Deep Generative Models

Lecture 5

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2023, Autumn

Recap of previous lecture

Jacobian matrix

Let $f : \mathbb{R}^m \to \mathbb{R}^m$ be a differentiable function.

$$\mathbf{z} = f(\mathbf{x}), \quad \mathbf{J} = \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \dots & \frac{\partial z_1}{\partial x_m} \\ \dots & \dots & \dots \\ \frac{\partial z_m}{\partial x_1} & \dots & \frac{\partial z_m}{\partial x_m} \end{pmatrix} \in \mathbb{R}^{m \times m}$$

Change of variable theorem (CoV)

Let $\mathbf{x}$ be a random variable with density function $p(\mathbf{x})$ and $f : \mathbb{R}^m \to \mathbb{R}^m$ is a differentiable, invertible function (diffeomorphism). If $\mathbf{z} = f(\mathbf{x})$, $\mathbf{x} = f^{-1}(\mathbf{z}) = g(\mathbf{z})$, then

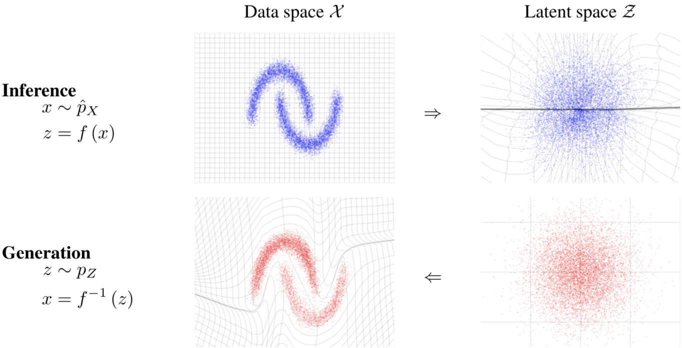
$$p(\mathbf{x}) = p(\mathbf{z})|\det(\mathbf{J}_f)| = p(\mathbf{z}) \left|\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right)\right| = p(f(\mathbf{x})) \left|\det\left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

$$p(\mathbf{z}) = p(\mathbf{x})|\det(\mathbf{J}_g)| = p(\mathbf{x}) \left|\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}}\right)\right| = p(g(\mathbf{z})) \left|\det\left(\frac{\partial g(\mathbf{z})}{\partial \mathbf{z}}\right)\right|.$$

Recap of previous lecture

Definition

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



Log likelihood

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

Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

Recap of previous lecture

Forward KL for flow model

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

Reverse KL for flow model

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

Flow KL duality

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

- $p(\mathbf{z})$ is a base distribution; $\pi(\mathbf{x})$ is a data distribution;
- $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z})$, $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$;
- $\mathbf{x} \sim \pi(\mathbf{x})$, $\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x})$, $\mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta})$.

Papamakarios G. et al. Normalizing flows for probabilistic modeling and inference, 2019

Recap of previous lecture

Flow log-likelihood

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

The main challenge is a determinant of the Jacobian.

Linear flows

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

- LU-decomposition
$$\mathbf{W} = \mathbf{P}\mathbf{L}\mathbf{U}.$$
- QR-decomposition
$$\mathbf{W} = \mathbf{Q}\mathbf{R}.$$

Decomposition should be done only once in the beggining. Next, we fit decomposed matrices ($\mathbf{P}/\mathbf{L}/\mathbf{U}$ or $\mathbf{Q}/\mathbf{R}$).

Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018
Hoogeboom E., et al. Emerging convolutions for generative normalizing flows, 2019

Recap of previous lecture

Consider an autoregressive model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}), \quad p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}) = \mathcal{N}\left(\mu_j(\mathbf{x}_{1:j-1}), \sigma_j^2(\mathbf{x}_{1:j-1})\right).$$

Gaussian autoregressive NF

$$\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x}) \quad \Rightarrow \quad z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}.$$

- We have an **invertible** and **differentiable** transformation from $p(\mathbf{z})$ to $p(\mathbf{x}|\boldsymbol{\theta})$.
- Jacobian of such transformation is triangular!

Generation function $g_{\boldsymbol{\theta}}(\mathbf{z})$ is **sequential**.
Inference function $f_{\boldsymbol{\theta}}(\mathbf{x})$ is **not sequential**.

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

Gaussian autoregressive NF

$$\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x}) \quad \Rightarrow \quad z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}.$$

- Sampling is sequential, density estimation is parallel.
- Forward KL is a natural loss.

Forward transform: $f_{\boldsymbol{\theta}}(\mathbf{x})$

$$z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}$$

Inverse transform: $g_{\boldsymbol{\theta}}(\mathbf{z})$

$$x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1})$$

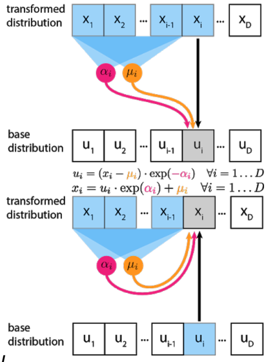


image credit: https://blog.evjang.com/2018/01/nf2.html

Outline

1. RealNVP: coupling layer
2. Normalizing flows as VAE model
3. Discrete data vs continuous model
   - Discretization of continuous distribution
   - Dequantization of discrete data

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RealNVP

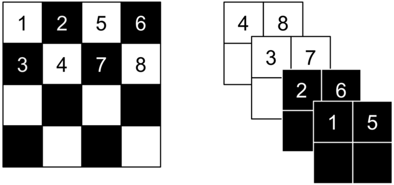
Let split $\mathbf{x}$ and $\mathbf{z}$ in two parts:

$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}].$$

Coupling layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}_1) + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}_1). \end{cases} \qquad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_1)) \odot \frac{1}{\boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{x}_1)}. \end{cases}$$

Image partitioning



- Checkerboard ordering uses masking.
- Channelwise ordering uses splitting.

Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

RealNVP

Coupling layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}_1) + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}_1). \end{cases} \quad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_1)) \odot \frac{1}{\boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{x}_1)}. \end{cases}$$

Estimating the density takes 1 pass, sampling takes 1 pass!

Jacobian

$$\det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) = \det \begin{pmatrix} \mathbf{I}_d & 0_{d \times m-d} \\ \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_1} & \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_2} \end{pmatrix} = \prod_{j=1}^{m-d} \frac{1}{\sigma_j(\mathbf{x}_1)}.$$

Gaussian AR NF

$$\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x}) \quad \Rightarrow \quad z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}.$$

How to get RealNVP coupling layer from gaussian AR NF?

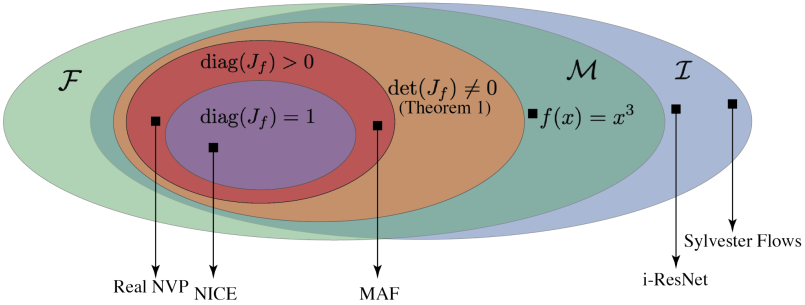
Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

Glow samples

Glow model: coupling layer + linear flows (1x1 convs)

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

Venn diagram for Normalizing flows



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

Song Y., Meng C., Ermon S. Mintnet: Building invertible neural networks with masked convolutions, 2019

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VAE vs Normalizing flows

	VAE	**NF**
Objective	ELBO $\mathcal{L}$	Forward KL/MLE
Encoder	stochastic $\mathbf{z} \sim q(\mathbf{z}\|\mathbf{x}, \boldsymbol{\phi})$	deterministic $\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x})$ $q(\mathbf{z}\|\mathbf{x}, \boldsymbol{\theta}) = \delta(\mathbf{z} - f_{\boldsymbol{\theta}}(\mathbf{x}))$
Decoder	stochastic $\mathbf{x} \sim p(\mathbf{x}\|\mathbf{z}, \boldsymbol{\theta})$	deterministic $\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z})$ $p(\mathbf{x}\|\mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - g_{\boldsymbol{\theta}}(\mathbf{z}))$
Parameters	$\boldsymbol{\phi}, \boldsymbol{\theta}$	$\boldsymbol{\theta} \equiv \boldsymbol{\phi}$

Theorem

MLE for normalizing flow is equivalent to maximization of ELBO for VAE model with deterministic encoder and decoder:

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - f^{-1}(\mathbf{z}, \boldsymbol{\theta})) = \delta(\mathbf{x} - g_{\boldsymbol{\theta}}(\mathbf{z}));$$

$$q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) = \delta(\mathbf{z} - f_{\boldsymbol{\theta}}(\mathbf{x})).$$

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows, 2020

Normalizing flow as VAE

Proof

1. Dirac delta function property

$$\mathbb{E}_{\delta(\mathbf{x}-\mathbf{y})} f(\mathbf{x}) = \int \delta(\mathbf{x}-\mathbf{y}) f(\mathbf{x}) d\mathbf{x} = f(\mathbf{y}).$$

2. CoV theorem and Bayes theorem:

$$p(\mathbf{x}|\boldsymbol{\theta}) = p(\mathbf{z})|\det(\mathbf{J}_f)|;$$

$$p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) = \frac{p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z})}{p(\mathbf{x}|\boldsymbol{\theta})}; \quad \Rightarrow \quad p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})|\det(\mathbf{J}_f)|.$$

3. Log-likelihood decomposition

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\theta}) + KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) = \mathcal{L}(\boldsymbol{\theta}).$$

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows, 2020

Normalizing flow as VAE

Proof

ELBO objective:

$$\mathcal{L} = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \left[\log p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta}) - \log \frac{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})}{p(\mathbf{z})} \right]$$
$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \left[\log \frac{p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} + \log p(\mathbf{z}) \right].$$

1. Dirac delta function property:
$$\mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \log p(\mathbf{z}) = \int \delta(\mathbf{z} - f_{\boldsymbol{\theta}}(\mathbf{x})) \log p(\mathbf{z}) d\mathbf{z} = \log p(f_{\boldsymbol{\theta}}(\mathbf{x})).$$
2. CoV theorem and Bayes theorem:
$$\mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \log \frac{p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \log \frac{p(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})|\det(\mathbf{J}_f)|}{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} = \log|\det \mathbf{J}_f|.$$
3. Log-likelihood decomposition
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\theta}) = \log p(f_{\boldsymbol{\theta}}(\mathbf{x})) + \log|\det \mathbf{J}_f|.$$

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows, 2020

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Discrete data vs continuous model

Let our data $\mathbf{y}$ comes from discrete distribution $\Pi(\mathbf{y})$ and we have continuous model $p(\mathbf{x}|\boldsymbol{\theta}) = \text{NN}(\mathbf{x}, \boldsymbol{\theta})$.

- Images (and not only images) are discrete data, pixels lie in the integer domain ($\{0, 255\}$).
- By fitting a continuous density model $p(\mathbf{x}|\boldsymbol{\theta})$ to discrete data $\Pi(\mathbf{y})$, one can produce a degenerate solution with all probability mass on discrete values.

Discrete model

- Use **discrete** model (e.x. $P(\mathbf{y}|\boldsymbol{\theta}) = \text{Cat}(\boldsymbol{\pi}(\boldsymbol{\theta}))$).
- Minimize any suitable divergence measure $D(\Pi, P)$.
- NF works only with continuous data $\mathbf{x}$ (there are discrete NF, see papers below).
- If pixel value is not presented in the train data, it won't be predicted.

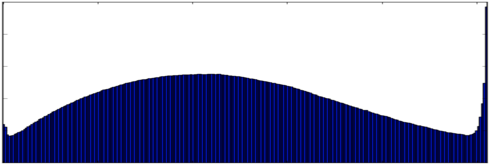
Hoogeboom E. et al. Integer discrete flows and lossless compression, 2019
Tran D. et al. Discrete flows: Invertible generative models of discrete data, 2019

Discrete data vs continuous model

Continuous model

- Use **continuous** model (e.x. $p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{x}))$), but
  - **discretize** model (make the model outputs discrete): transform $p(\mathbf{x}|\boldsymbol{\theta})$ to $P(\mathbf{y}|\boldsymbol{\theta})$;
  - **dequantize** data (make the data continuous): transform $\Pi(\mathbf{y})$ to $\pi(\mathbf{x})$.
- Continuous distribution knows numerical relationships.

CIFAR-10 pixel values distribution



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

Outline

Discretization of continuous distribution

Model discretization through CDF

$$F(\mathbf{x}|\boldsymbol{\theta}) = \int_{-\infty}^{\mathbf{x}} p(\mathbf{x}'|\boldsymbol{\theta}) d\mathbf{x}'; \quad P(\mathbf{y}|\boldsymbol{\theta}) = F(\mathbf{y} + 0.5|\boldsymbol{\theta}) - F(\mathbf{y} - 0.5|\boldsymbol{\theta})$$

Mixture of logistic distributions

$$p(x|\mu, s) = \frac{\exp^{-(x-\mu)/s}}{s(1 + \exp^{-(x-\mu)/s})^2}; \quad p(x|\boldsymbol{\pi}, \boldsymbol{\mu}, \mathbf{s}) = \sum_{k=1}^{K} \pi_k p(x|\mu_k, s_k).$$

PixelCNN++

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}); \quad p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k p(x|\mu_k, s_k).$$

Here, $\pi_k = \pi_{k,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})$, $\mu_k = \mu_{k,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})$, $s_k = s_{k,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})$.

For the pixel edge cases of 0, replace $y - 0.5$ by $-\infty$, and for 255 replace $y + 0.5$ by $+\infty$.

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

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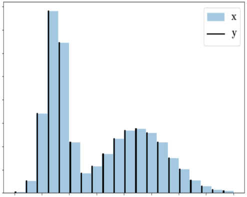
Uniform dequantization

Let dequantize discrete distribution $\Pi(\mathbf{y})$ to continuous distribution $\pi(\mathbf{x})$ in the following way: $\mathbf{x} = \mathbf{y} + \mathbf{u}$, where $\mathbf{u} \sim U[0, 1]$.

Theorem

Fitting continuous model $p(\mathbf{x}|\boldsymbol{\theta})$ on uniformly dequantized data is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

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



Proof

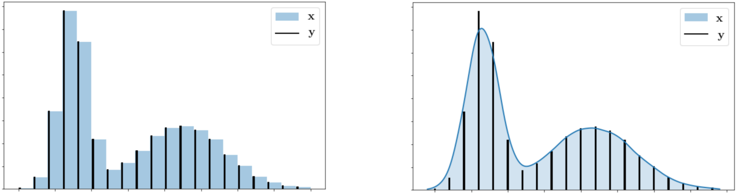
$$\mathbb{E}_\pi \log p(\mathbf{x}|\boldsymbol{\theta}) = \int \pi(\mathbf{x}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{x} = \sum \Pi(\mathbf{y}) \int_{U[0,1]} \log p(\mathbf{y}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \leq$$

$$\leq \sum \Pi(\mathbf{y}) \log \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} =$$

$$= \sum \Pi(\mathbf{y}) \log P(\mathbf{y}|\boldsymbol{\theta}) = \mathbb{E}_\Pi \log P(\mathbf{y}|\boldsymbol{\theta}).$$

Theis L., Oord A., Bethge M. A note on the evaluation of generative models. 2015

Variational dequantization



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

Introduce variational dequantization noise distribution $q(\mathbf{u}|\mathbf{y})$, which tells what kind of noise we have to add to our discrete data. Treat it as an approximate posterior as in VAE model.

Variational dequantization

Variational lower bound

$$\log P(\mathbf{y}|\boldsymbol{\theta}) = \left[\log \int q(\mathbf{u}|\mathbf{y}) \frac{p(\mathbf{y}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{y})} d\mathbf{u}\right] \geq$$

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

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

Flow++: flow-based variational dequantization

Let $\mathbf{u} = g_{\boldsymbol{\lambda}}(\boldsymbol{\epsilon}, \mathbf{y})$ is a flow model with base distribution $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$:

$$q(\mathbf{u}|\mathbf{y}) = p(f_{\boldsymbol{\lambda}}(\mathbf{u}, \mathbf{y})) \cdot \left|\det \frac{\partial f_{\boldsymbol{\lambda}}(\mathbf{u}, \mathbf{y})}{\partial \mathbf{u}}\right|.$$

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

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

Summary

- Gaussian autoregressive flow is an autoregressive model with triangular Jacobian. It has fast inference function and slow generation function. Forward KL is a natural loss function.
- The RealNVP coupling layer is an effective type of flow (special case of AR flows) that has fast inference and generation modes.
- NF models could be treated as VAE model with deterministic encoder and decoder.
- Lots of data are discrete. We able to discretize the model or to dequantize our data to use continuous model.
- Uniform dequantization is the simplest form of dequantization. Variational dequantization is a more natural type that uses variational inference.