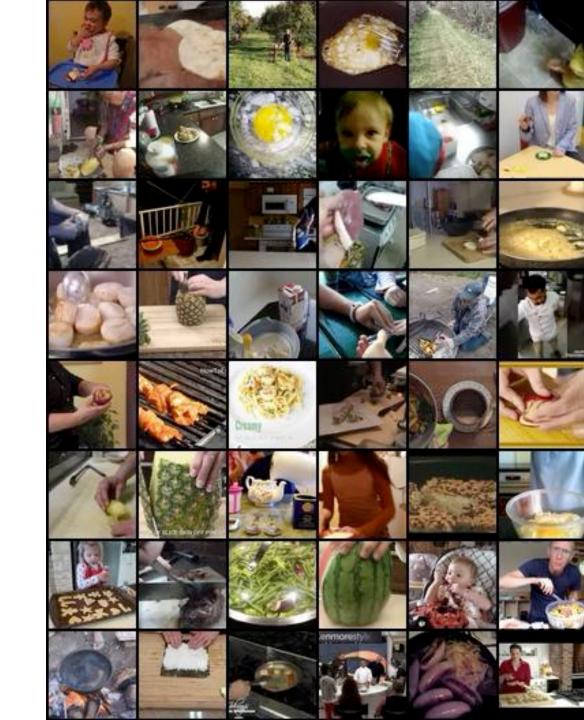


Previously on COMP547

- 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

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Differences from Autoregressive Models from last lecture

Lecture overview

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

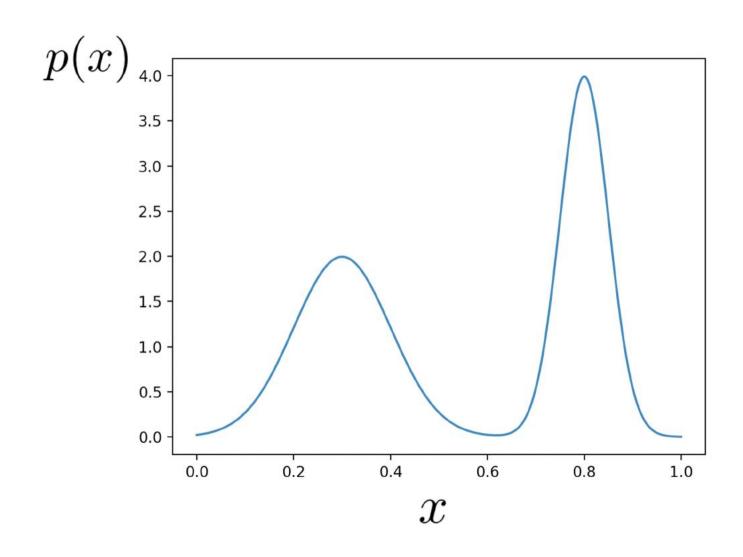
Disclaimer: Much of the material and slides for this lecture were borrowed from

- —Pieter Abbeel, Peter Chen, Jonathan Ho, Aravind Srinivas' Berkeley CS294-158 class
- —Chin-Wei Huang slides on Normalizing Flows

Lecture overview

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- 2-D Flows
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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:

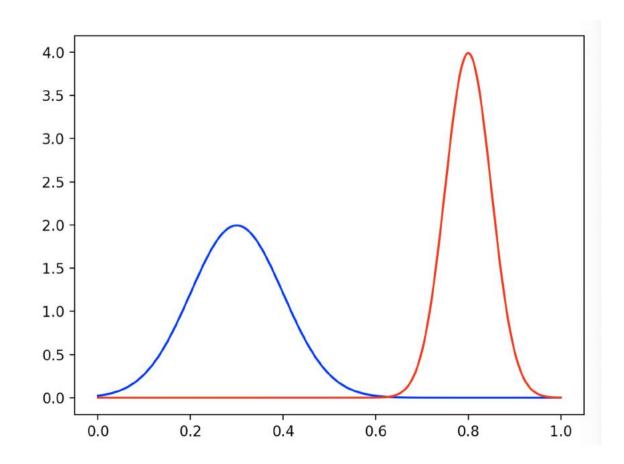
$$\min_{\theta} \mathbb{E}_x \left[-\log p_{\theta}(x) \right]$$

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

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



Aside on Mixtures of Gaussians

Do mixtures of Gaussians work for high-dimensional data?

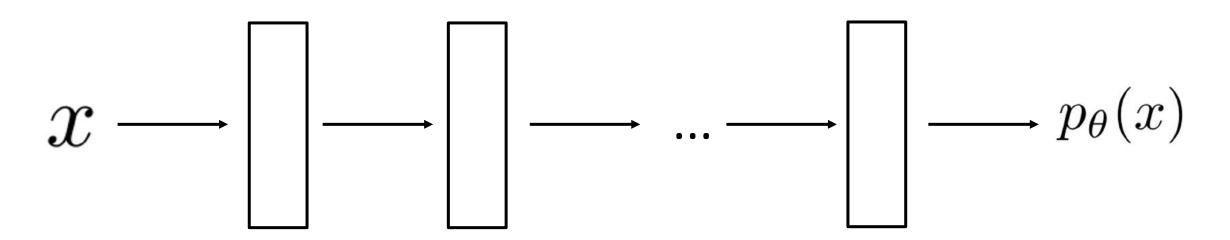
Not really. The sampling process is:

- 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?

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

- How to sample?
- Latent representation?

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

Flows: Main Idea

$$x \longrightarrow \boxed{\boxed{}} \longrightarrow \boxed{\boxed{}} \longrightarrow \dots \longrightarrow \boxed{\boxed{}} \longrightarrow p_{\theta}(x)$$

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

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

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

$$z \sim p_{Z}(z)$$

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

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

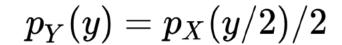
Change of Variable Density Needs to Be Normalized

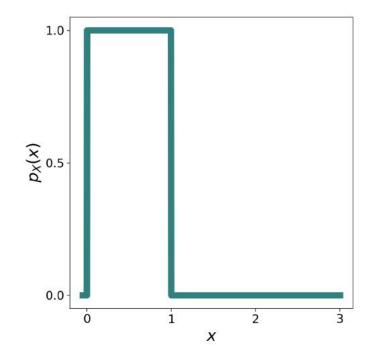
$$X \sim p_X$$

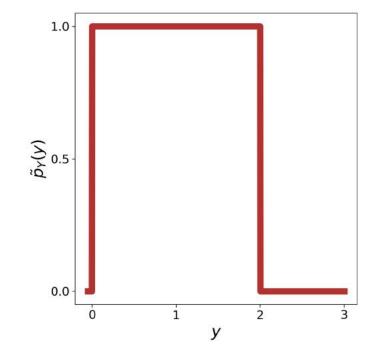
$$p_X(x) = egin{cases} 1 & ext{for } 0 \leq x \leq 1 \ 0 & ext{else} \end{cases}$$

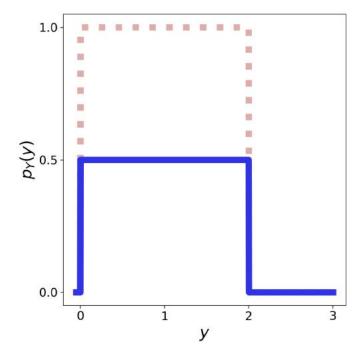
$$Y := 2X$$

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









Flows: Training

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

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

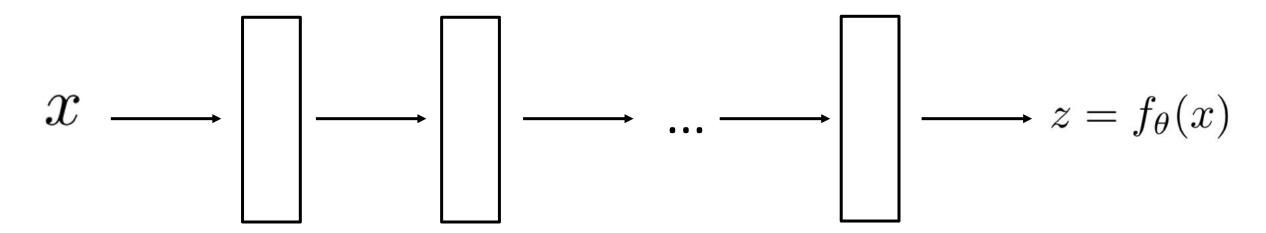
$$p_{\theta}(x^{(i)}) = p_{Z}(z^{(i)}) \left| \frac{\partial z}{\partial x}(x^{(i)}) \right|$$

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

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

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

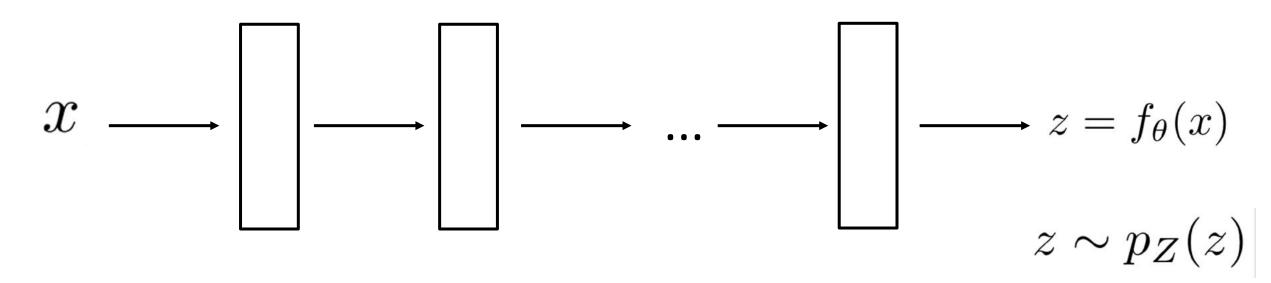
Flows: Sampling



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

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

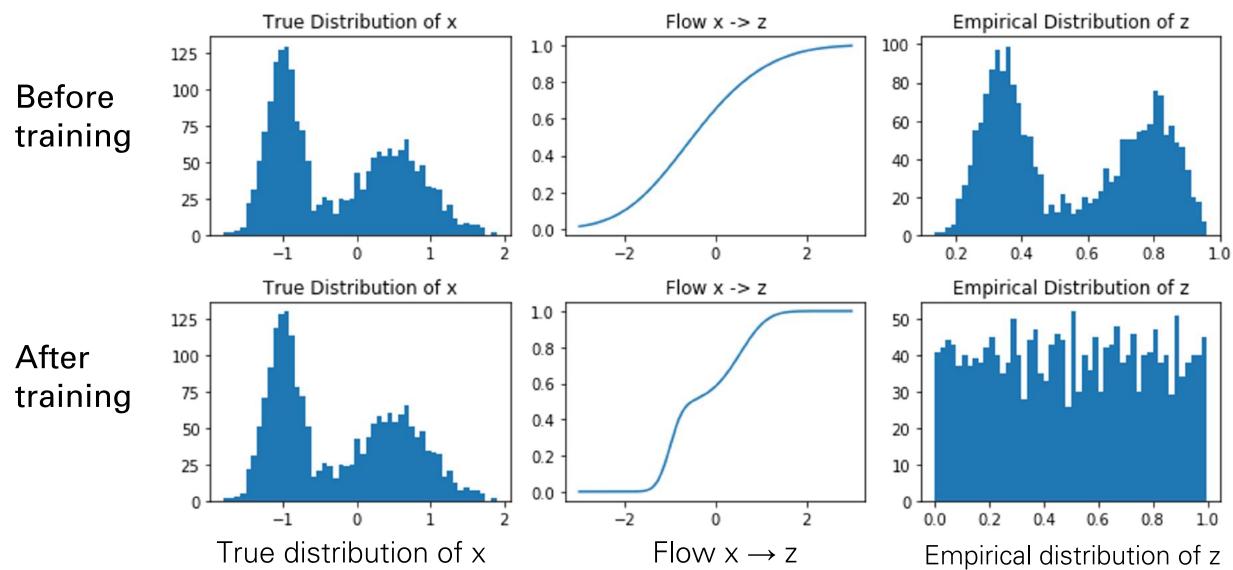
What do we need to keep in mind for f?



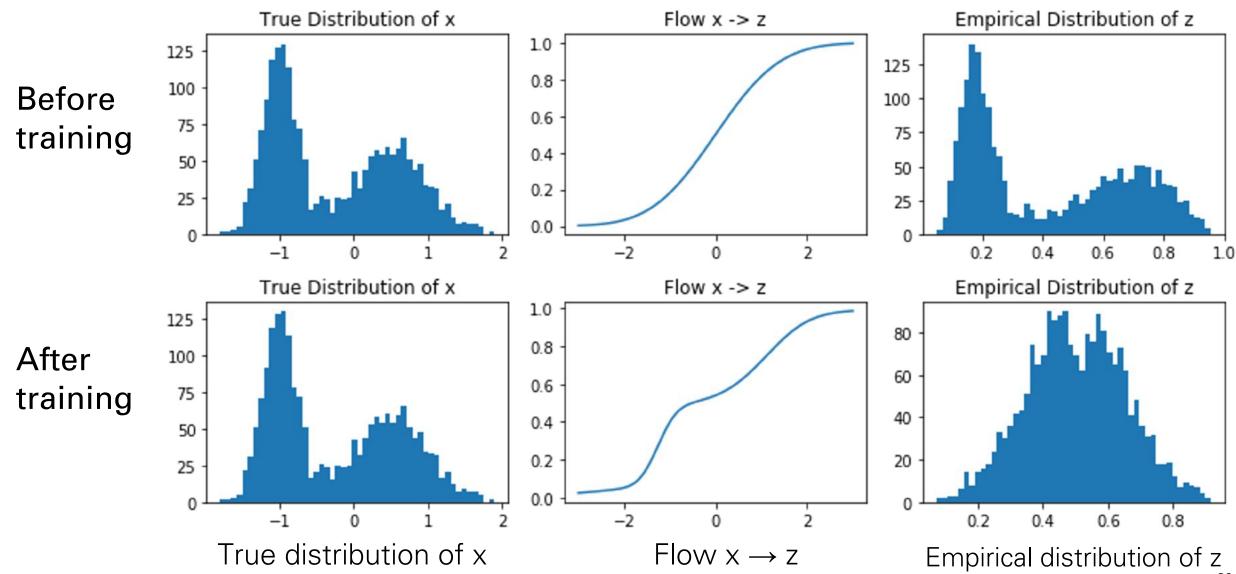
Recall, change of variable formula requires

• f_{θ} Invertible & differentiable

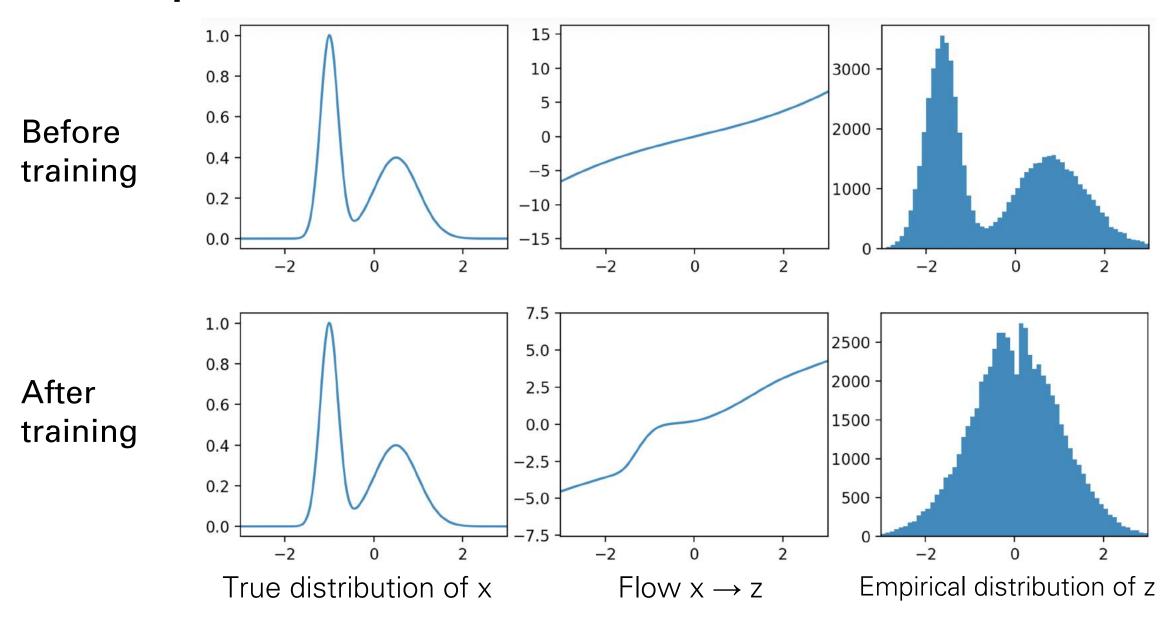
Example: Flow to Uniform z



Example: Flow to Beta(5,5) z



Example: Flow to Gaussian z



Practical Parameterizations of Flows

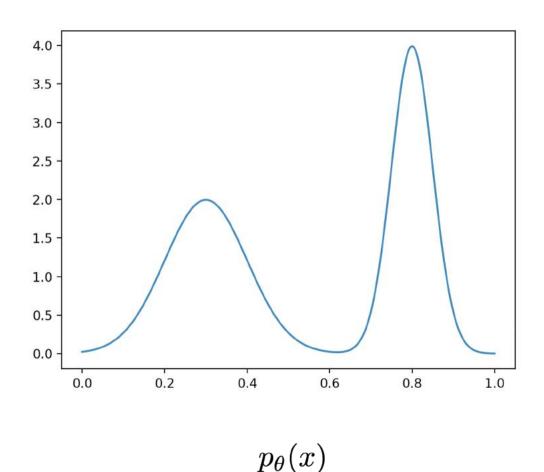
Requirement: Invertible and Differentiable

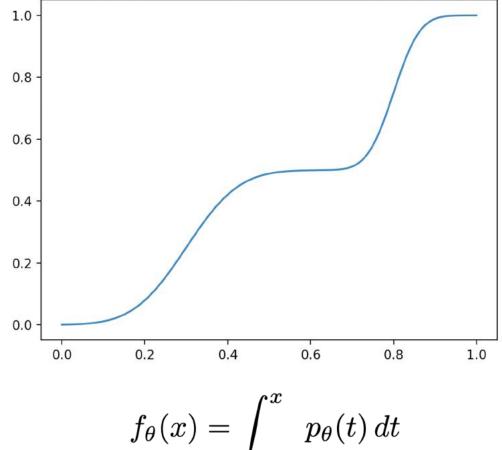
- Cumulative Density Functions
 - E.g. Gaussian mixture density, mixture of logistics
- Neural Net
 - If each layer flow, then sequencing of layers = flow
 - Each layer:
 - ReLU?
 - Sigmoid?
 - Tanh?

How general are flows?

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

Refresher: Cumulative Density Function (CDF)





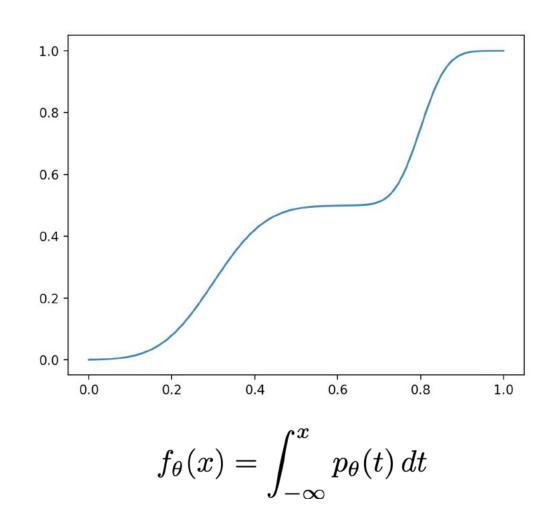
Sampling via inverse CDF

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]



How general are flows?

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

 \rightarrow can turn any (smooth) p(x) into any (smooth) p(z)

Lecture overview

- Foundations of Flows (1-D)
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2-D Autoregressive Flow

$$x_1 \to z_1 = f_{\theta}(x_1)$$
$$x_2 \to z_2 = f_{\phi}(x_1, x_2)$$

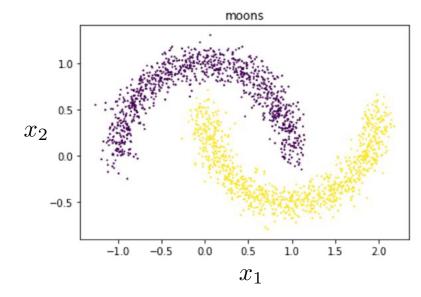
$$\max_{\theta,\phi} \sum_{i} \log p_{z_1}(f_{\theta}(x_1)) + \log \left| \frac{dz_1}{dx_1} \right| + \log p_{z_2}(f_{\phi}(x_1, x_2)) + \log \left| \frac{dz_2}{dx_2} \right|$$

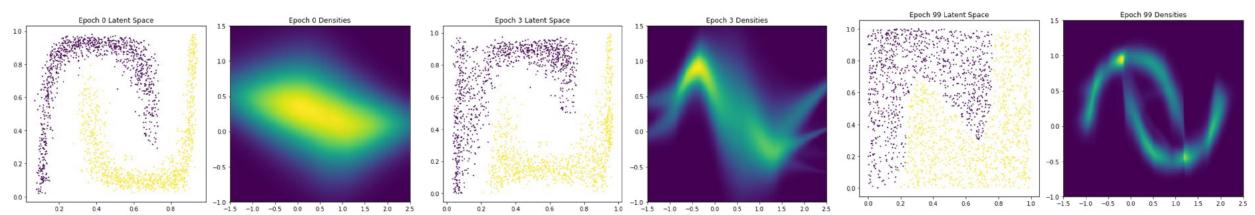
$$\frac{dz_1}{dx_1} = \frac{df_{\theta}(x_1)}{dx_1}, \frac{dz_2}{dx_2} = \frac{df_{\phi}(x_1, x_2)}{dx_2}$$

2-D Autoregressive Flow: Two Moons

Architecture:

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

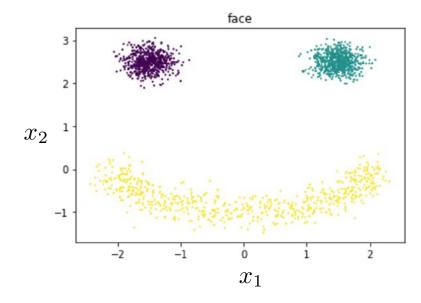


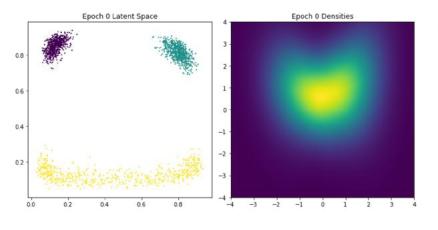


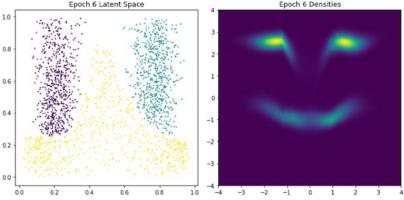
2-D Autoregressive Flow: Face

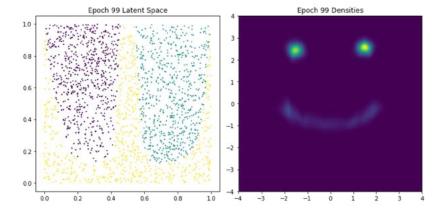
Architecture:

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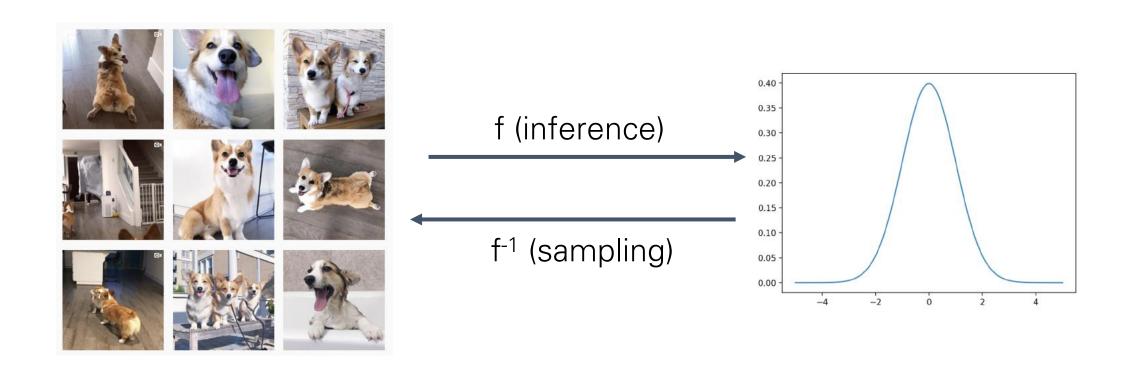




Lecture overview

- Foundations of Flows (1-D)
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High-dimensional data



x and z must have the same dimension

Lecture overview

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

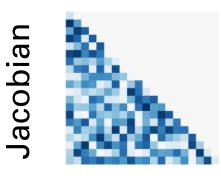
Architectural Taxonomy

Sparse connection

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

1. Autoregressive

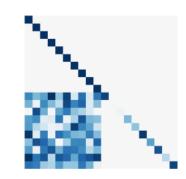
IAF/MAF/NAF SOS polynomial **UMNN**



(Lower triangular)

2. Block coupling

NICE/RealNVP/Glow Cubic Spline Flow Neural Spline Flow



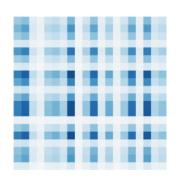
(Lower triangular + structured)

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)

Autoregressive flows

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

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

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

$$egin{align} z_1 &= f_{ heta}(x_1) & x_1 &= f_{ heta}^{-1}(z_1) \ z_2 &= f_{ heta}(x_2; x_1) & x_2 &= f_{ heta}^{-1}(z_2; x_1) \ z_3 &= f_{ heta}(x_3; x_1, x_2) & x_3 &= f_{ heta}^{-1}(z_3; x_1, x_2) \ \end{array}$$

Inverse autoregressive flows

- The inverse of an autoregressive flow is also a flow, called the inverse autoregressive flow (IAF)
 - $-x \rightarrow z$ has the same structure as the **sampling** in an autoregressive model
 - $-z \rightarrow x$ 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

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 previous lecture [e.g. RNN, masking]

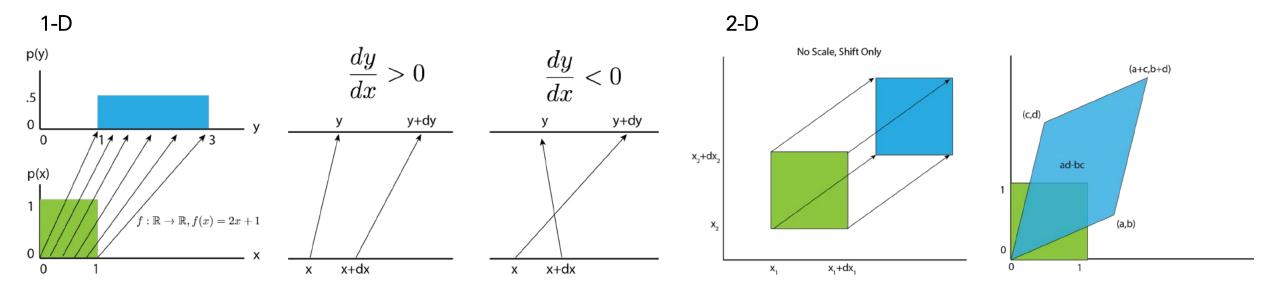
Lecture overview

- Foundations of Flows (1-D)
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Change of MANY variables

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

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



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:

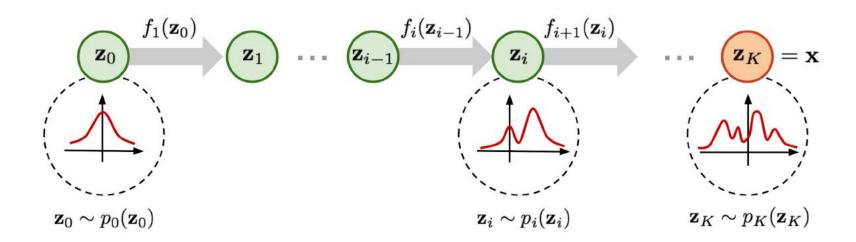
$$\arg\min_{\theta} \mathbb{E}_{\mathbf{x}} \left[-\log p_{\theta}(\mathbf{x}) \right] = \mathbb{E}_{\mathbf{x}} \left[-\log p(f_{\theta}(\mathbf{x})) - \log \det \left| \frac{\partial f_{\theta}(\mathbf{x})}{\partial \mathbf{x}} \right| \right]$$

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

Chaining Invertible Mappings (Composition)

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

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



$$rac{\partial f(x)}{\partial x} = rac{f_S(x_{S-1})}{\partial x_{S-1}} \cdots rac{f_2(x_1)}{\partial x_1} rac{f_1(x_0)}{\partial x_0} \qquad egin{matrix} x_s = f_s(x_{s-1}) \ x_0 = x \end{matrix}$$

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

Chain rule

Determinant of matrix product

Affine flows

- Another name for affine flow: multivariate Gaussian.
 - Parameters: an invertible matrix A and a vector b

$$-f(x) = A^{-1}(x-b)$$

- Sampling: x = Az + b , where $z \sim \mathcal{N}(0, I)$ $x \sim \mathcal{N}(b, AA^T)$
- Log likelihood is expensive when dimension is large.
 - The Jacobian of f is A^{-1}
 - Log likelihood involves calculating $\det(A)$

Elementwise flows

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

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

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

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

NICE/RealNVP

Affine coupling layer

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

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

- 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

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

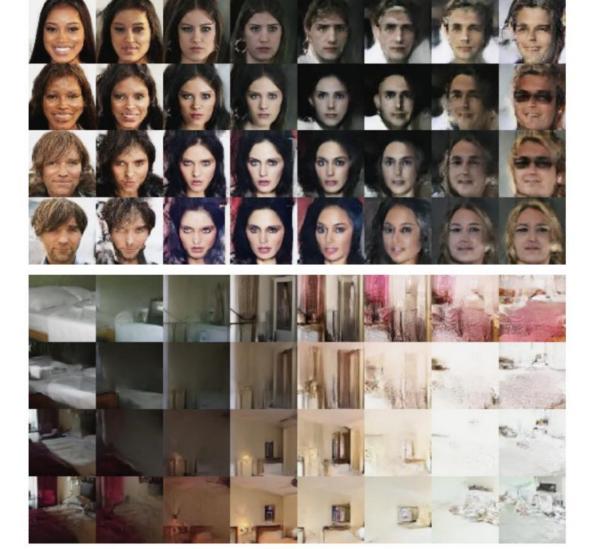
$$rac{\partial \mathbf{z}}{\partial \mathbf{x}} = egin{bmatrix} I & 0 \ rac{\partial \mathbf{z}_{d/2:d}}{\partial \mathbf{x}_{1:d/2}} & \mathrm{diag}(s_{ heta}(\mathbf{x}_{1:d/2})) \end{bmatrix}$$

• 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: 32×32×c image

- Layer 1: (Checkerboard ×3, channel squeeze, channel ×3)
 - Split result to get x_1 : $16\times16\times2c$ and z_1 : $16\times16\times2c$ (fine-grained latents)
- Layer 2: (Checkerboard ×3, channel squeeze, channel ×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 ×3, channel squeeze, channel ×3)
 - Get z_3 : $4\times4\times16c$ (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

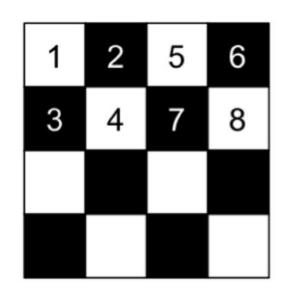
$$f(x) = b \odot x + (1 - b) \odot (x \odot \exp(s_{-}(b \odot x)) + m(b \odot x))$$

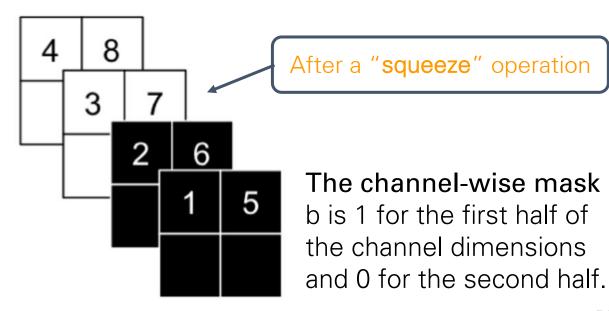
RealNVP: How to partition variables?

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

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

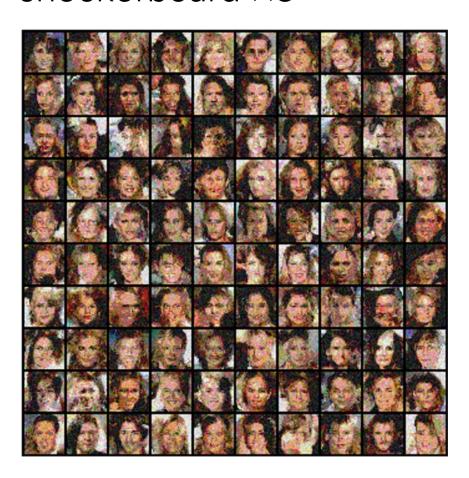
The spatial checkerboard pattern mask has value 1 where the sum of spatial coordinates is odd, and 0 otherwise.



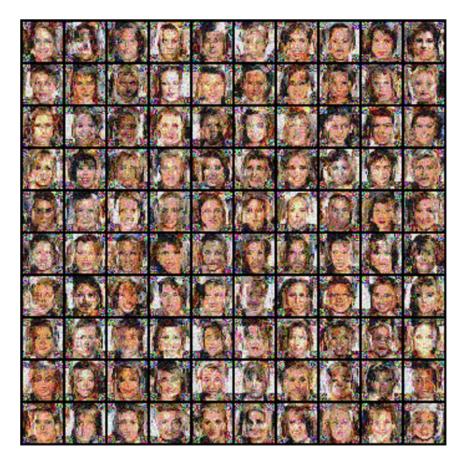


Good vs Bad Partitioning

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



(Mask top half; mask bottom half; mask left half; mask right half) ×2



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 - -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

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

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

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

- 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.

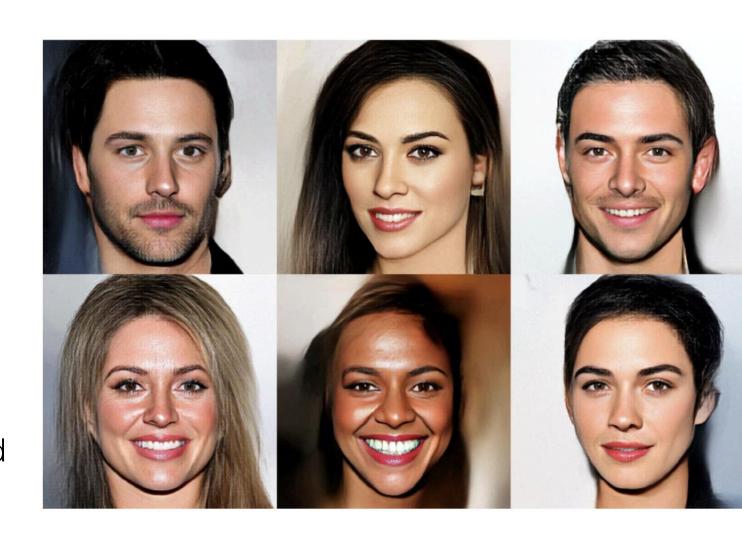
Table 2. CIFAR10 ablation results after 400 epochs of training. Models not converged for the purposes of ablation study.

Ablation	bits/dim	parameters
	2 202	22 21 5
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 (<u>link</u>)
 - Replacing permutation with 1x1 convolution (soft permutation)
 - Large-scale training

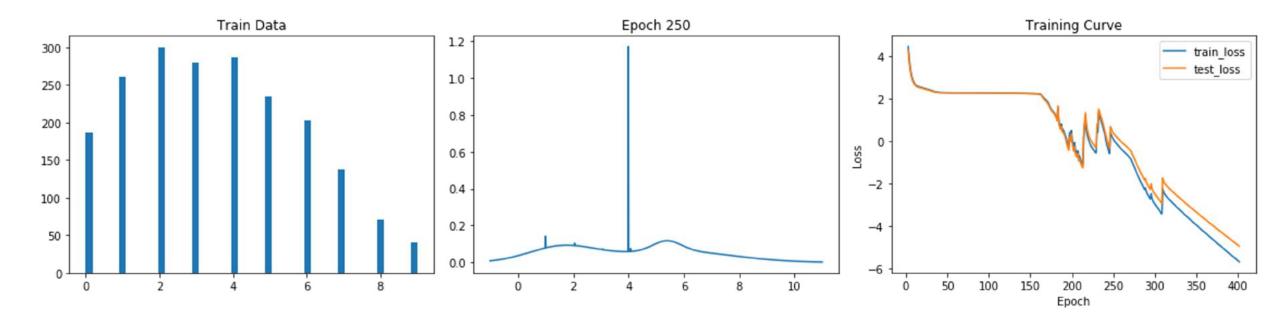
- Continuous time flows (FFJORD)
 - Allows for unrestricted architectures. Invertibility and fast log probability computation guaranteed.



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

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

Continuous flows for discrete data

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

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

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

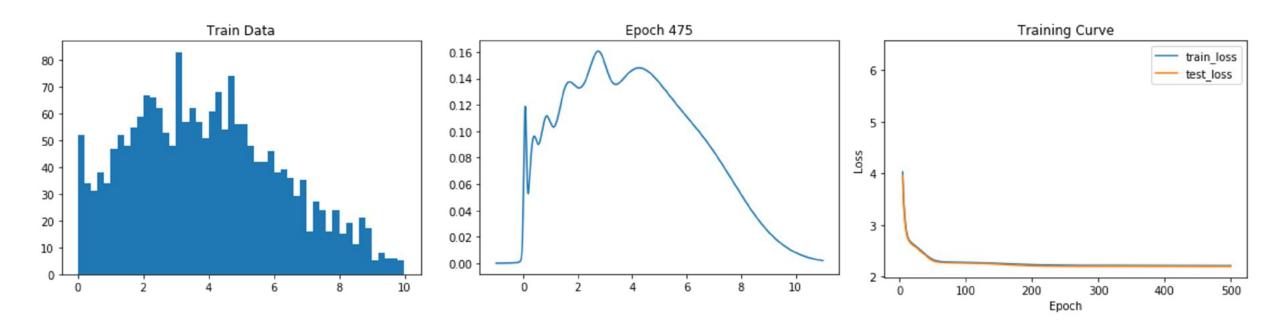
$$\mathbb{E}_{\mathbf{y} \sim p_{\text{data}}} \left[\log p_{\text{model}}(\mathbf{y}) \right] = \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \int_{[0,1)^D} \log p_{\text{model}}(\mathbf{x} + \mathbf{u}) d\mathbf{u}$$

$$\leq \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \log \int_{[0,1)^D} p_{\text{model}}(\mathbf{x} + \mathbf{u}) d\mathbf{u}$$

$$= \mathbb{E}_{\mathbf{x} \sim P_{\text{data}}} \left[\log P_{\text{model}}(\mathbf{x}) \right]$$

[Theis, Oord, Bethge, 2016]

Flow on Discrete Data With Dequantization



Applications

FloWaveNet

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

Yeven, Ceven Context Flow block $\exp(s)$ x M flows Change Order $s(x_{odd}, c_{odd})$ x N blocks Flow Affine Coupling $m(x_{odd}, c_{odd})$ Squeeze Non-causal ActNorm WaveNet Xodd, Codd x, cx, cXeven, Ceven

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



Yodd, Codd

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