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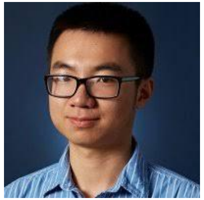
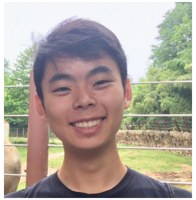
CS294-158 Deep Unsupervised Learning

Lecture 3 Likelihood Models: Flow Models

Pieter Abbeel, Xi (Peter) Chen, Jonathan Ho, Aravind Srinivas, Alex Li, Wilson Yan

UC Berkeley

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!)

    $p_\theta(x)$
  - For new x, ability to eva $p_\theta(x)$
  - Ability to sample from
  - 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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$p_\theta(x)$

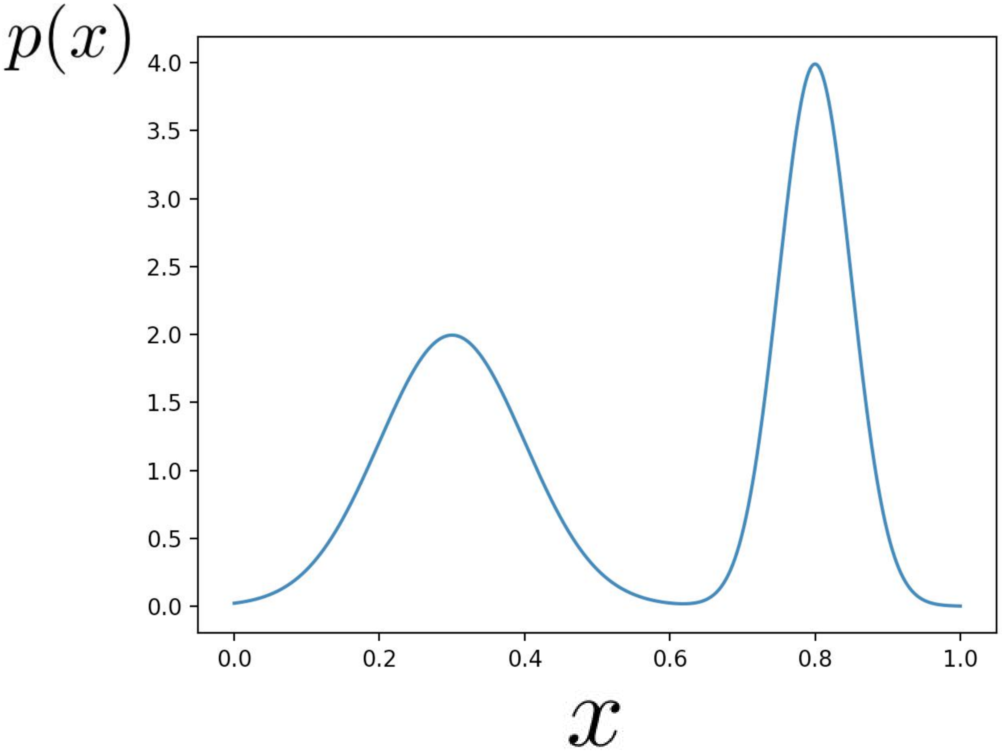
  - For new x, ability to eva $p_\theta(x)$
  - Ability to sample from
  - And, ideally, *a latent representation* that's meaningful

- Differences from Autoregressive Models from last lecture

Outline

- ***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:

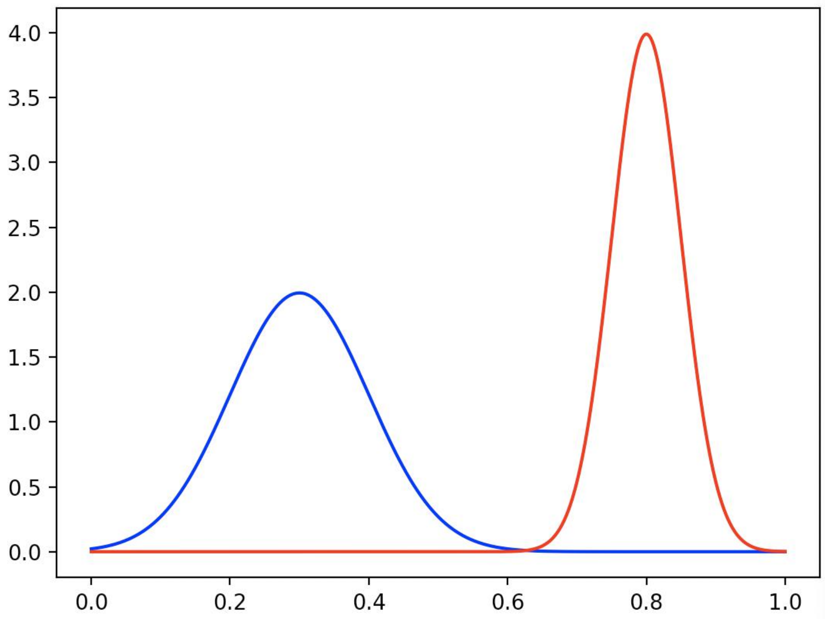
$$\min_\theta \mathbb{E}_x \left[-\log p_\theta(x) \right]$$

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

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



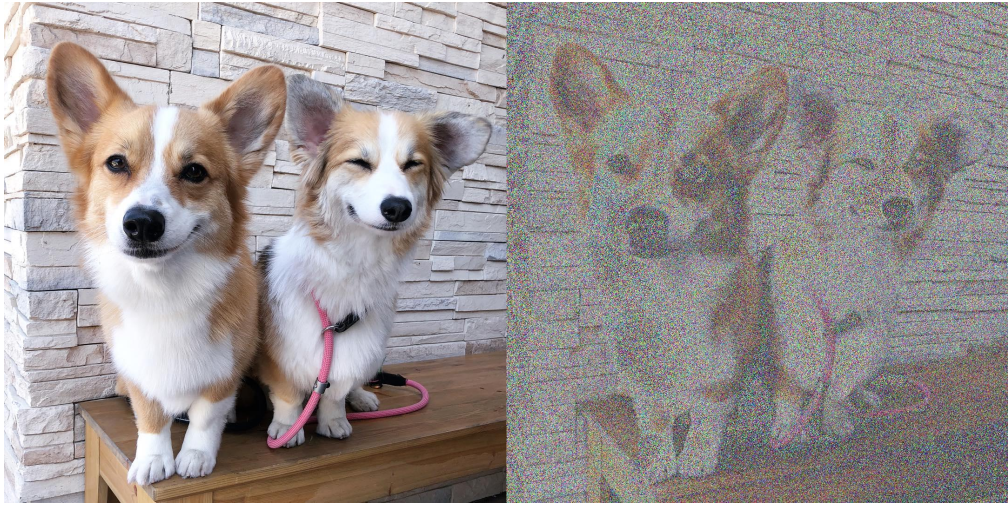
Aside on Mixtures of Gaussians

Do mixtures of Gaussians work for high-dimensional data?

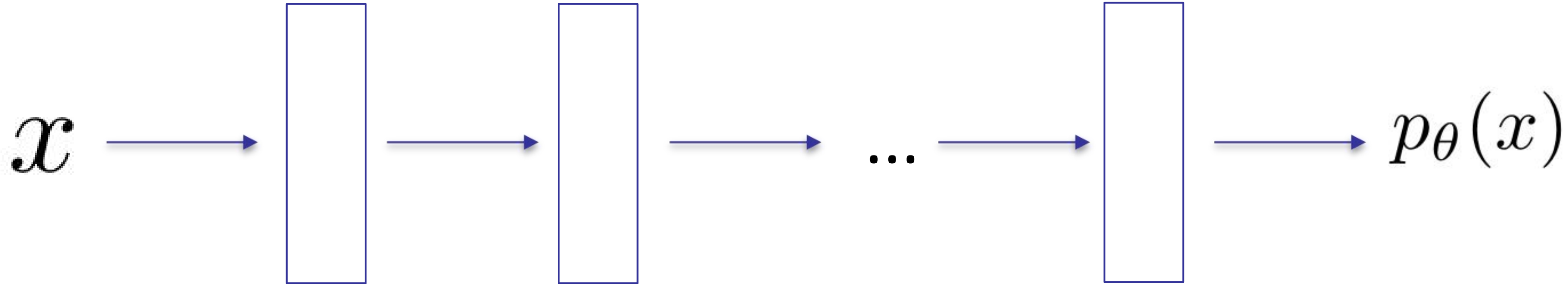
Not really. The sampling process is:

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?

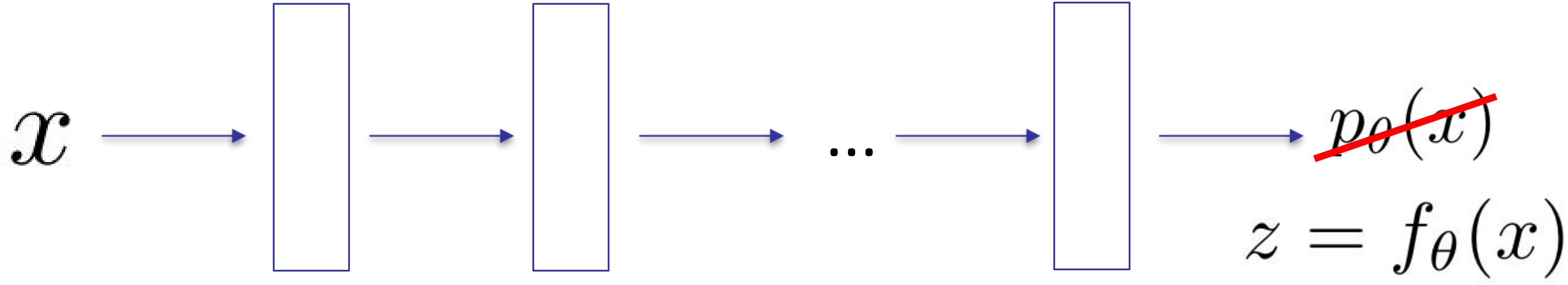


- How to ensure proper distribution?

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

- How to sample?
- Latent representation?

Flows: Main Idea

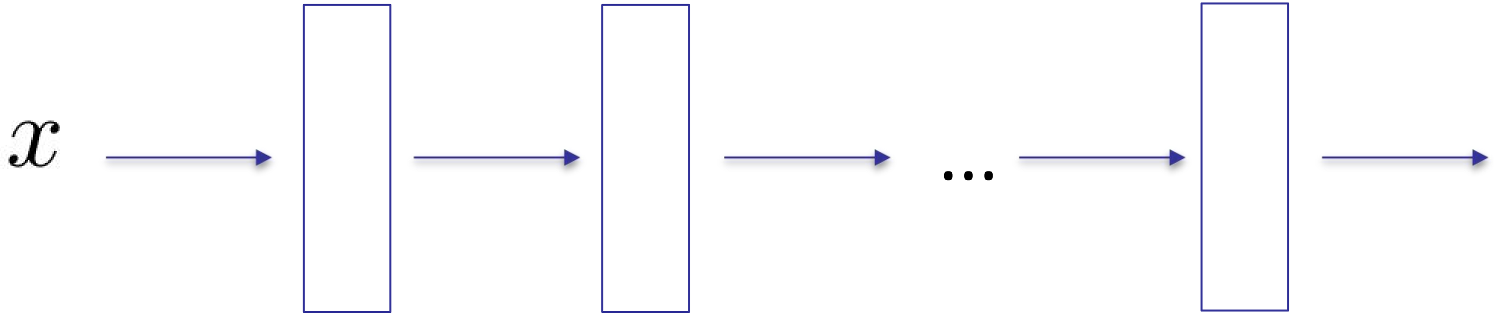


Generally: $z \sim p_Z(z)$

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

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

Flows: Training



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

$$z \sim p_Z(z)$$

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

Change of Variables

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

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

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

Note: requires f_θ invertible & differentiable

Flows: Training

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

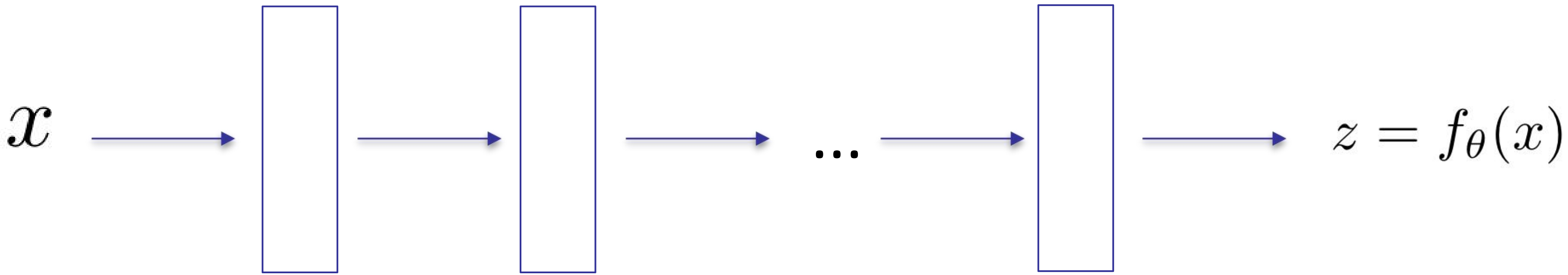
$$z^{(i)} = f_\theta(x^{(i)})$$

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

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

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

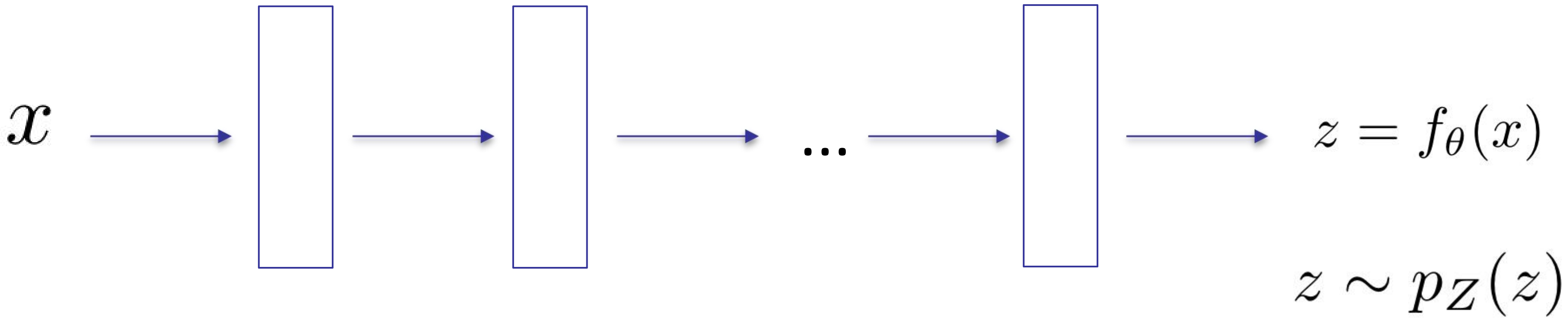
Flows: Sampling



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

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

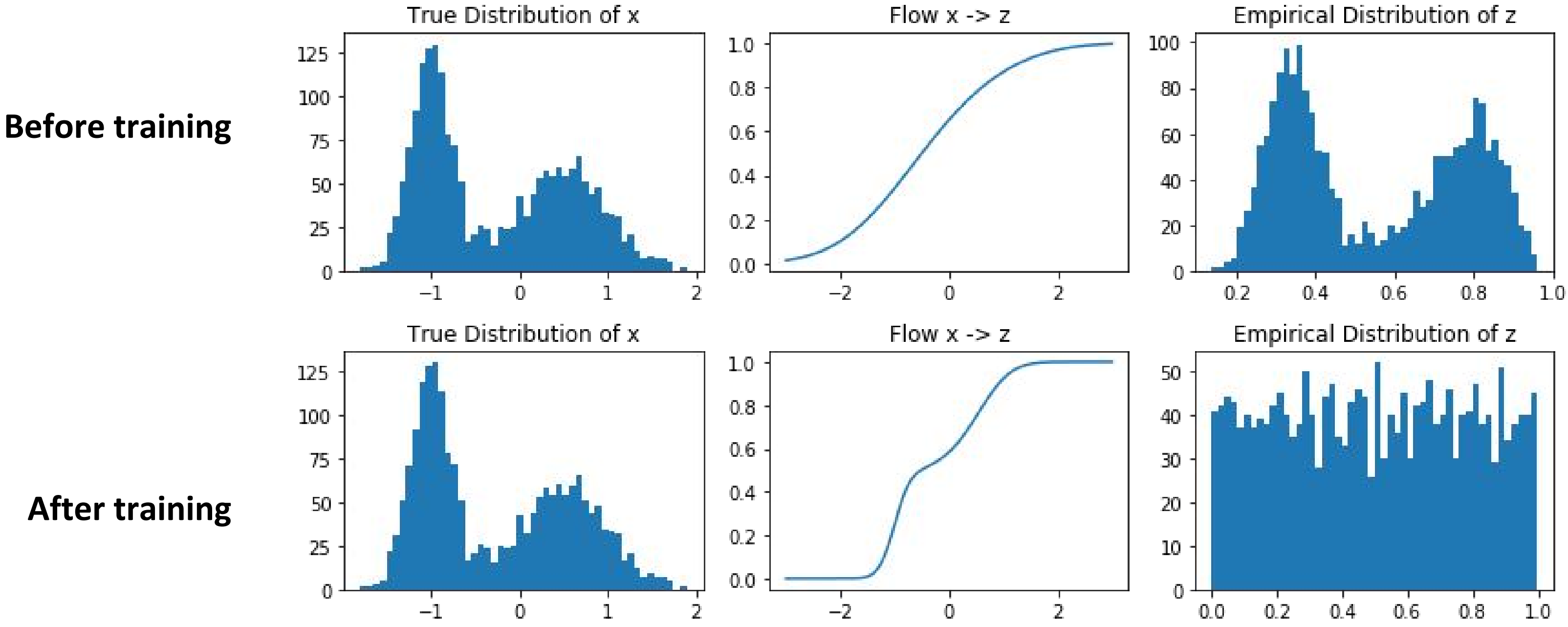
What do we need to keep in mind for f?



Recall, change of variable formula requires

- f_θ Invertible & differentiable

Example: Flow to Uniform z



True distribution of x

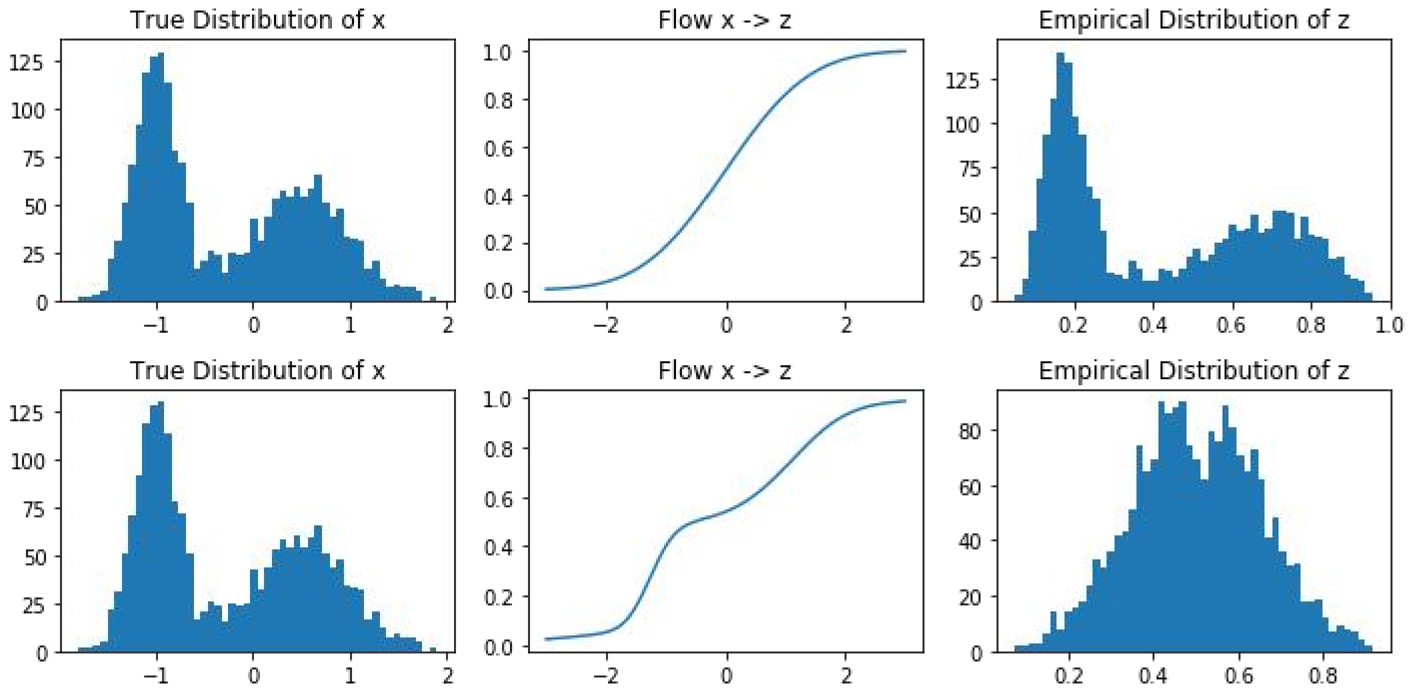
Flow x → z

Empirical distribution of z

Example: Flow to Beta(5,5) z

Before training

After training

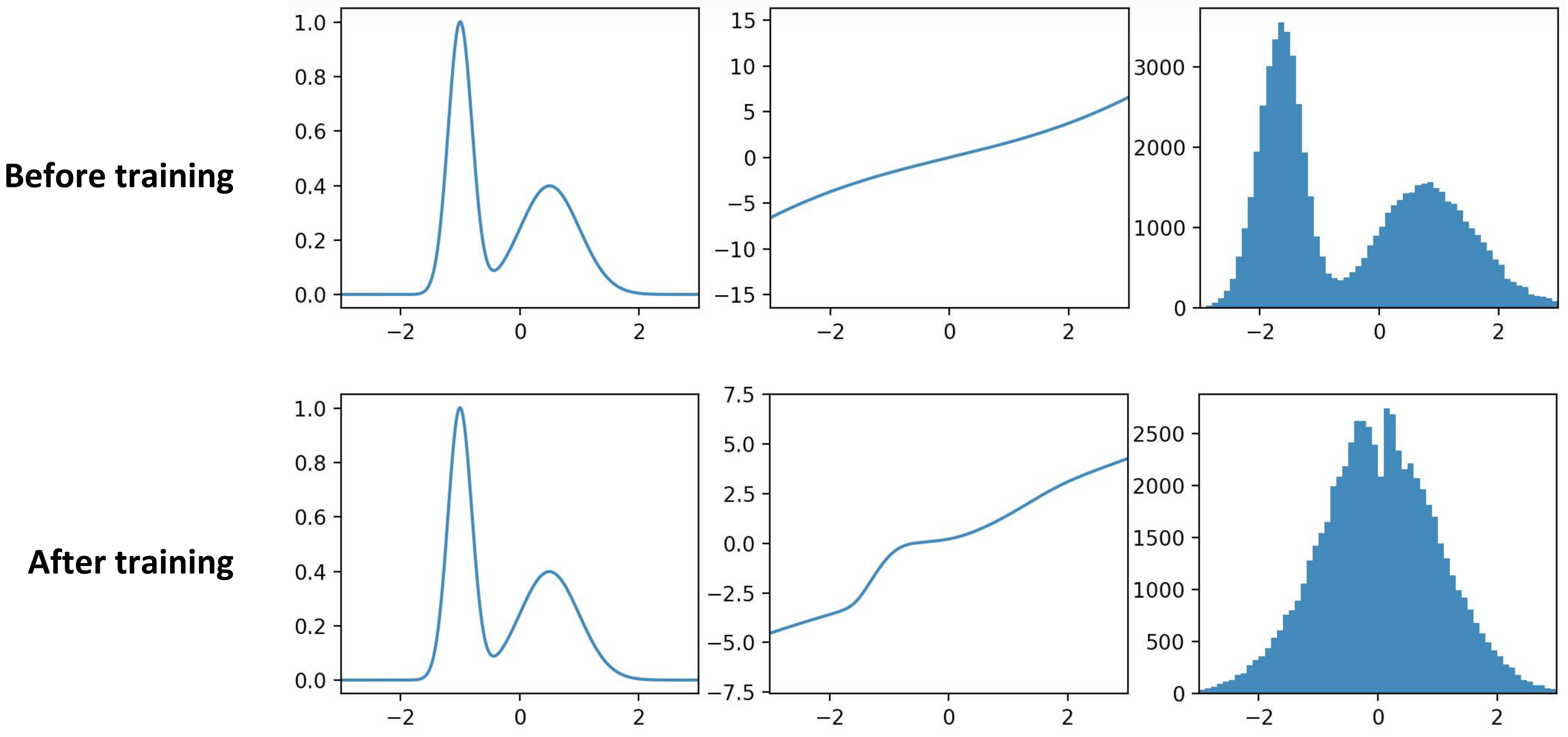


True distribution of x

Flow x → z

Empirical distribution of z

Example: Flow to Gaussian z



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

Practical Parameterizations of Flows

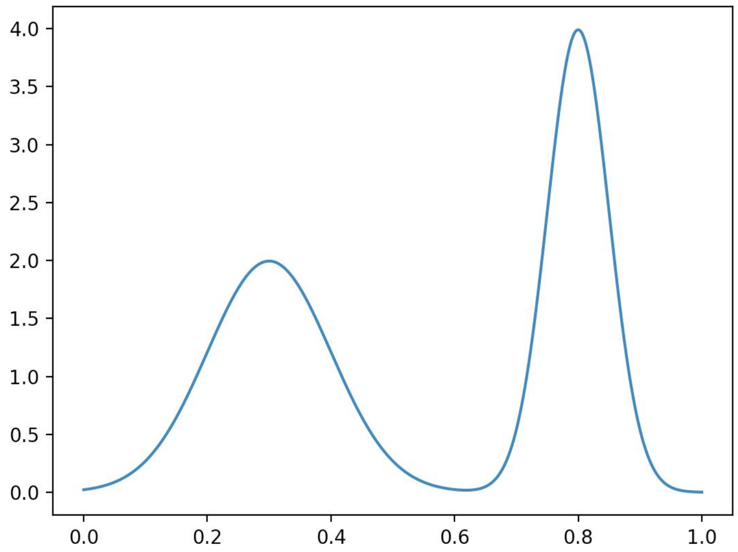
Requirement: Invertible and Differentiable

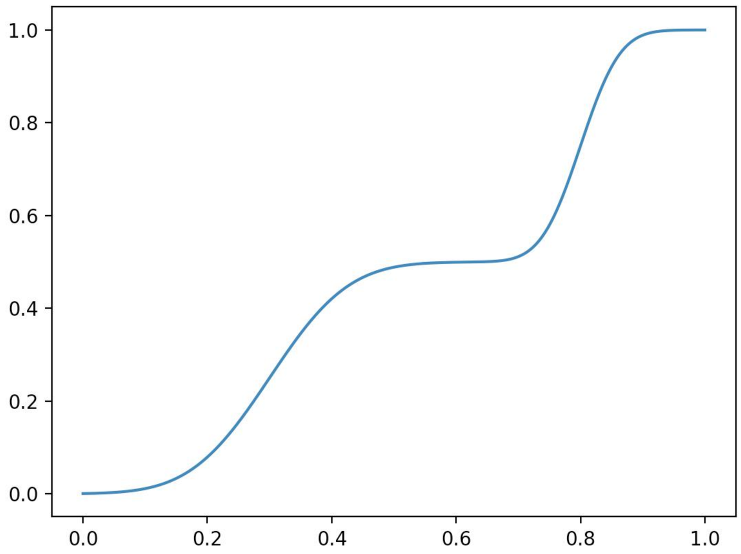
- Cumulative Density Functions
  - E.g. Gaussian mixture density, mixture of logistics
- Neural Net
  - If each layer flow, then sequencing of layers = flow
  - Each layer:
    - ReLU?
    - Sigmoid?
    - Tanh?

How general are flows?

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

Refresher: Cumulative Density Function (CDF)





$$p_\theta(x)$$

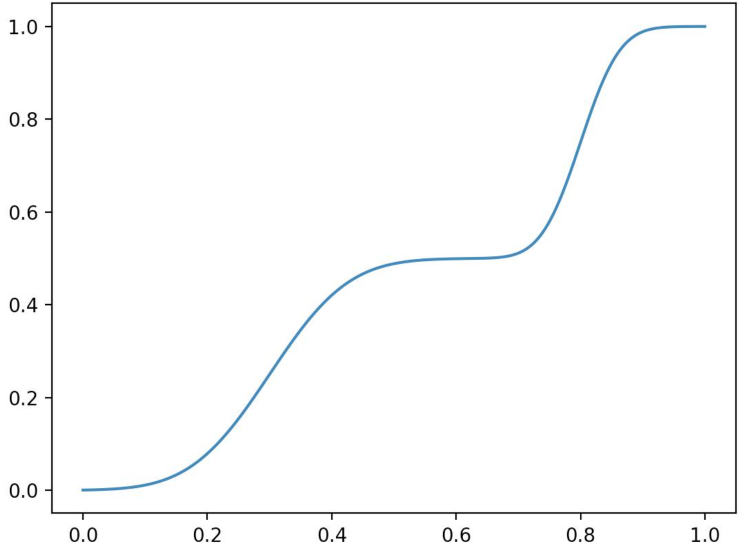
$$f_\theta(x) = \int_{-\infty}^{x} p_\theta(t)\, dt$$

Sampling via inverse CDF

Sampling from the model:

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

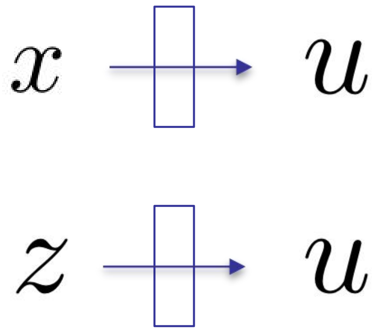
The CDF is an invertible, differentiable map from data to [0, 1]



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

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)

Outline

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

2-D Autoregressive Flow

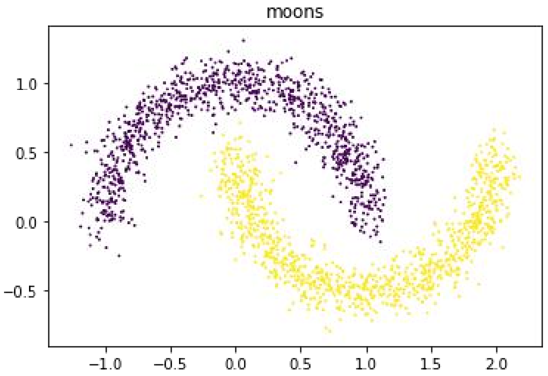
$$x_1 \rightarrow z_1 = f_\theta(x_1)$$

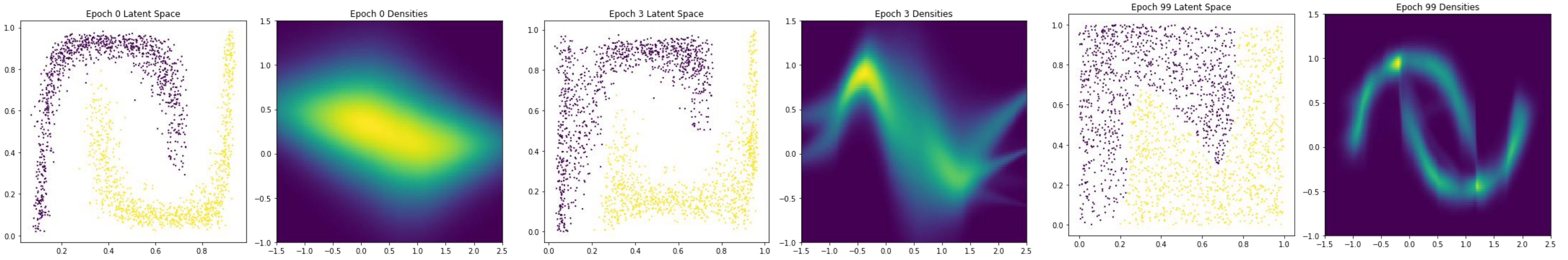
$$x_2 \rightarrow z_2 = f_\theta(x_1, x_2)$$

2-D Autoregressive Flow: Two Moons

Architecture:

- Base distribution: Uniform[0,1]^2
- x1: mixture of 5 Gaussians
- x2: mixture of 5 Gaussians, conditioned on x1

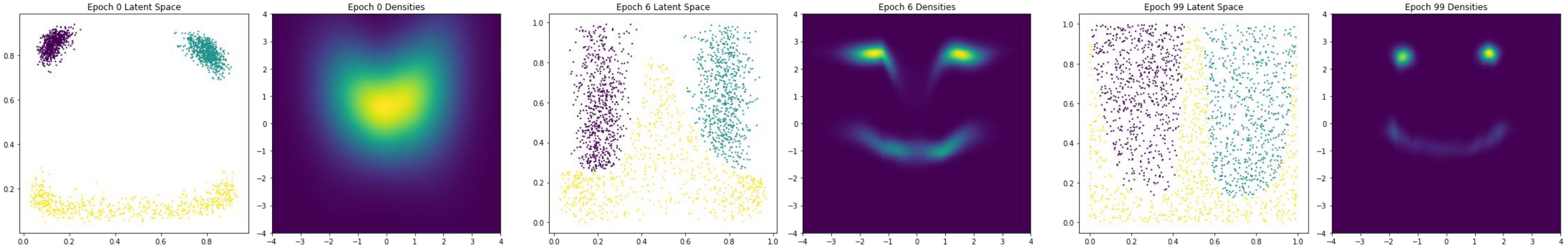




2-D Autoregressive Flow: Face

Architecture:

- Base distribution: Uniform[0,1]^2
- x1: mixture of 5 Gaussians
- x2: mixture of 5 Gaussians, conditioned on x1



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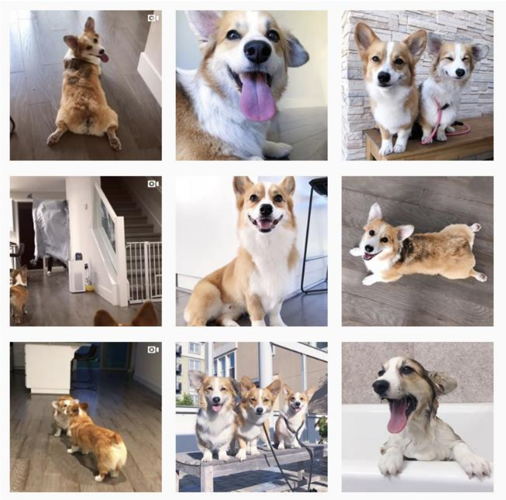
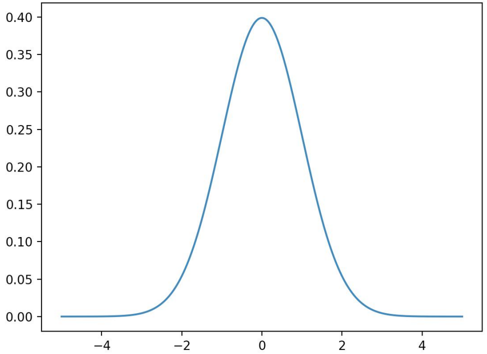
High-dimensional data



f (inference)

f^{-1} (sampling)



x and z must have the same dimension

Outline

- 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**

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

- 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

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

Inverse autoregressive flows

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

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

$$x_1 = f_\theta(z_1)$$
$$x_2 = f_\theta(z_2; z_1)$$
$$x_3 = f_\theta(z_3; z_1, z_2)$$

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

AF and IAF

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

- E.g. 1MP image → 1M layers…

Can do parameter sharing as in Autoregressive Models from lecture 2 [e.g. RNN, masking]

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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!

Constructing flows: composition

- **Flows can be composed**

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

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

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

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

- 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 $z \sim N(0, I)$
- 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: $x_{1:d/2}$, $x_{d/2+1:d}$

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

- Invertible! Note that s_θ and t_θ can be arbitrary neural nets with **no restrictions**.
  - Think of them as **data-parameterized elementwise flows**.

NICE/RealNVP

- It also has a tractable Jacobian determinant

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

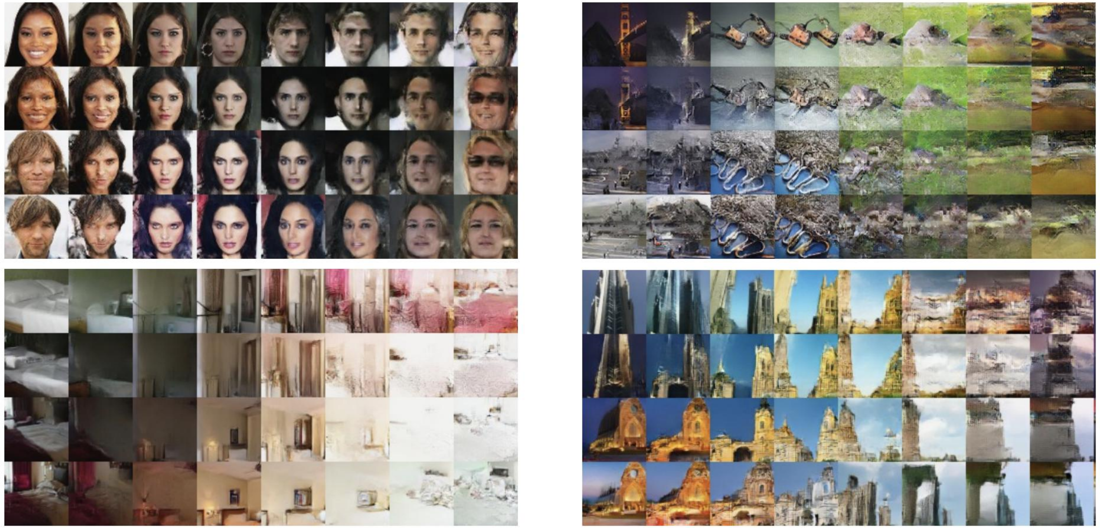
$$
\frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{bmatrix} I & 0 \\ \frac{\partial \mathbf{z}_{d/2:d}}{\partial \mathbf{x}_{1:d/2}} & \mathrm{diag}(s_\theta(\mathbf{x}_{1:d/2})) \end{bmatrix}
$$

- 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



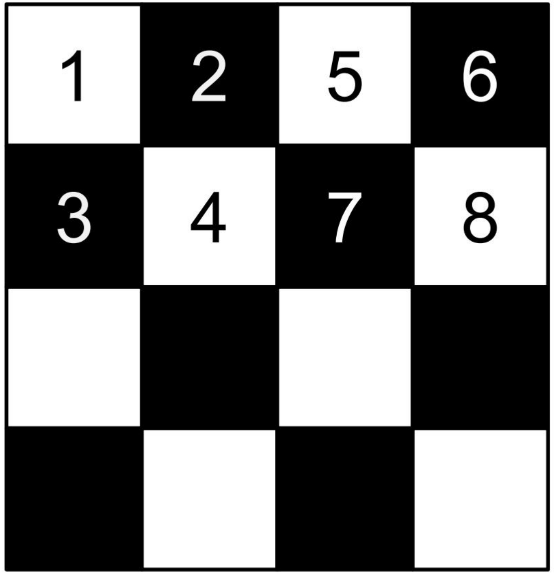
[Dinh et al. Density estimation using Real NVP. ICLR 2017]

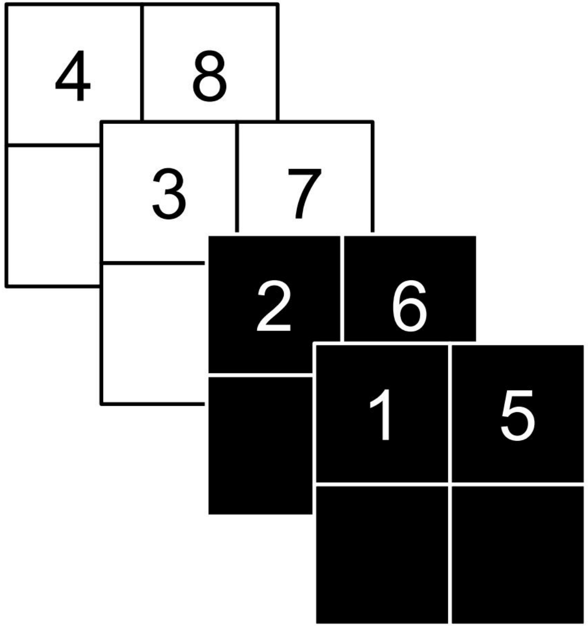
RealNVP Architecture

Input x: 32x32xc image

- Layer 1: (Checkerboard x3, channel squeeze, channel x3)
  - Split result to get x1: 16x16x2c and z1: 16x16x2c (fine-grained latents)
- Layer 2: (Checkerboard x3, channel squeeze, channel x3)
  - Split result to get x2: 8x8x4c and z2: 8x8x4c (coarser latents)
- Layer 3: (Checkerboard x3, channel squeeze, channel x3)
  - Get z3: 4x4x16c (latents for highest-level details)

RealNVP: How to partition variables?





Good vs Bad Partitioning

Checkerboard x4; channel squeeze; channel x3; channel unsqueeze; checkerboard x3

(Mask top half; mask bottom half; mask left half; mask right half) x2

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Choice of coupling transformation

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

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

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

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

- 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. Still an

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**

Other classes of flows

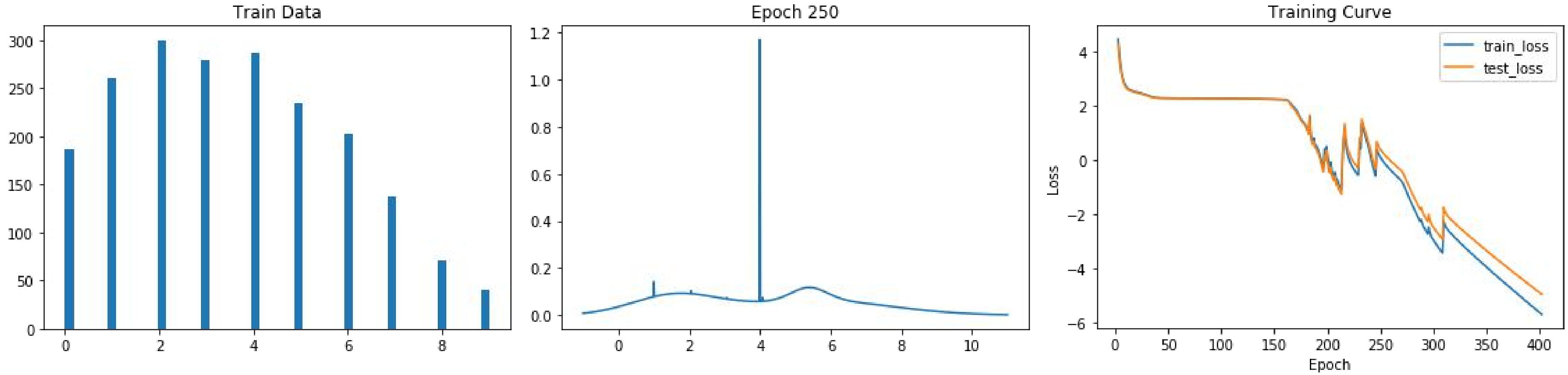
- Glow (link)
  - Invertible 1x1 convolutions
  - Large-scale training

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

Outline

- 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

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

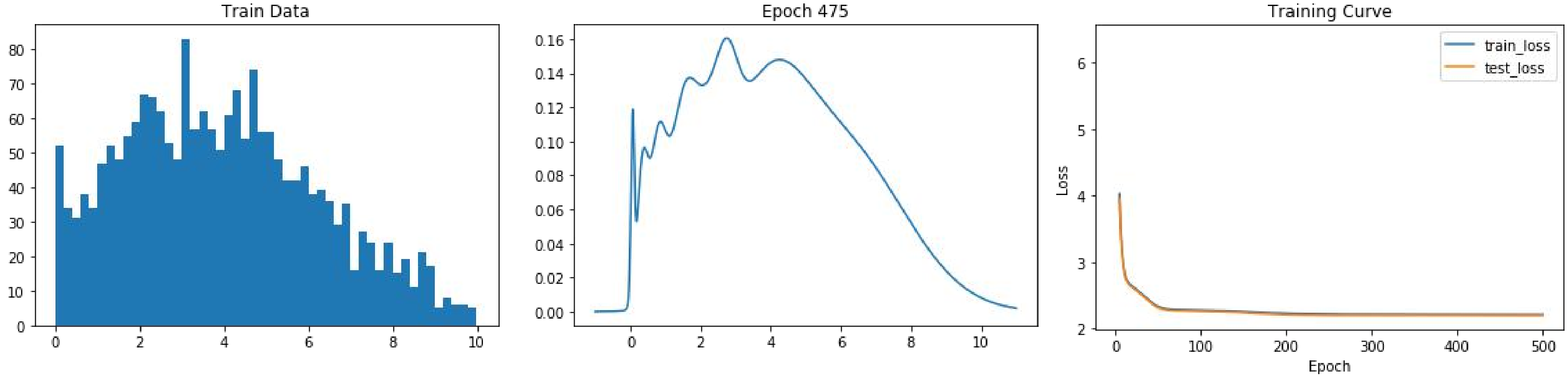
Continuous flows for discrete data

- 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



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.

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