

Deep Generative Models

Lecture 6

Roman Isachenko



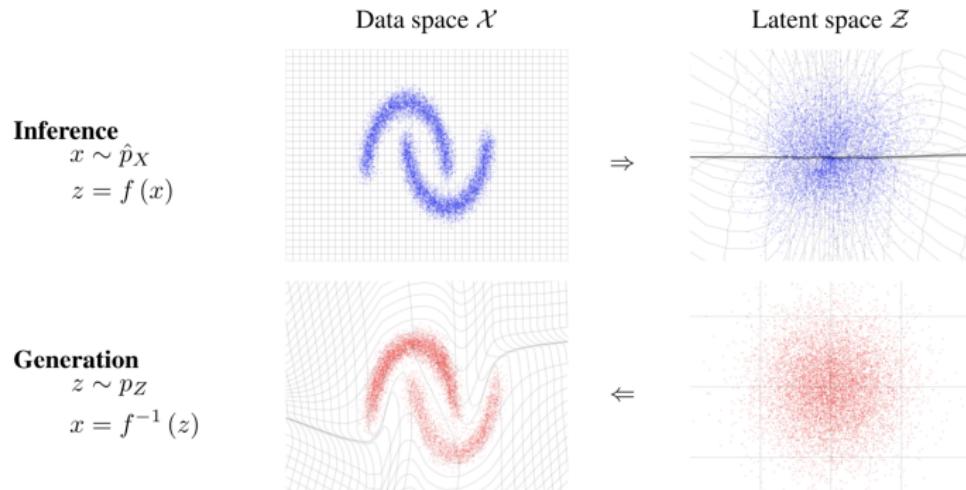
Autumn, 2022

Recap of previous lecture

MLE problem

$$p(\mathbf{x}|\boldsymbol{\theta}) = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x}, \boldsymbol{\theta})) \left| \det \left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right|$$

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f(\mathbf{x}, \boldsymbol{\theta})) + \log |\det(\mathbf{J}_f)| \rightarrow \max_{\boldsymbol{\theta}}$$



Recap of previous lecture

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f(\mathbf{x}, \boldsymbol{\theta})) + \log |\det(\mathbf{J}_f)| \rightarrow \max_{\boldsymbol{\theta}}$$

Definition

Normalizing flow is a *differentiable, invertible* mapping from data \mathbf{x} to the noise \mathbf{z} .

- ▶ **Normalizing** means that the inverse flow takes samples from $p(\mathbf{x})$ and normalizes them into samples from density $p(\mathbf{z})$.
- ▶ **Flow** refers to the trajectory followed by samples from $p(\mathbf{z})$ as they are transformed by the sequence of transformations

$$\mathbf{z} = f_K \circ \cdots \circ f_1(\mathbf{x}); \quad \mathbf{x} = f_1^{-1} \circ \cdots \circ f_K^{-1}(\mathbf{z}) = g_1 \circ \cdots \circ g_K(\mathbf{z})$$

Log likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f_K \circ \cdots \circ f_1(\mathbf{x})) + \sum_{k=1}^K \log |\det(\mathbf{J}_{f_k})|,$$

where $\mathbf{J}_{f_k} = \frac{\partial \mathbf{f}_k}{\partial \mathbf{f}_{k-1}}$.

Recap of previous lecture

Forward KL for flow model

$$\log p(\mathbf{x}|\theta) = \log p(f(\mathbf{x}, \theta)) + \log |\det(\mathbf{J}_f)|$$

Reverse KL for flow model

$$KL(p||\pi) = \mathbb{E}_{p(\mathbf{z})} [\log p(\mathbf{z}) - \log |\det(\mathbf{J}_g)| - \log \pi(g(\mathbf{z}, \theta))]$$

Flow KL duality

$$\arg \min_{\theta} KL(\pi(\mathbf{x})||p(\mathbf{x}|\theta)) = \arg \min_{\theta} KL(p(\mathbf{z}|\theta)||p(\mathbf{z})).$$

- ▶ $p(\mathbf{z})$ is a base distribution; $\pi(\mathbf{x})$ is a data distribution;
- ▶ $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} = g(\mathbf{z}, \theta)$, $\mathbf{x} \sim p(\mathbf{x}|\theta)$;
- ▶ $\mathbf{x} \sim \pi(\mathbf{x})$, $\mathbf{z} = f(\mathbf{x}, \theta)$, $\mathbf{z} \sim p(\mathbf{z}|\theta)$;

Recap of previous lecture

Flow log-likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f(\mathbf{x}, \boldsymbol{\theta})) + \log |\det(\mathbf{J}_f)|$$

The main challenge is a determinant of the Jacobian.

Residual flows: planar/Sylvester

$$g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{u} \sigma(\mathbf{w}^T \mathbf{z} + b); \quad g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{A} \sigma(\mathbf{B}\mathbf{z} + \mathbf{b}).$$

Matrix determinant lemma for calculating the Jacobian.

Linear flows

$$\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) = \mathbf{W}\mathbf{x}, \quad \mathbf{W} \in \mathbb{R}^{m \times m}, \quad \boldsymbol{\theta} = \mathbf{W}, \quad \mathbf{J}_f = \mathbf{W}$$

Matrix decompositions (LU or QR helps to parametrize matrix \mathbf{W} and reduce the cost of computing the $\det(\mathbf{J})$).

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Berg R. et al. Sylvester normalizing flows for variational inference, 2018

Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018

Recap of previous lecture

Gaussian autoregressive flow (MAF)

$$\mathbf{x} = g(\mathbf{z}, \theta) \Rightarrow x_i = \sigma_i(\mathbf{x}_{1:i-1}) \cdot z_i + \mu_i(\mathbf{x}_{1:i-1}).$$

$$\mathbf{z} = f(\mathbf{x}, \theta) \Rightarrow z_i = (x_i - \mu_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\sigma_i(\mathbf{x}_{1:i-1})}.$$

Generation function $g(\mathbf{z}, \theta)$ is **sequential**. Inference function $f(\mathbf{x}, \theta)$ is **not sequential**.

Inverse autoregressive flow (IAF)

$$\mathbf{x} = g(\mathbf{z}, \theta) \Rightarrow x_i = \tilde{\sigma}_i(\mathbf{z}_{1:i-1}) \cdot z_i + \tilde{\mu}_i(\mathbf{z}_{1:i-1})$$

$$\mathbf{z} = f(\mathbf{x}, \theta) \Rightarrow z_i = (x_i - \tilde{\mu}_i(\mathbf{z}_{1:i-1})) \cdot \frac{1}{\tilde{\sigma}_i(\mathbf{z}_{1:i-1})}.$$

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

Outline

1. Autoregressive flows
2. RealNVP: coupling layer
3. Discrete data vs continuous model
 - Discretization of continuous distribution
 - Dequantization

Outline

1. Autoregressive flows
2. RealNVP: coupling layer
3. Discrete data vs continuous model
 - Discretization of continuous distribution
 - Dequantization

Autoregressive flows

$$x_j = \tau(z_j, c(\mathbf{z}_{1:j-1})) \Leftrightarrow z_j = \tau^{-1}(x_j, c(\mathbf{z}_{1:j-1}))$$

- ▶ $\tau(\cdot, \cdot)$ – coupling law (invertible by first argument, differentiable).
- ▶ $c(\cdot)$ – coupling function (do not need to be invertible, could be neural network).

Coupling law $\tau(\cdot, \cdot)$

- ▶ $\tau(x, c) = x + c$ – additive;
- ▶ $\tau(x, c) = x \odot c_1 + c_2$ – affine.

What is the Jacobian for the additive/affine coupling law?

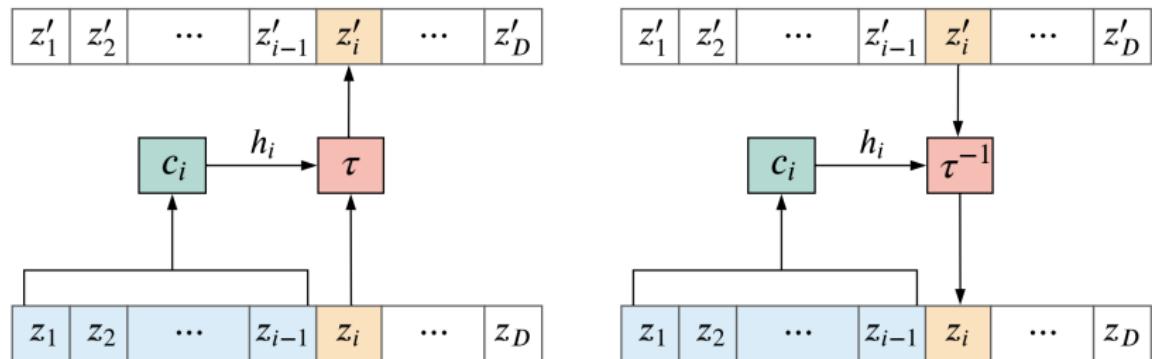
Jacobian

$$\det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) = \prod_{j=1}^m \frac{\partial x_j}{\partial z_j} = \prod_{j=1}^m \frac{\partial \tau(z_j, c(\mathbf{z}_{1:j-1}))}{\partial z_j}$$

Autoregressive flows

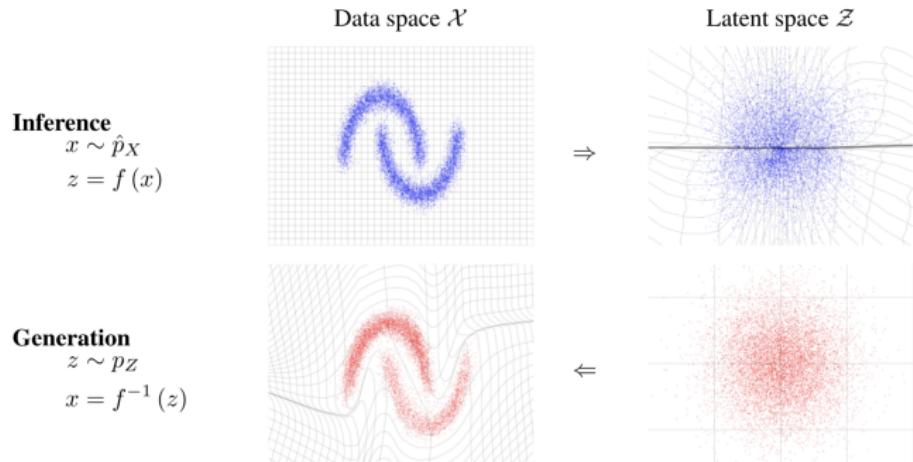
Forward and inverse transforms

$$x_j = \tau(z_j, c(\mathbf{z}_{1:j-1})) \Leftrightarrow z_j = \tau^{-1}(x_j, c(\mathbf{z}_{1:j-1}))$$



- ▶ Forward transform is **not sequential**.
- ▶ Inverse transform is **sequential**.

Autoregressive flows



- ▶ AF performs parallel inference that is useful for density estimation tasks (forward KL or MLE).
- ▶ IAF performs parallel generation that is useful for optimization of reverse KL.

Outline

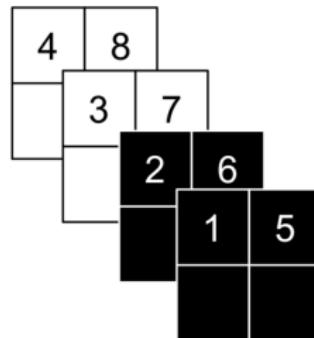
1. Autoregressive flows
2. RealNVP: coupling layer
3. Discrete data vs continuous model
 - Discretization of continuous distribution
 - Dequantization

RealNVP

Coupling layer

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \tau(\mathbf{x}_{d:m}, c(\mathbf{x}_{1:d})); \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \tau^{-1}(\mathbf{z}_{d:m}, c(\mathbf{z}_{1:d})). \end{cases}$$

Image partitioning



Checkerboard ordering uses masking, channelwise ordering uses splitting.

Affine coupling law

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \mathbf{x}_{d:m} \odot c_1(\mathbf{x}_{1:d}, \theta) + c_2(\mathbf{x}_{1:d}, \theta). \end{cases}$$

$$\begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = (\mathbf{z}_{d:m} - c_2(\mathbf{z}_{1:d}, \theta)) \cdot \frac{1}{c_1(\mathbf{z}_{1:d}, \theta)}. \end{cases}$$

Jacobian

$$\det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) = \det \begin{pmatrix} \mathbf{I}_d & 0_{d \times m-d} \\ \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{1:d}} & \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}} \end{pmatrix} = \prod_{j=1}^{m-d} c_1(\mathbf{x}_{1:d}, \theta)_j.$$

Non-Volume Preserving (the determinant of Jacobian $\neq 1$).

AF vs IAF vs RealINVP

MADE/AF

$$\mathbf{x} = \sigma(\mathbf{z}) \odot \mathbf{z} + \boldsymbol{\mu}(\mathbf{x}).$$

Estimating the density $p(\mathbf{x}|\theta)$ - 1 pass, sampling - m passes.

IAF

$$\mathbf{x} = \tilde{\sigma}(\mathbf{z}) \odot \mathbf{z} + \tilde{\boldsymbol{\mu}}(\mathbf{z}).$$

Estimating the density $p(\mathbf{x}|\theta)$ - m passes, sampling - 1 pass.

RealINVP

$$\begin{cases} \mathbf{x}_{1:d} &= \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} &= \mathbf{z}_{d:m} \odot c_1(\mathbf{z}_{1:d}, \theta) + c_2(\mathbf{z}_{1:d}, \theta). \end{cases}$$

Estimating the density $p(\mathbf{x}|\theta)$ - 1 pass, sampling - 1 pass.

AF vs IAF vs RealINVP

RealINVP

$$\begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \mathbf{z}_{d:m} \odot c_1(\mathbf{z}_{1:d}, \boldsymbol{\theta}) + c_2(\mathbf{z}_{1:d}, \boldsymbol{\theta}). \end{cases}$$

- ▶ Calculating the density $p(\mathbf{x}|\boldsymbol{\theta})$ - 1 pass.
- ▶ Sampling - 1 pass.

RealINVP is a special case of AF and IAF:

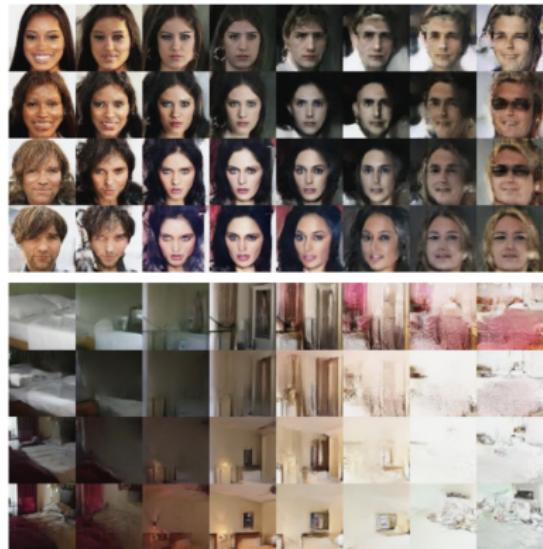
AF

$$\begin{cases} \mu_j = 0, \sigma_j = 1, j = 1, \dots, d; \\ \mu_j, \sigma_j - \text{functions of } \mathbf{x}_{1:d}, j = d + 1, \dots, m. \end{cases}$$

IAF

$$\begin{cases} \tilde{\mu}_j = 0, \tilde{\sigma}_j = 1, j = 1, \dots, d; \\ \tilde{\mu}_j, \tilde{\sigma}_j - \text{functions of } \mathbf{z}_{1:d}, j = d + 1, \dots, m. \end{cases}$$

RealNVP samples



Linear flows

RealNVP

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \tau(\mathbf{x}_{d:m}, c(\mathbf{x}_{1:d})); \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \tau^{-1}(\mathbf{z}_{d:m}, c(\mathbf{z}_{1:d})). \end{cases}$$

- ▶ First step is a **split** operator which decouples a variable into 2 subparts: \mathbf{x}_1 and \mathbf{x}_2 (usually channel-wise).
- ▶ We should **permute** components between different layers.

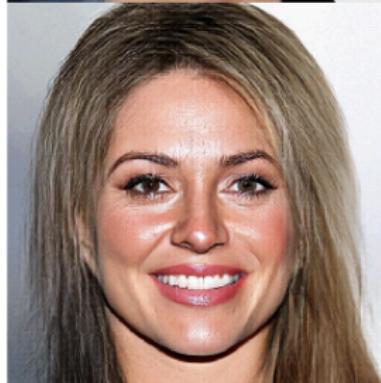
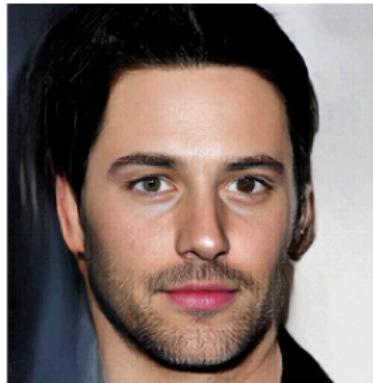
$$\mathbf{z} = \mathbf{W}\mathbf{x}, \quad \mathbf{W} \in \mathbb{R}^{m \times m}$$

In general, we need $O(m^3)$ to invert matrix.

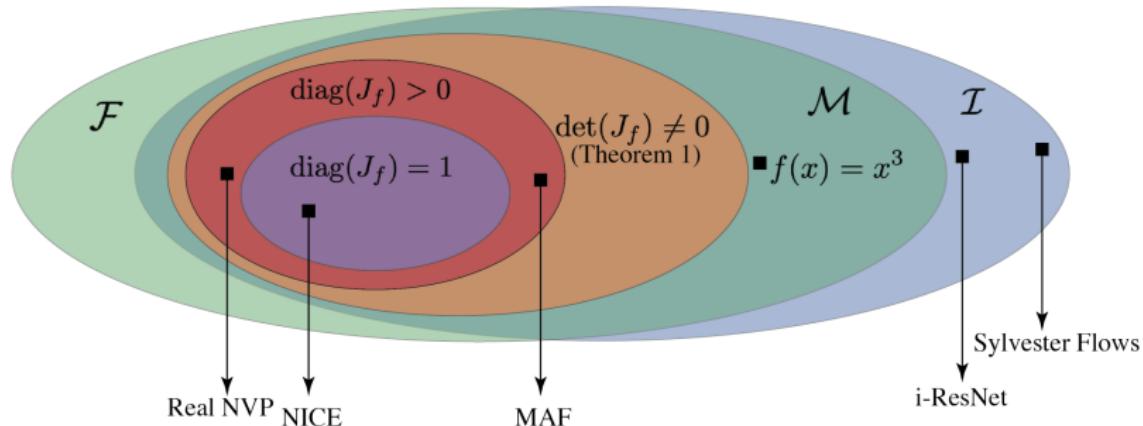
Invertibility

- ▶ Diagonal matrix $O(m)$.
- ▶ Triangular matrix $O(m^2)$.
- ▶ It is impossible to parametrize all invertible matrices.

Glow samples



Venn diagram for Normalizing flows



- ▶ \mathcal{I} – invertible functions.
- ▶ \mathcal{F} – continuously differentiable functions whose Jacobian is lower triangular.
- ▶ \mathcal{M} – invertible functions from \mathcal{F} .

Outline

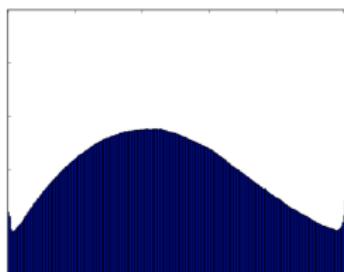
1. Autoregressive flows
2. RealNVP: coupling layer
3. Discrete data vs continuous model
 - Discretization of continuous distribution
 - Dequantization

Outline

1. Autoregressive flows
2. RealNVP: coupling layer
3. Discrete data vs continuous model
 - Discretization of continuous distribution
 - Dequantization

PixelCNN++

CIFAR-10 pixel values distribution



- ▶ Standard PixelCNN outputs softmax probabilities for values $\{0, 255\}$ (256 outputs feature maps).
- ▶ Categorical distribution do not know anything about numerical relationships (220 is close to 221 and far from 15).
- ▶ If pixel value is not presented in the training dataset, it won't be predicted.
- ▶ (Look at the edges of the distributions: they have higher probability mass).

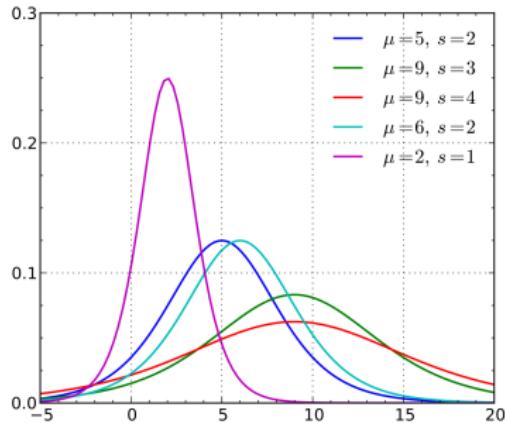
Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

PixelCNN++

Mixture of logistic distributions

$$p(x|\mu, s) = \frac{\exp^{-(x-\mu)/s}}{s(1 + \exp^{-(x-\mu)/s})^2};$$

$$p(x|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi}) = \sum_{k=1}^K \pi_k p(x|\mu_k, s_k);$$



To adopt probability calculation to discrete values:

$$P_d(x|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi}) = P(x + 0.5|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi}) - P(x - 0.5|\boldsymbol{\mu}, \mathbf{s}, \boldsymbol{\pi})$$

For the edge case of 0, replace $x - 0.5$ by $-\infty$, and for 255 replace $x + 0.5$ by $+\infty$.

Outline

1. Autoregressive flows
2. RealNVP: coupling layer
3. Discrete data vs continuous model
 - Discretization of continuous distribution
 - Dequantization

Dequantization

- ▶ Images are discrete data, pixels lie in the $\{0, 255\}$ integer domain (the model is $P(\mathbf{x}|\theta) = \text{Categorical}(\pi(\theta))$).
- ▶ Flow is a continuous model (it works with continuous data \mathbf{x}).

By fitting a continuous density model to discrete data, one can produce a degenerate solution with all probability mass on discrete values.

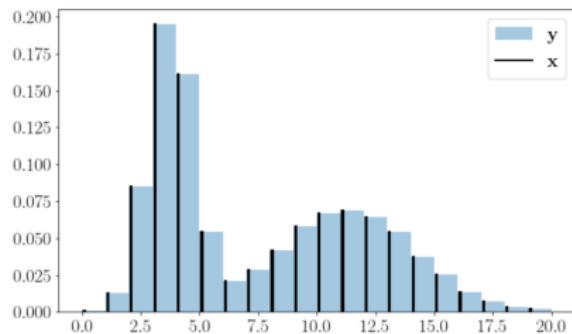
How to convert a discrete data distribution to a continuous one?

Uniform dequantization

$$\mathbf{x} \sim \text{Categorical}(\boldsymbol{\pi})$$

$$\mathbf{u} \sim U[0, 1]$$

$$\mathbf{y} = \mathbf{x} + \mathbf{u} \sim \text{Continuous}$$



Uniform dequantization

Theorem

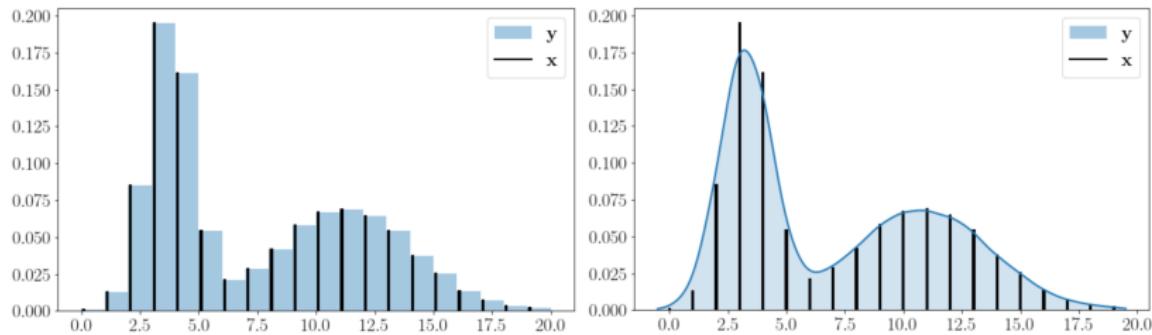
Fitting continuous model $p(\mathbf{y}|\theta)$ on uniformly dequantized data $\mathbf{y} = \mathbf{x} + \mathbf{u}$, $\mathbf{u} \sim U[0, 1]$ is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

$$P(\mathbf{x}|\theta) = \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\theta) d\mathbf{u}$$

Proof

$$\begin{aligned}\mathbb{E}_\pi \log p(\mathbf{y}|\theta) &= \int \pi(\mathbf{y}) \log p(\mathbf{y}|\theta) d\mathbf{y} = \\ &= \sum \pi(\mathbf{x}) \int_{U[0,1]} \log p(\mathbf{x} + \mathbf{u}|\theta) d\mathbf{u} \leq \\ &\leq \sum \pi(\mathbf{x}) \log \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\theta) d\mathbf{u} = \\ &= \sum \pi(\mathbf{x}) \log P(\mathbf{x}|\theta) = \mathbb{E}_\pi \log P(\mathbf{x}|\theta).\end{aligned}$$

Variational dequantization



- ▶ $p(y|\theta)$ assign uniform density to unit hypercubes $x + U[0, 1]$ (left fig).
- ▶ Neural network density models are smooth function approximators (right fig).
- ▶ Smooth dequantization is more natural.

How to perform the smooth dequantization?

Flow++

Variational dequantization

Introduce variational dequantization noise distribution $q(\mathbf{u}|\mathbf{x})$ and treat it as an approximate posterior.

Variational lower bound

$$\begin{aligned}\log P(\mathbf{x}|\theta) &= \left[\log \int q(\mathbf{u}|\mathbf{x}) \frac{p(\mathbf{x} + \mathbf{u}|\theta)}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} \right] \geq \\ &\geq \int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x} + \mathbf{u}|\theta)}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} = \mathcal{L}(q, \theta).\end{aligned}$$

Uniform dequantization bound

$$\log P(\mathbf{x}|\theta) = \log \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\theta) d\mathbf{u} \geq \int_{U[0,1]} \log p(\mathbf{x} + \mathbf{u}|\theta) d\mathbf{u}.$$

Uniform dequantization is a special case of variational dequantization ($q(\mathbf{u}|\mathbf{x}) = U[0, 1]$).

Flow++

Variational lower bound

$$\mathcal{L}(q, \theta) = \int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x} + \mathbf{u}|\theta)}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u}.$$

Let $\mathbf{u} = g(\epsilon, \mathbf{x}, \lambda)$ is a flow model with base distribution $\epsilon \sim p(\epsilon) = \mathcal{N}(0, \mathbf{I})$:

$$q(\mathbf{u}|\mathbf{x}) = p(g^{-1}(\mathbf{u}, \mathbf{x}, \lambda)) \cdot \left| \det \frac{\partial g^{-1}(\mathbf{u}, \mathbf{x}, \lambda)}{\partial \mathbf{u}} \right|.$$

Flow-based variational dequantization

$$\log P(\mathbf{x}|\theta) \geq \mathcal{L}(\lambda, \theta) = \int p(\epsilon) \log \left(\frac{p(\mathbf{x} + g(\epsilon, \mathbf{x}, \lambda)|\theta)}{p(\epsilon) \cdot |\det \mathbf{J}_g|^{-1}} \right) d\epsilon.$$

If $p(\mathbf{x} + \mathbf{u}|\theta)$ is also a flow model, it is straightforward to calculate stochastic gradient of this ELBO.

Flow-based variational dequantization

$$\log P(\mathbf{x}|\theta) \geq \int p(\epsilon) \log \left(\frac{p(\mathbf{x} + g(\epsilon, \mathbf{x}, \lambda))}{p(\epsilon) \cdot |\det \mathbf{J}_g|^{-1}} \right) d\epsilon.$$

Table 1. Unconditional image modeling results in bits/dim

Model family	Model	CIFAR10	ImageNet 32x32	ImageNet 64x64
Non-autoregressive	RealNVP (Dinh et al., 2016)	3.49	4.28	—
	Glow (Kingma & Dhariwal, 2018)	3.35	4.09	3.81
	IAF-VAE (Kingma et al., 2016)	3.11	—	—
	Flow++ (ours)	3.08	3.86	3.69
Autoregressive	Multiscale PixelCNN (Reed et al., 2017)	—	3.95	3.70
	PixelCNN (van den Oord et al., 2016b)	3.14	—	—
	PixelRNN (van den Oord et al., 2016b)	3.00	3.86	3.63
	Gated PixelCNN (van den Oord et al., 2016c)	3.03	3.83	3.57
	PixelCNN++ (Salimans et al., 2017)	2.92	—	—
	Image Transformer (Parmar et al., 2018)	2.90	3.77	—
	PixelSNAIL (Chen et al., 2017)	2.85	3.80	3.52

Summary

- ▶ AF/IAF is a special case of autoregressive flows.
- ▶ The RealINVP is an effective type of flow (special case of AR flows) that uses coupling layer.
- ▶ Dequantization allows to fit discrete data using continuous model.
- ▶ Uniform dequantization is the simplest form of dequantization. Variational dequantization is a more natural type that was proposed in Flow++ model.