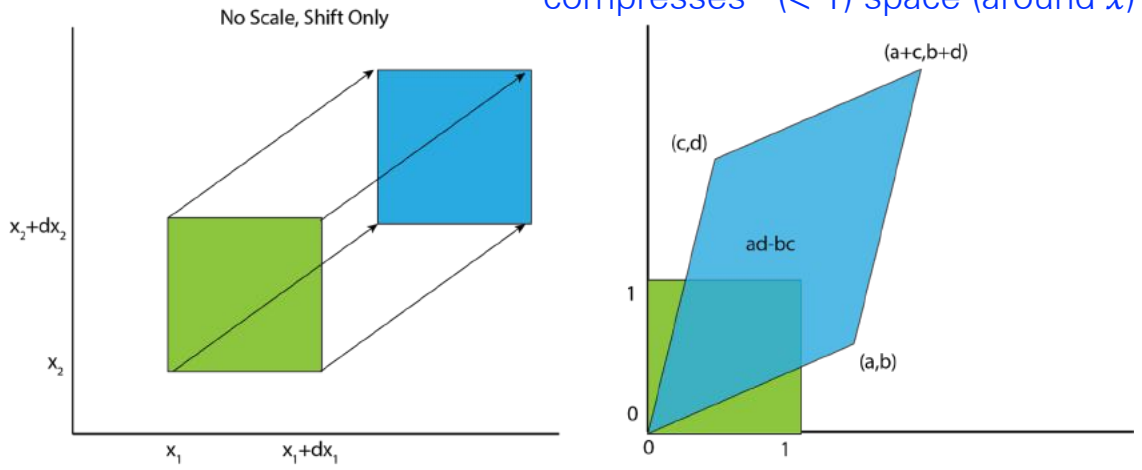
$$p_Y(y) = p_X(f^{-1}(y)) \left| \det \frac{\partial f^{-1}(y)}{\partial y} \right|$$

Jacobian Determinant: How much does f "stretches" (> 1) or "compresses" (< 1) space (around x)

1-D



2-D



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:

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

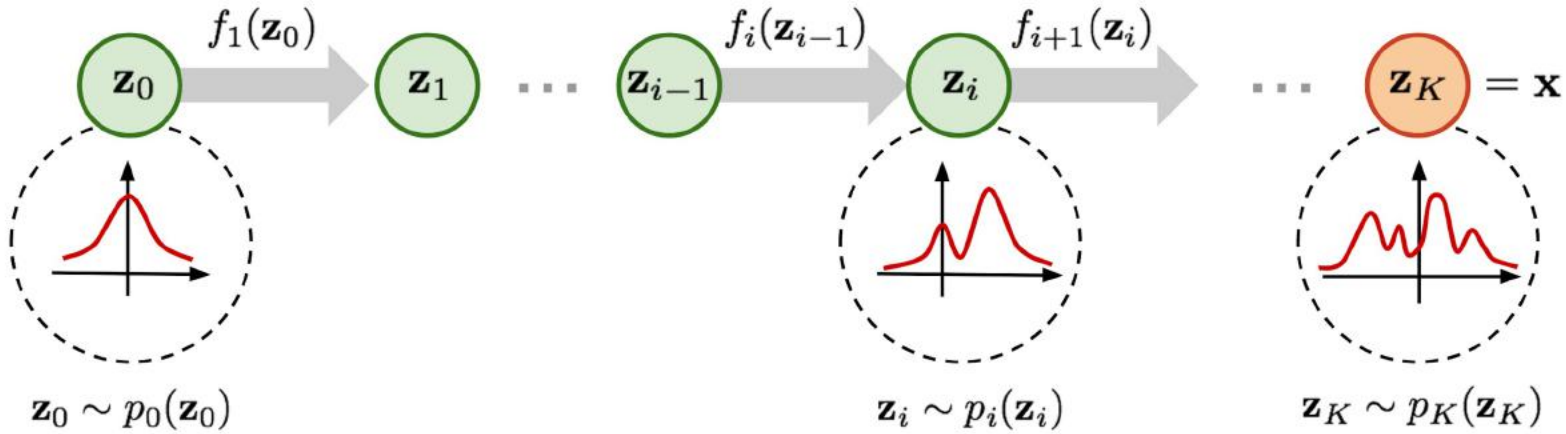
Train with maximum likelihood:

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

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

Chaining Invertible Mappings

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



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

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

Chain rule

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 $z \sim \mathcal{N}(0, I)$ $\qquad$ $x \sim \mathcal{N}(b, AA^T)$
- 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.

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

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

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

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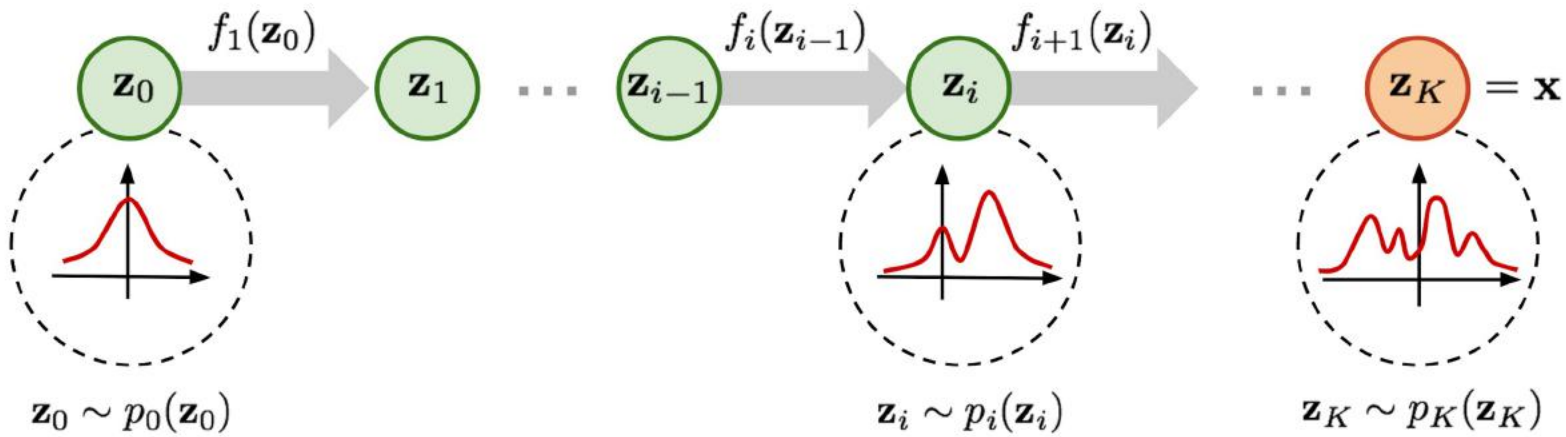

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Chain rule

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- Easy way to increase expressiveness

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

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

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_θ and t_θ can be arbitrary neural nets with **no restrictions**.
  - Think of them as **data-parameterized elementwise flows.**

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

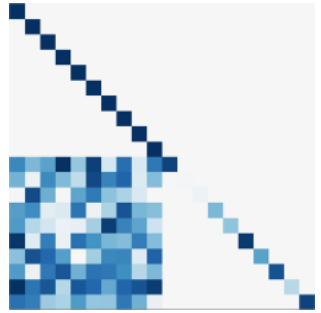
NICE/RealNVP

- It also has a tractable Jacobian determinant

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

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

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

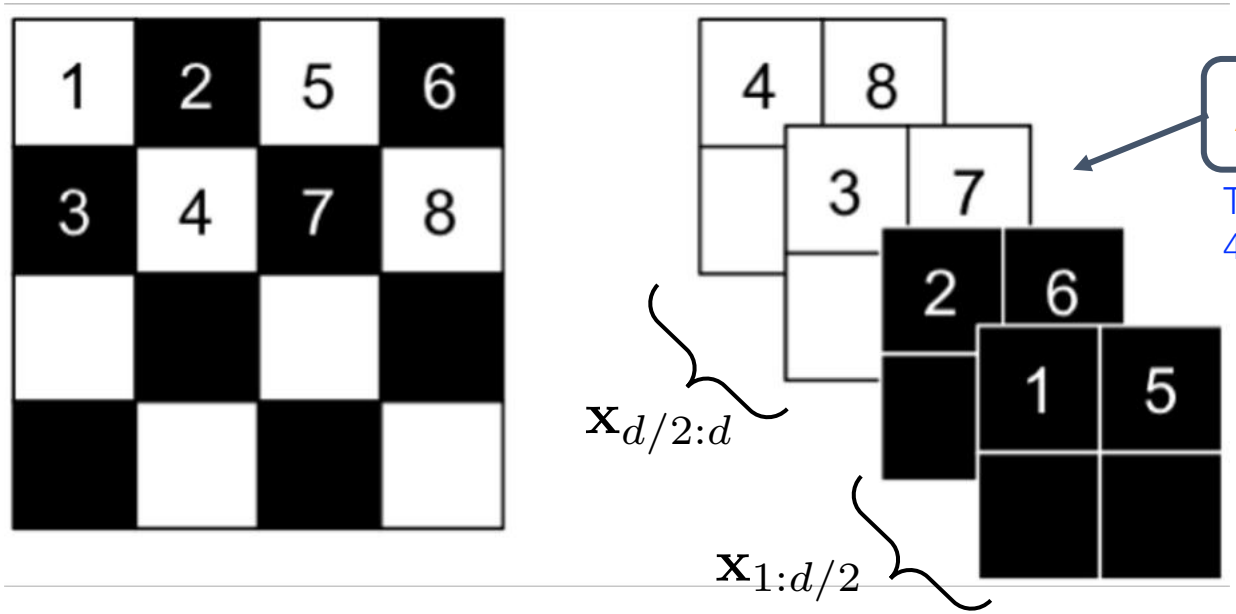
$$f(x) = b \odot x + (1 - b) \odot (x \odot \exp(s\_(b \odot x)) + m(b \odot x))$$

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

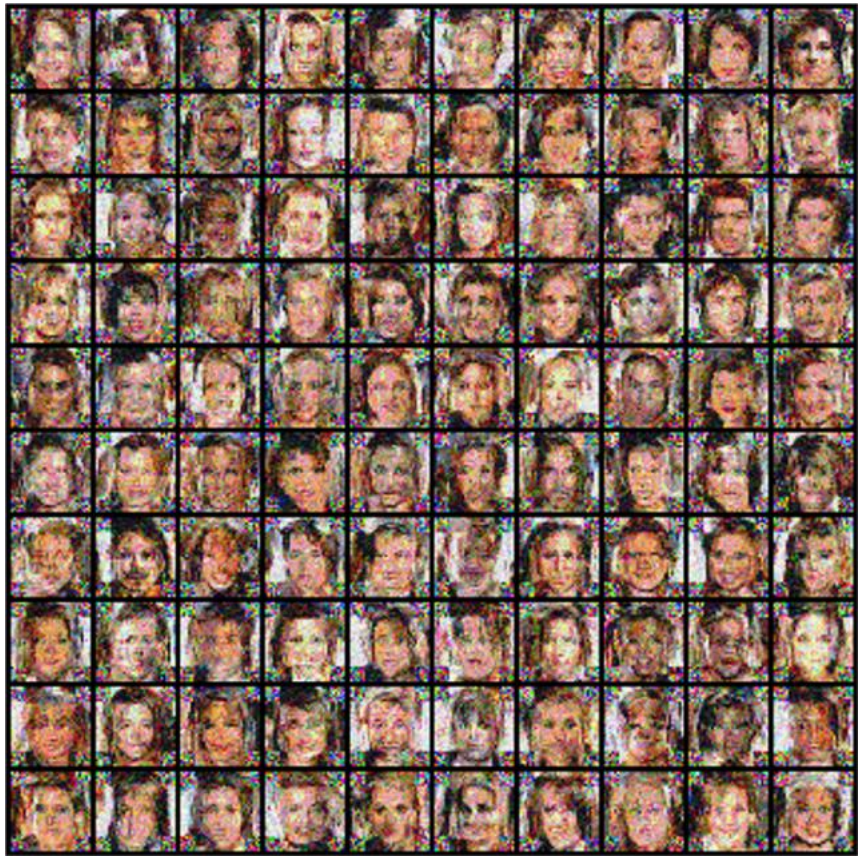
Input x: 32×32×c image

- 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 ×4; channel squeeze; channel ×3; channel unsqueeze; checkerboard ×3

(Mask top half; mask bottom half; mask left half; mask right half) ×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)

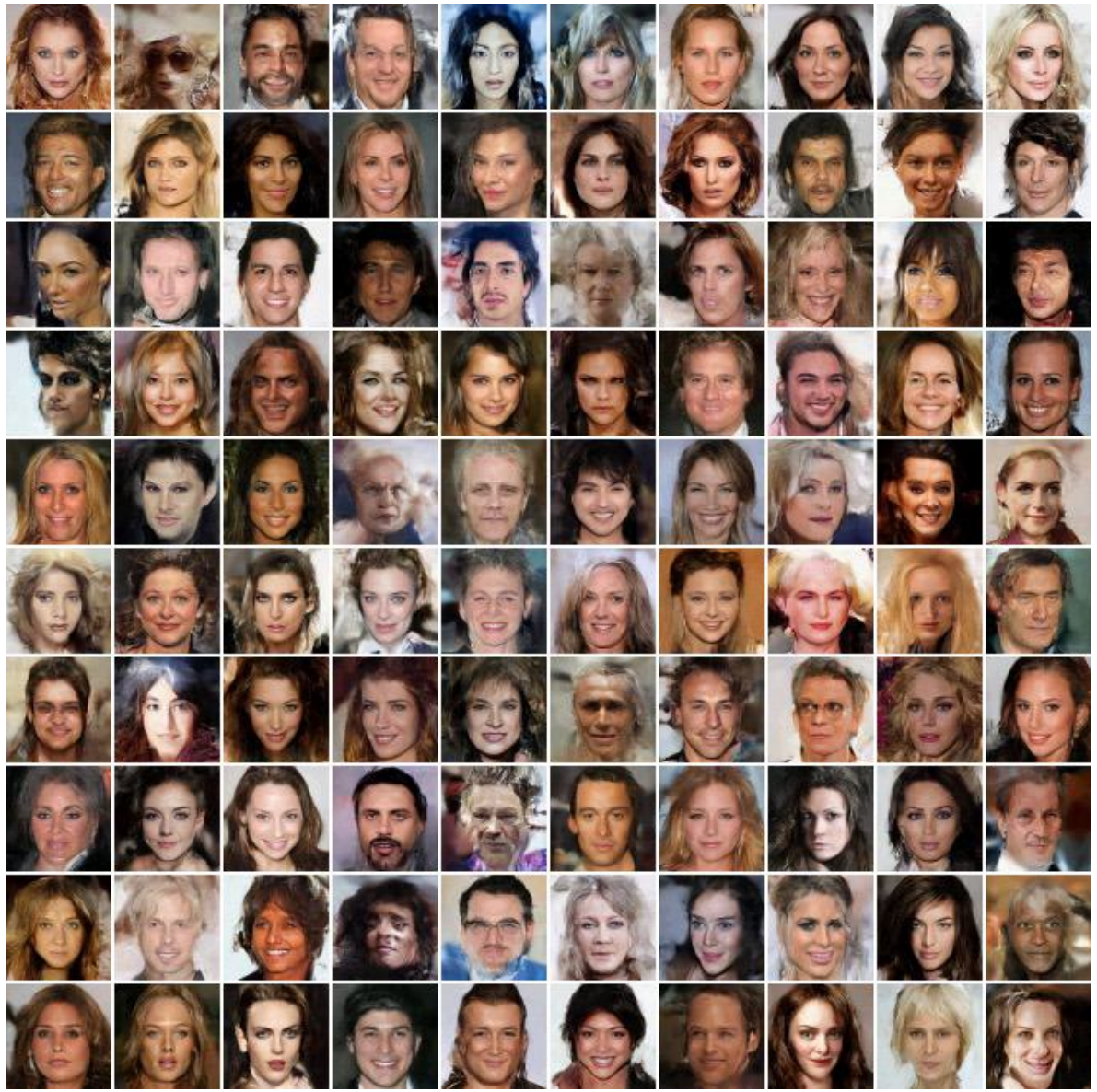
NN architecture also matters

- 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++

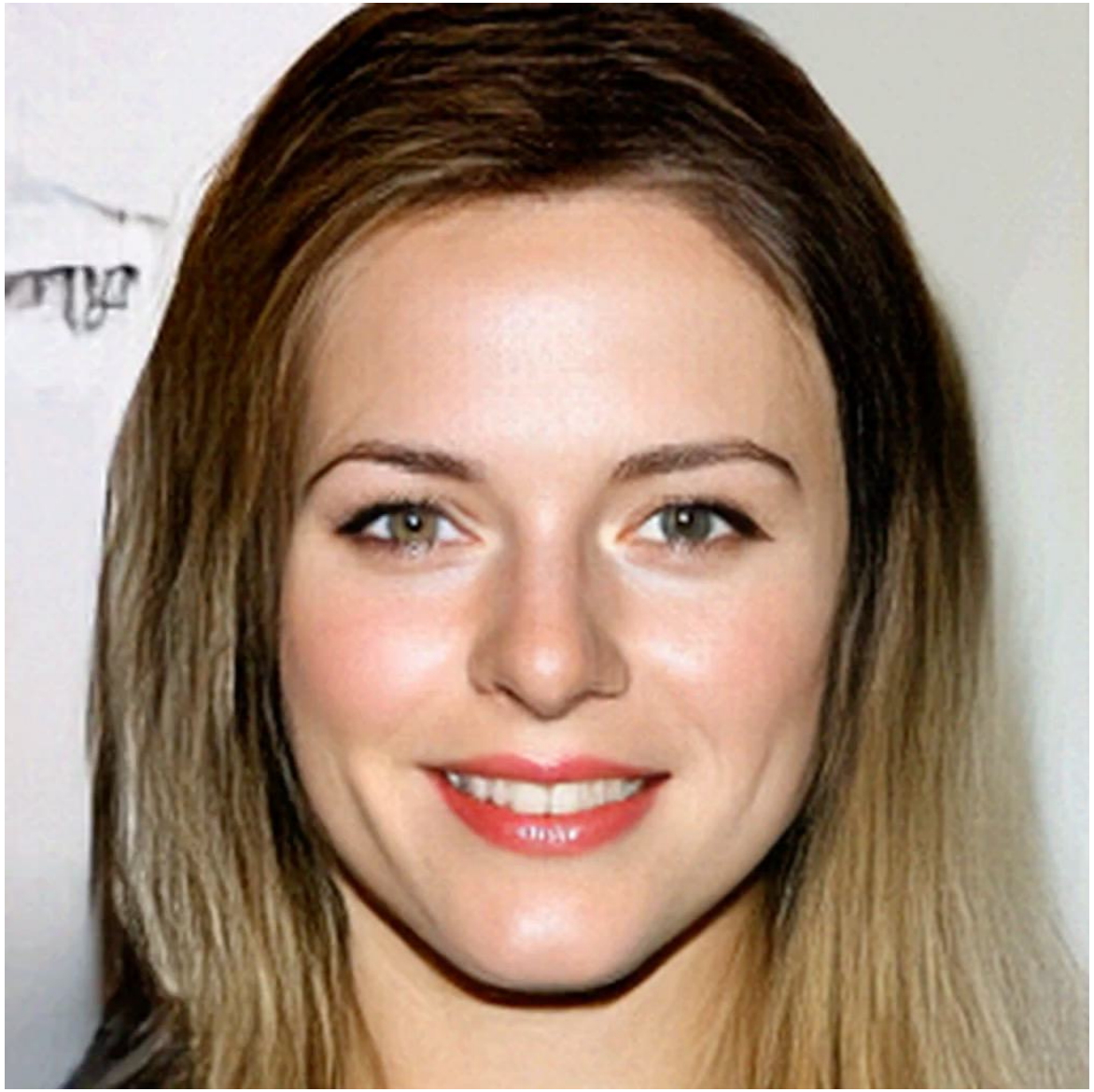


Samples from Flow++ trained on 64x64 CelebA

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

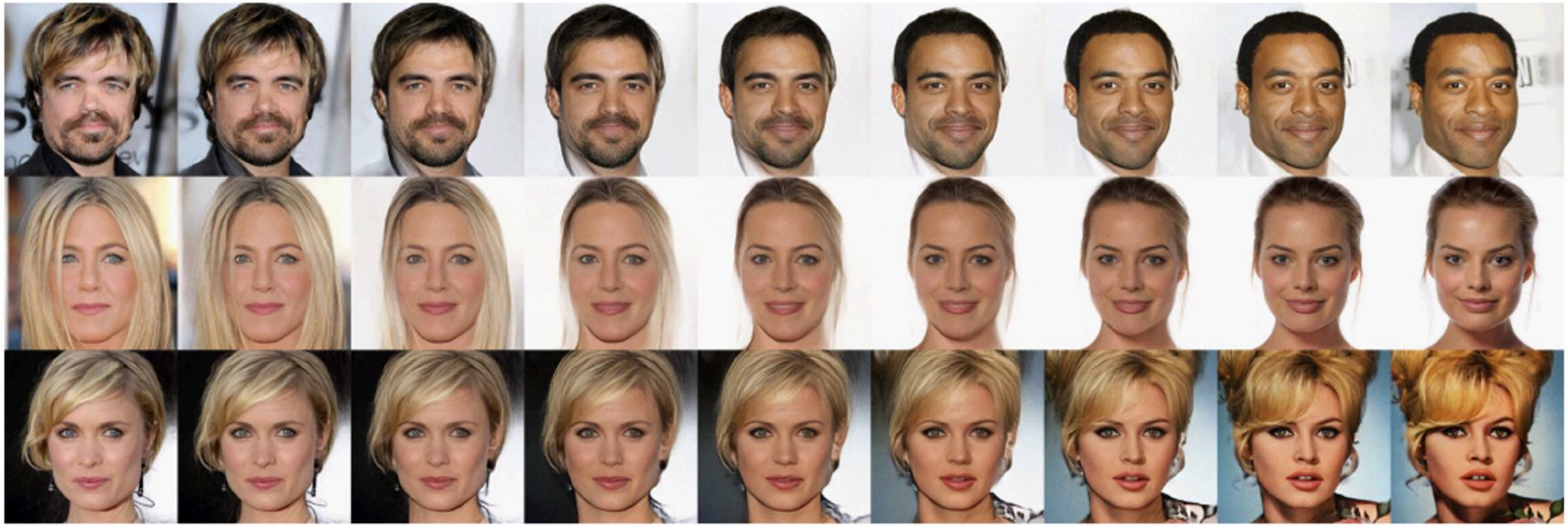
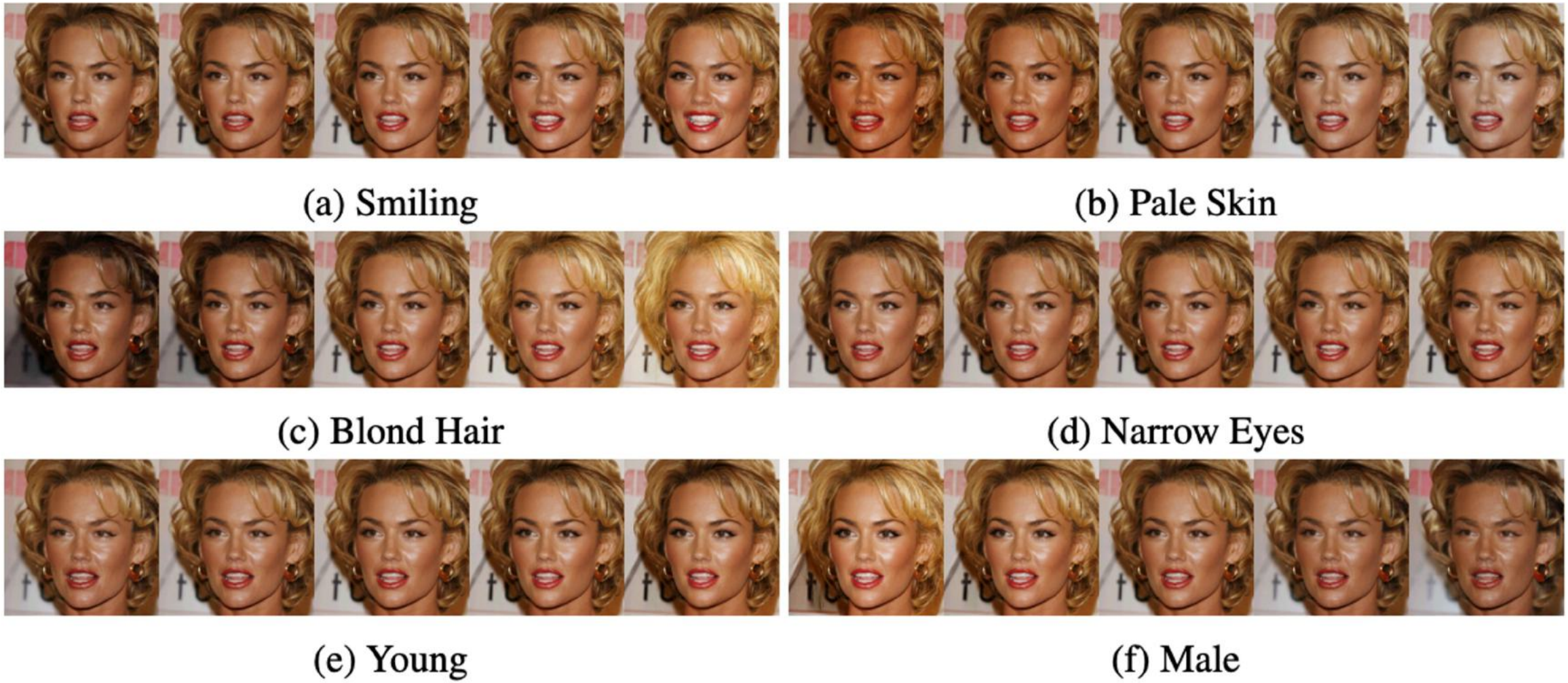


Figure 5: Linear interpolation in latent space between real images

Glow: Attribute Control



(a) Smiling (b) Pale Skin

(c) Blond Hair (d) Narrow Eyes

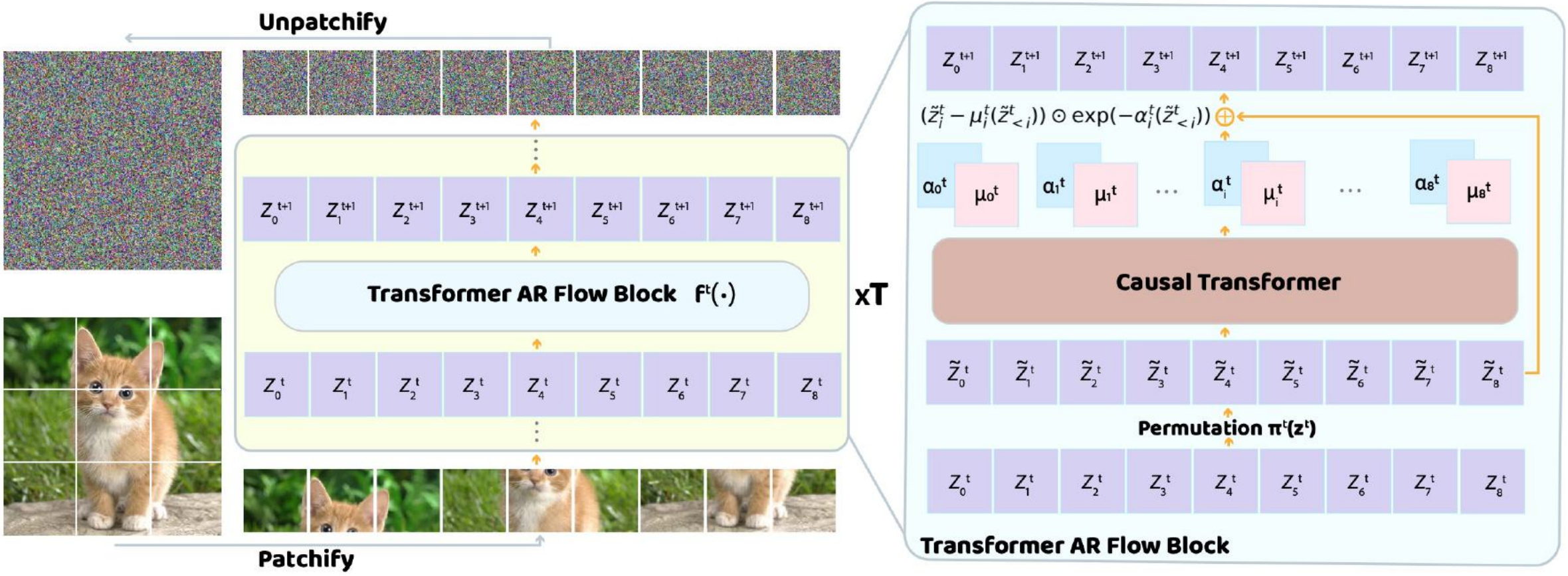
(e) Young (f) Male

How do Normalizing Flows perform?

Glow, 2018

StyleGAN, 2019

Modern Normalizing Flows



"Normalizing Flows are Capable Generative Models", Zhai et al., 2024

Modern Normalizing Flows

"Normalizing Flows are Capable Generative Models", Zhai et al., 2024

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

IAF/MAF/NAF
SOS polynomial
UMNN

2. Block coupling

NICE/RealNVP/Glow
Cubic Spline Flow
Neural Spline Flow

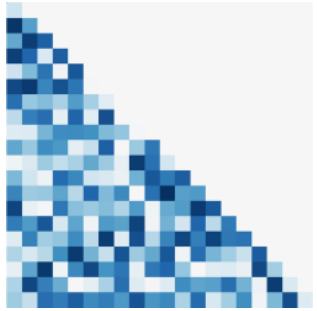
3. Det identity

Planar/Sylvester flows
Radial flow

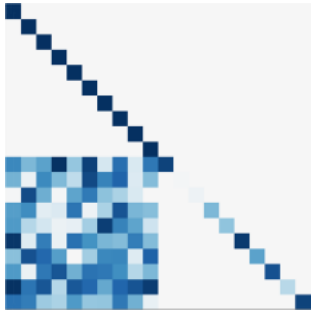
4. Stochastic estimation

Residual Flow
FFJORD

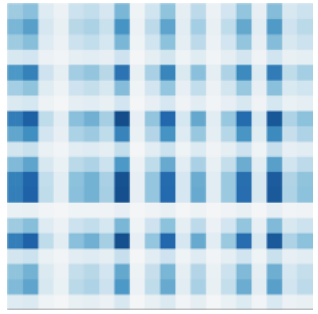
Jacobian



(Lower triangular)



(Lower triangular + structured)



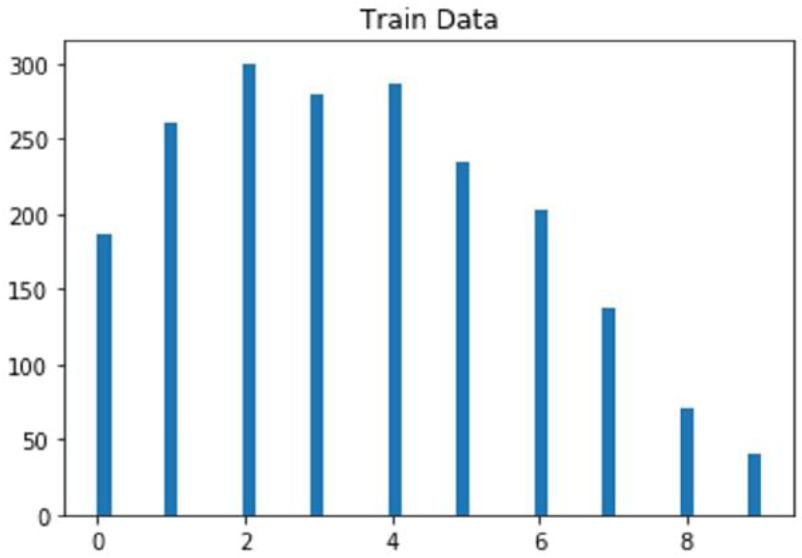
(Low rank)

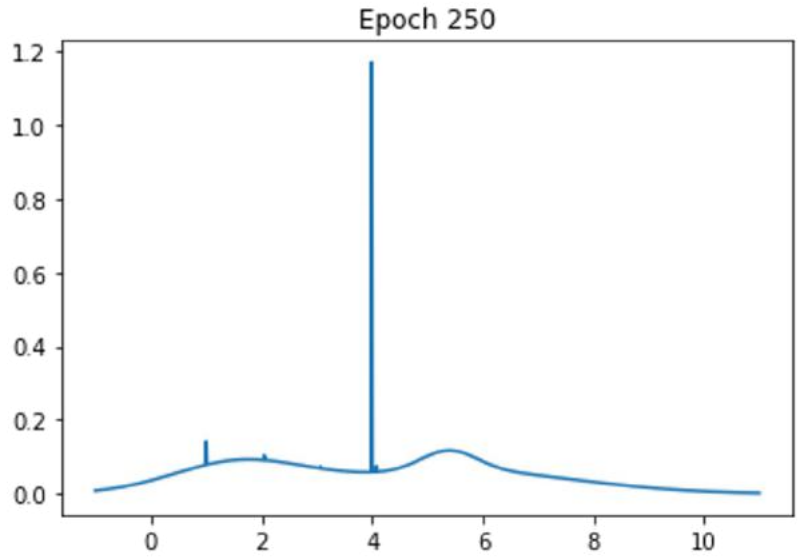
(Arbitrary)

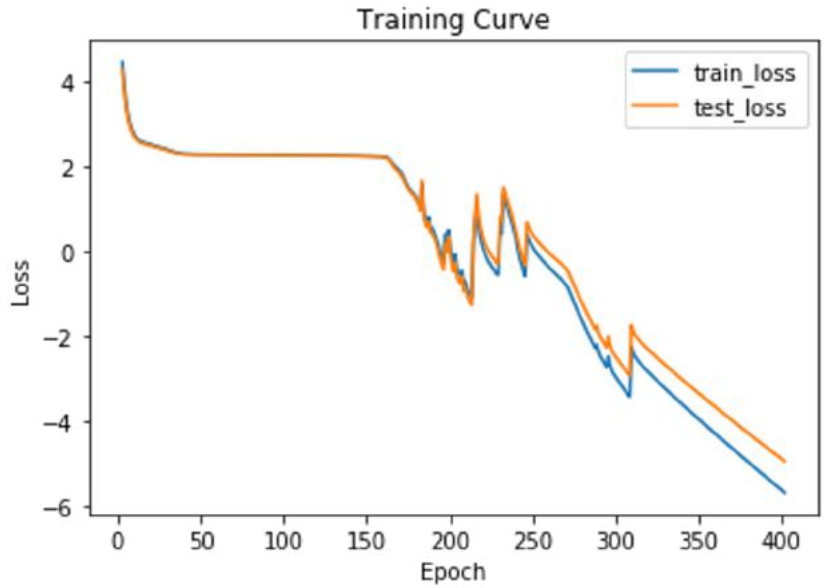
Lecture overview

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

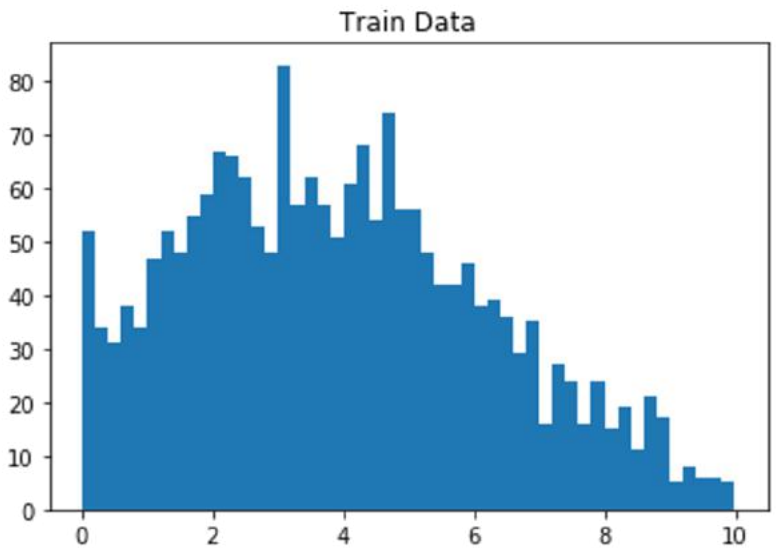
$$\mathbf{x} \in \{0, 1, 2, \ldots, 255\}$$

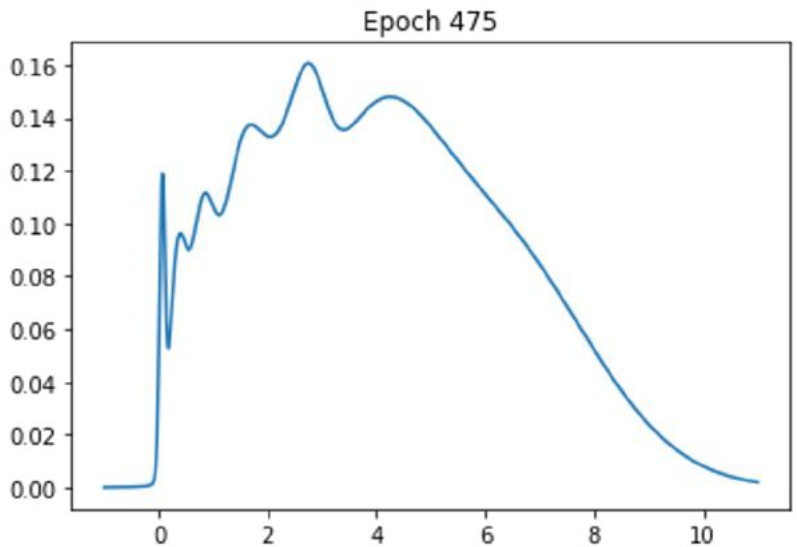
  - We draw noise u uniformly from $[0, 1)^D$

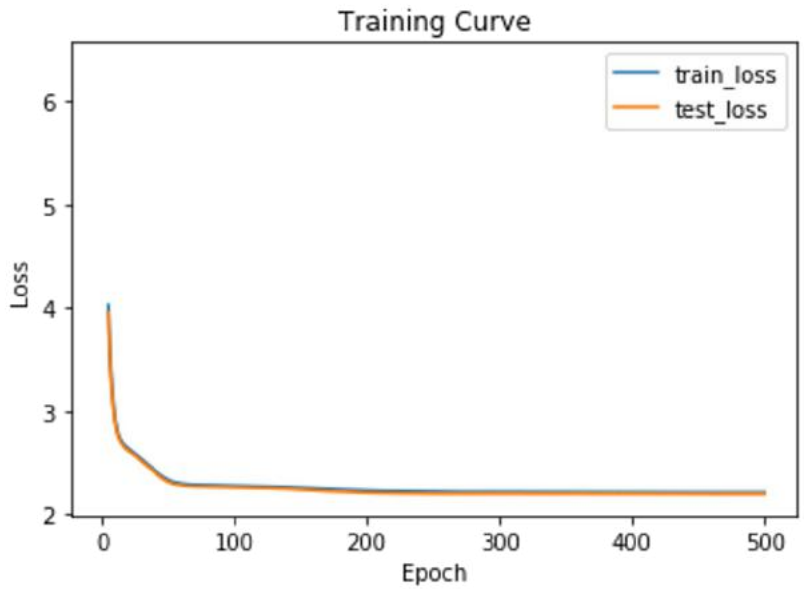
$$\begin{aligned}
\mathbb{E}_{\mathbf{y} \sim p_{\text{data}}} \left[\log p_{\text{model}}(\mathbf{y}) \right] &= \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \int_{[0,1)^D} \log p_{\text{model}}(\mathbf{x} + \mathbf{u}) \, d\mathbf{u} \\
&\leq \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \log \int_{[0,1)^D}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

[Theis, Oord, Bethge, 2016]

Flow on Discrete Data With Dequantization

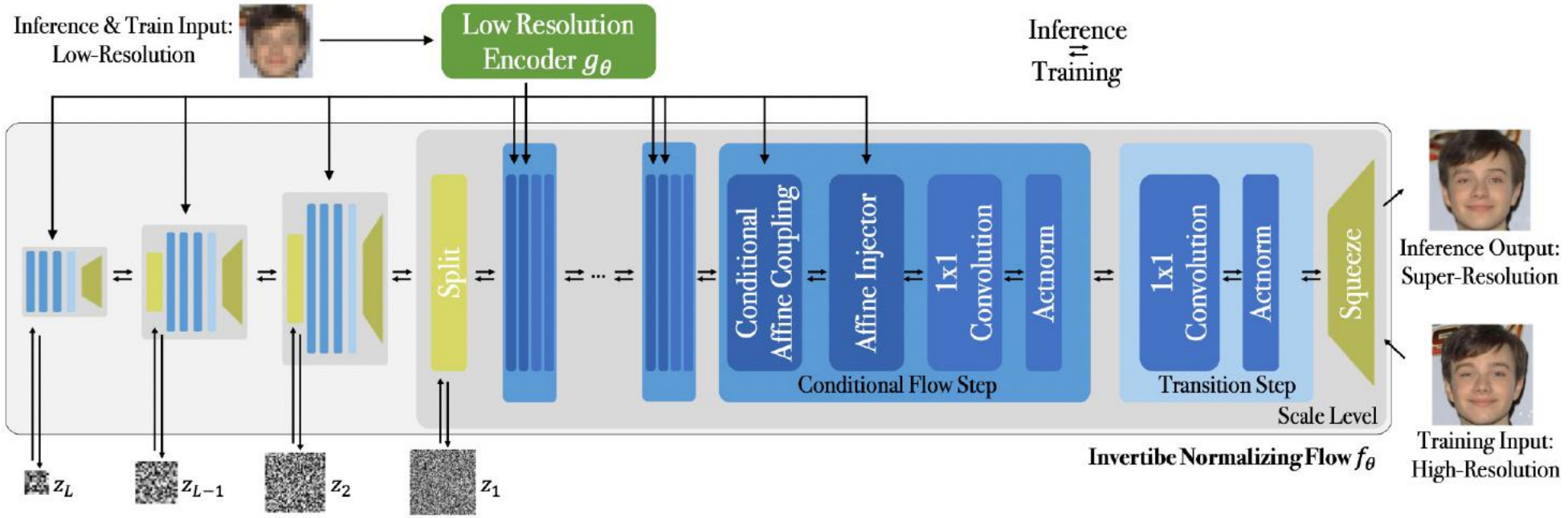






Applications: Super-Resolution

- 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

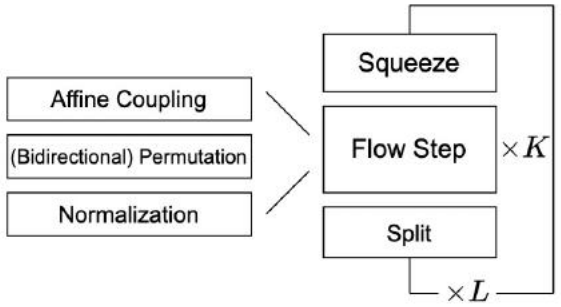


Figure 2: Non-autoregressive Language Flow model with Multi-Scale architecture.

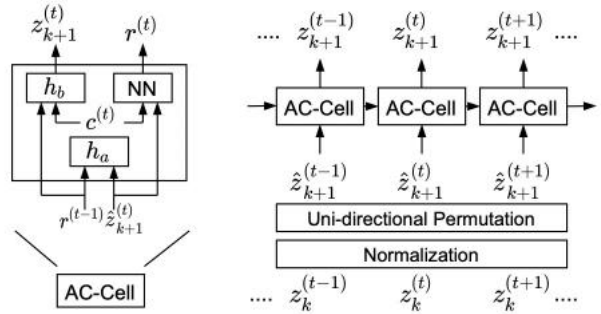


Figure 3: Autoregressive Language Generative Flow model. The whole autoregressive flow model contains multiple K steps. This figure illustrates one flow step from z_k to z_{k+1}.

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

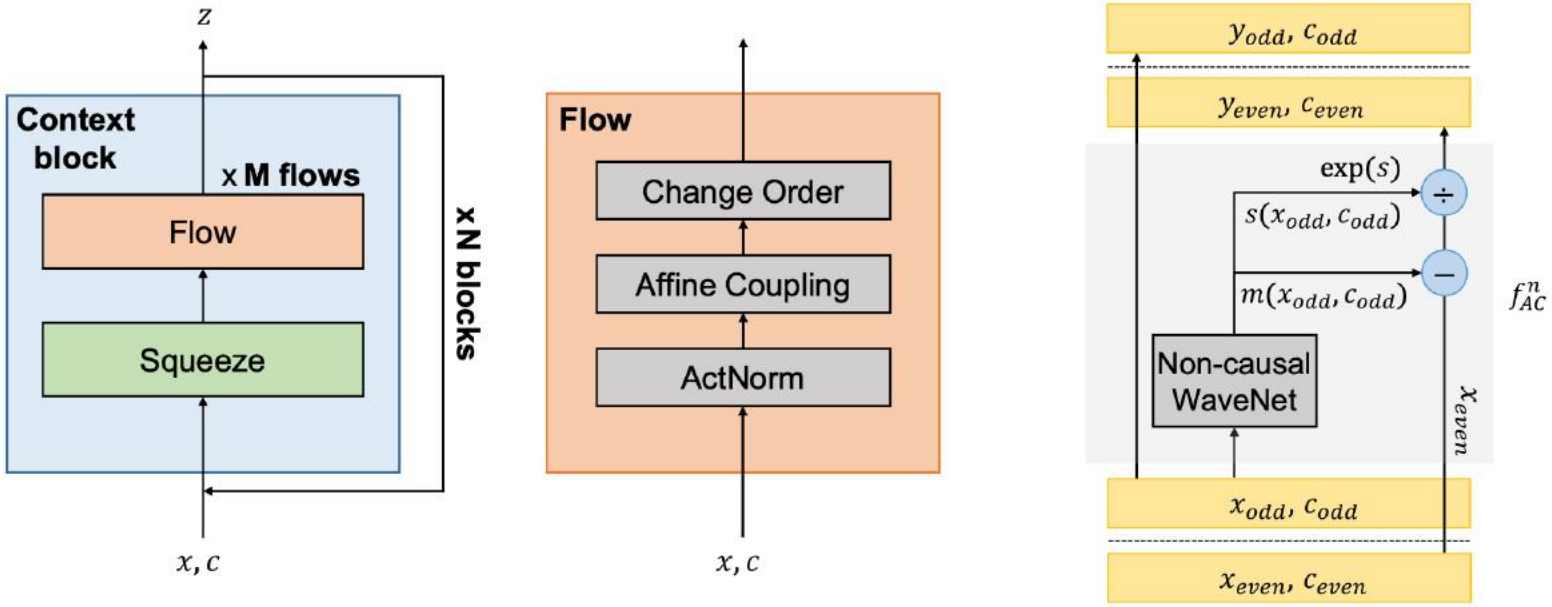
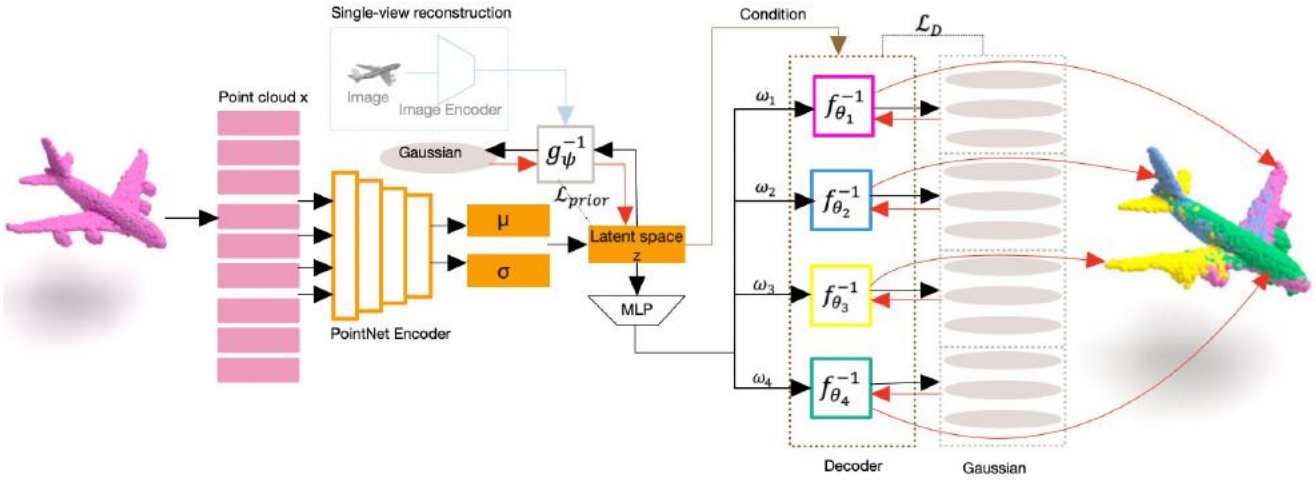
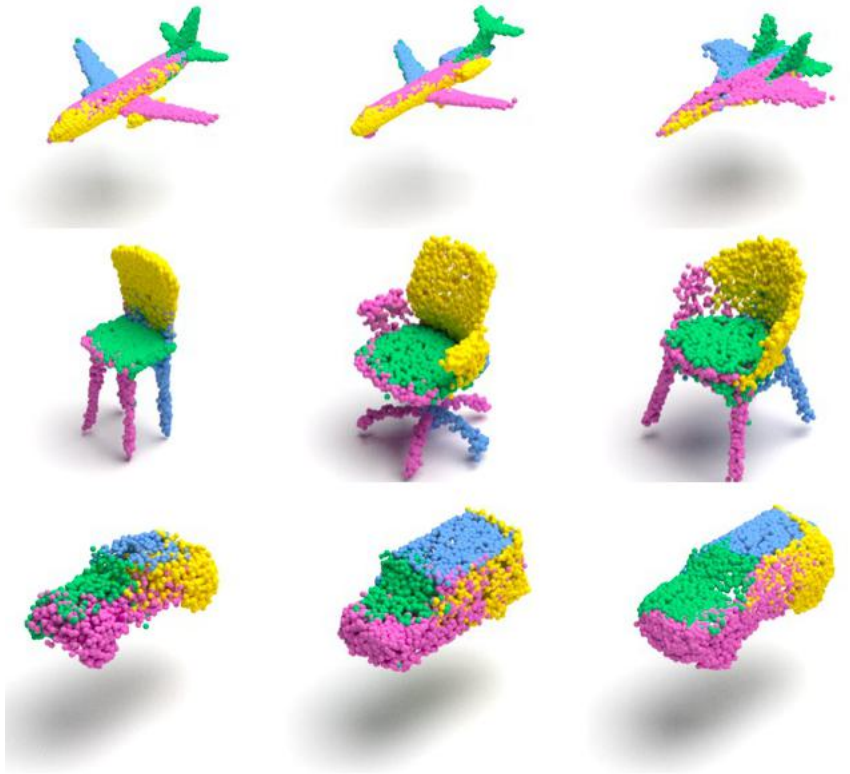


Figure 1. Schematic diagram of FloWaveNet. Left: an entire forward pass of the FloWaveNet consisting of N context blocks. Middle: an abstract diagram of the flow operation. Right: a detailed version of the affine coupling operation.

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:
Latent Variable Models