

Deep Generative Models

Lecture 2

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Recap of Previous Lecture

We're given i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^m$ drawn from some unknown distribution $\pi(\mathbf{x})$.

Objective

Our goal is to learn the distribution $\pi(\mathbf{x})$ so that we can:

- ▶ Evaluate $\pi(\mathbf{x})$ for new samples;
- ▶ Sample from $\pi(\mathbf{x})$ (i.e., generate novel samples $\mathbf{x} \sim \pi(\mathbf{x})$).

Rather than considering all possible probability distributions, we approximate $\pi(\mathbf{x})$ by a parameterized family $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

Divergence Minimization Task

- ▶ $D(\pi\|p) \geq 0$ for all $\pi, p \in \mathcal{P}$;
- ▶ $D(\pi\|p) = 0$ if and only if $\pi \equiv p$.

$$\min_{\boldsymbol{\theta}} D(\pi\|p)$$

Recap of Previous Lecture

Forward KL Divergence

$$\text{KL}(\pi \| p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\theta)} d\mathbf{x} \rightarrow \min_{\theta}$$

Reverse KL Divergence

$$\text{KL}(p \| \pi) = \int p(\mathbf{x}|\theta) \log \frac{p(\mathbf{x}|\theta)}{\pi(\mathbf{x})} d\mathbf{x} \rightarrow \min_{\theta}$$

Maximum Likelihood Estimation (MLE)

$$\theta^* = \arg \max_{\theta} \prod_{i=1}^n p(\mathbf{x}_i|\theta) = \arg \max_{\theta} \sum_{i=1}^n \log p(\mathbf{x}_i|\theta)$$

Maximum likelihood estimation is equivalent to minimizing the Monte Carlo estimate of the forward KL divergence.

Recap of Previous Lecture

Likelihood as Product of Conditionals

Let $\mathbf{x} = (x_1, \dots, x_m)$, and define $\mathbf{x}_{1:j} = (x_1, \dots, x_j)$. Then,

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^m p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}), \quad \log p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{j=1}^m \log p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$$

MLE for Autoregressive Models

$$\boldsymbol{\theta}^* = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^n \sum_{j=1}^m \log p(x_{ij}|\mathbf{x}_{i,1:j-1}, \boldsymbol{\theta})$$

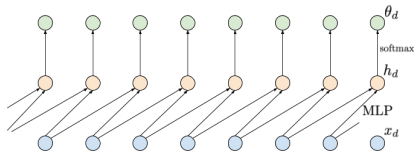
Sampling

$$\hat{x}_1 \sim p(x_1|\boldsymbol{\theta}), \quad \hat{x}_2 \sim p(x_2|\hat{x}_1, \boldsymbol{\theta}), \quad \dots, \quad \hat{x}_m \sim p(x_m|\hat{\mathbf{x}}_{1:m-1}, \boldsymbol{\theta})$$

The generated sample is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m)$.

Recap of Previous Lecture

Autoregressive MLP



Autoregressive Transformer

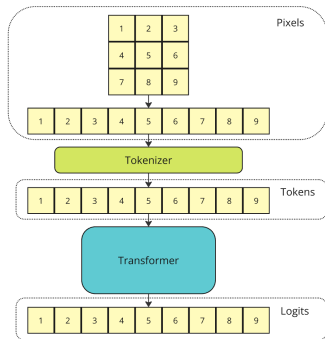
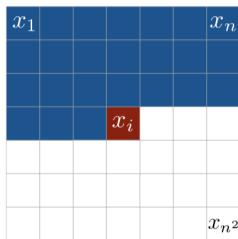


Image credit: https://jmtomczak.github.io/blog/2/2_ARM.html
Chen M. et al. Generative Pretraining from Pixels, 2020

Outline

1. Normalizing Flows (NF)

2. NF Examples

- Linear Normalizing Flows

- Gaussian Autoregressive NF

- Coupling Layer (RealNVP)

Outline

1. Normalizing Flows (NF)

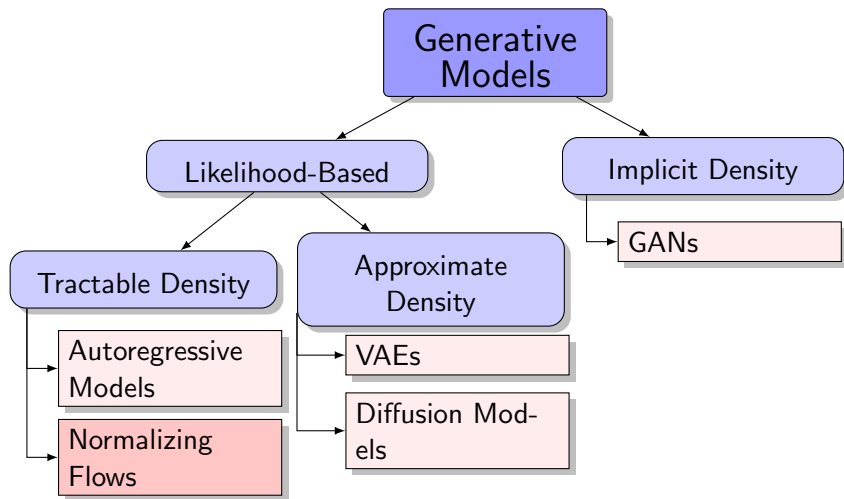
2. NF Examples

Linear Normalizing Flows

Gaussian Autoregressive NF

Coupling Layer (RealNVP)

Generative Models Zoo



Normalizing Flows: Prerequisites

Jacobian Matrix

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

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

Change of Variables Theorem (CoV)

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

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

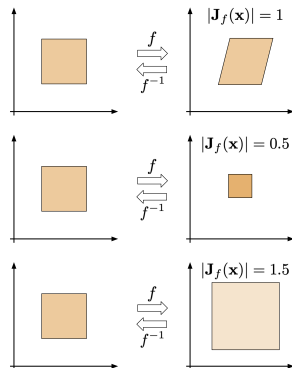
Jacobian Determinant

Inverse Function Theorem

If the function \mathbf{f} is invertible and its Jacobian is continuous and non-singular, then

$$\mathbf{J}_{\mathbf{f}^{-1}} = \mathbf{J}_{\mathbf{g}} = \mathbf{J}_{\mathbf{f}}^{-1}; \quad |\det(\mathbf{J}_{\mathbf{f}^{-1}})| = |\det(\mathbf{J}_{\mathbf{g}})| = \frac{1}{|\det(\mathbf{J}_{\mathbf{f}})|}$$

- ▶ \mathbf{x} and \mathbf{z} reside in the same space (\mathbb{R}^m).
- ▶ $\mathbf{f}_{\theta}(\mathbf{x})$ is a parameterized transformation.
- ▶ The determinant of the Jacobian $\mathbf{J} = \frac{\partial \mathbf{f}_{\theta}(\mathbf{x})}{\partial \mathbf{x}}$ quantifies how the volume is changed by the transformation.

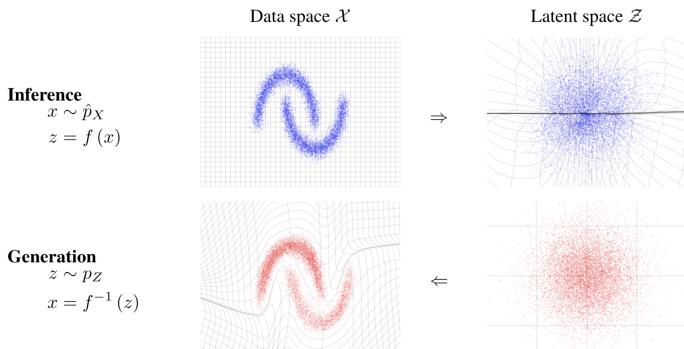


Fitting Normalizing Flows

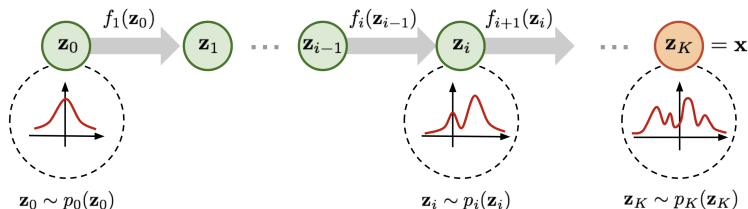
MLE Problem

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

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



Composition of Normalizing Flows



Theorem

If every $\{\mathbf{f}_k\}_{k=1}^K$ satisfies the conditions of the change-of-variables theorem, then the composition $\mathbf{f}(\mathbf{x}) = \mathbf{f}_K \circ \dots \circ \mathbf{f}_1(\mathbf{x})$ also satisfies them.

$$\begin{aligned} p(\mathbf{x}) &= p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \dots \frac{\partial \mathbf{f}_1}{\partial \mathbf{x}} \right) \right| = \\ &= p(\mathbf{f}(\mathbf{x})) \prod_{k=1}^K \left| \det \left(\frac{\partial \mathbf{f}_k}{\partial \mathbf{f}_{k-1}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \prod_{k=1}^K |\det(\mathbf{J}_{\mathbf{f}_k})| \end{aligned}$$

Normalizing Flows (NF)

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

Definition

A normalizing flow is a *differentiable, invertible* mapping that transforms data \mathbf{x} to latent noise \mathbf{z} .

- ▶ **Normalizing** refers to mapping samples from $\pi(\mathbf{x})$ to a base distribution $p(\mathbf{z})$.
- ▶ **Flow** describes the sequence of transformations that maps samples from $p(\mathbf{z})$ to the target, more complex distribution.

$$\mathbf{z} = \mathbf{f}_K \circ \dots \circ \mathbf{f}_1(\mathbf{x}); \quad \mathbf{x} = \mathbf{f}_1^{-1} \circ \dots \circ \mathbf{f}_K^{-1}(\mathbf{z}) = \mathbf{g}_1 \circ \dots \circ \mathbf{g}_K(\mathbf{z})$$

Log-Likelihood

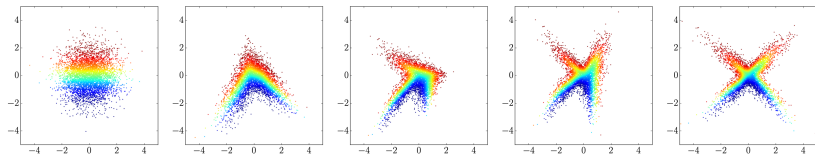
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_K \circ \dots \circ \mathbf{f}_1(\mathbf{x})) + \sum_{k=1}^K \log |\det(\mathbf{J}_{\mathbf{f}_k})|$$

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

Note: Here we consider only **continuous** random variables.

Normalizing Flows

Example: 4-Step NF



NF Log-Likelihood

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

What's the computational complexity of evaluating this determinant?

Requirements

- ▶ Efficient computation of the Jacobian $\mathbf{J}_{\mathbf{f}} = \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})}{\partial \mathbf{x}}$
- ▶ Efficient inversion of the transformation $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$

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Jacobian Structure

Normalizing Flows Log-Likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) + \log \left| \det \left(\frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

The principal computational challenge is evaluating the Jacobian determinant.

What is $\det(\mathbf{J})$ in These Cases?

Consider a linear layer $\mathbf{z} = \mathbf{W}\mathbf{x}$, $\mathbf{W} \in \mathbb{R}^{m \times m}$.

1. \mathbf{z} is a permutation of \mathbf{x} .
2. z_j depends only on x_j .

$$\log \left| \det \left(\frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \log \left| \prod_{j=1}^m \frac{\partial f_{j,\boldsymbol{\theta}}(x_j)}{\partial x_j} \right| = \sum_{j=1}^m \log \left| \frac{\partial f_{j,\boldsymbol{\theta}}(x_j)}{\partial x_j} \right|$$

3. z_j depends only on $\mathbf{x}_{1:j}$ (autoregressive dependency).

Linear Normalizing Flows

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

In general, matrix inversion has computational complexity $O(m^3)$.

Invertibility

- ▶ Diagonal matrix: $O(m)$.
- ▶ Triangular matrix: $O(m^2)$.
- ▶ Directly parameterizing the full group of invertible matrices is infeasible.

Invertible 1×1 Convolution

$\mathbf{W} \in \mathbb{R}^{c \times c}$ acts as the kernel of a 1×1 convolution with c input and c output channels. Calculating or differentiating $\det(\mathbf{W})$ incurs a cost of $O(c^3)$. It is critical that \mathbf{W} is invertible.

Linear Normalizing Flows

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

Matrix Decompositions

► LU Decomposition:

$$\mathbf{W} = \mathbf{P}\mathbf{L}\mathbf{U},$$

where \mathbf{P} is a permutation matrix, \mathbf{L} is lower triangular with positive diagonal, and \mathbf{U} is upper triangular with positive diagonal.

► QR Decomposition:

$$\mathbf{W} = \mathbf{Q}\mathbf{R},$$

where \mathbf{Q} is orthogonal, and \mathbf{R} is upper triangular with positive diagonal.

Decomposition is performed only at initialization; the decomposed matrices ($\mathbf{P}, \mathbf{L}, \mathbf{U}$ or \mathbf{Q}, \mathbf{R}) are optimized during training.

Kingma D. P., et al. *Glow: Generative Flow with Invertible 1x1 Convolutions*, 2018
Hoogeboom E., et al. *Emerging Convolutions for Generative Normalizing Flows*, 2019

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Gaussian Autoregressive Model

Consider the autoregressive model:

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^m p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}), \quad p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}) = \mathcal{N}(\mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}), \sigma_{j,\boldsymbol{\theta}}^2(\mathbf{x}_{1:j-1}))$$

Sampling

$$x_j = \sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}), \quad z_j \sim \mathcal{N}(0, 1)$$

Inverse Transformation

$$z_j = \frac{x_j - \mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})}{\sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})}$$

- ▶ This gives an **invertible** and **differentiable** transformation from $p(\mathbf{z})$ to $p(\mathbf{x}|\boldsymbol{\theta})$.
- ▶ This model is called an autoregressive (AR) NF with base distribution $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.
- ▶ The Jacobian matrix of this transformation is triangular.

Gaussian Autoregressive NF

$$\mathbf{x} = \mathbf{g}_\theta(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_{j,\theta}(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_{j,\theta}(\mathbf{x}_{1:j-1})$$

$$\mathbf{z} = \mathbf{f}_\theta(\mathbf{x}) \quad \Rightarrow \quad z_j = \frac{x_j - \mu_{j,\theta}(\mathbf{x}_{1:j-1})}{\sigma_{j,\theta}(\mathbf{x}_{1:j-1})}$$

To generate samples, apply $\mathbf{g}_\theta(\mathbf{z})$ sequentially;
inference via $\mathbf{f}_\theta(\mathbf{x})$ is parallelizable.

Forward KL for NFs

$$\text{KL}(\pi \| p) = -\mathbb{E}_{\pi(\mathbf{x})} [\log p(\mathbf{f}_\theta(\mathbf{x})) + \log |\det(\mathbf{J}_f)|] + \text{const}$$

- ▶ Computing $\mathbf{f}_\theta(\mathbf{x})$ and its Jacobian is necessary.
- ▶ One must be able to evaluate the density $p(\mathbf{z})$.
- ▶ The inverse $\mathbf{g}_\theta(\mathbf{z}) = \mathbf{f}_\theta^{-1}(\mathbf{z})$ is only needed for sampling.

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RealNVP

Split \mathbf{x} and \mathbf{z} into two parts:

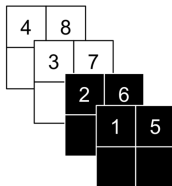
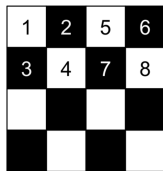
$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}]$$

Coupling Layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1 \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \sigma_{\theta}(\mathbf{z}_1) + \mu_{\theta}(\mathbf{z}_1) \end{cases}$$

$$\begin{cases} \mathbf{z}_1 = \mathbf{x}_1 \\ \mathbf{z}_2 = (\mathbf{x}_2 - \mu_{\theta}(\mathbf{x}_1)) \odot \frac{1}{\sigma_{\theta}(\mathbf{x}_1)} \end{cases}$$

Image Partitioning



- ▶ Checkerboard ordering corresponds to masking.
- ▶ Channelwise ordering relies on splitting.

RealNVP

Coupling Layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1 \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \sigma_{\theta}(\mathbf{z}_1) + \mu_{\theta}(\mathbf{z}_1) \end{cases} \quad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1 \\ \mathbf{z}_2 = (\mathbf{x}_2 - \mu_{\theta}(\mathbf{x}_1)) \odot \frac{1}{\sigma_{\theta}(\mathbf{x}_1)} \end{cases}$$

In both training and sampling, only a single forward pass is needed!

Jacobian

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

Gaussian AR NF

$$\mathbf{x} = \mathbf{g}_{\theta}(\mathbf{z}) \quad \Rightarrow \quad \mathbf{x}_j = \sigma_{j,\theta}(\mathbf{x}_{1:j-1}) \cdot \mathbf{z}_j + \mu_{j,\theta}(\mathbf{x}_{1:j-1})$$

$$\mathbf{z} = \mathbf{f}_{\theta}(\mathbf{x}) \quad \Rightarrow \quad \mathbf{z}_j = (\mathbf{x}_j - \mu_{j,\theta}(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_{j,\theta}(\mathbf{x}_{1:j-1})}.$$

How can the RealNVP layer be derived as a special instance of the Gaussian autoregressive NF?

Glow: Coupling Layers + Linear Flows (1×1 Convolutions)



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

Summary

- ▶ The change-of-variables theorem provides a method for computing a random variable's density under an invertible transformation.
- ▶ Normalizing flows transform a simple base distribution into a complex one via a sequence of invertible mappings, each with efficient Jacobian determinants.
- ▶ This enables exact likelihood computation, thanks to the change-of-variables formula.
- ▶ Linear NFs capture invertible matrices by using matrix decompositions.
- ▶ Gaussian autoregressive NFs are AR models with triangular Jacobians.
- ▶ The RealNVP coupling layer provides an efficient normalizing flow (a special case of AR NF), supporting fast inference and sampling.