Deep Generative Models

Lecture 2

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Recap of Previous Lecture

We're given **finite** number of i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^m$ drawn from an **unknown** distribution $p_{\text{data}}(\mathbf{x})$.

Objective

Our aim is to learn a distribution $p_{\text{data}}(\mathbf{x})$ that allows us to:

- Generate new samples from $p_{\text{data}}(\mathbf{x})$ (sample $\mathbf{x} \sim p_{\text{data}}(\mathbf{x})$) — **generation**.
- Evaluate $p_{\text{data}}(\mathbf{x})$ on novel data (answering "How likely is an object $\mathbf{x}$?") — **density estimation**;

Divergence Minimization Task

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

$$\min_{\boldsymbol{\theta}} D(p_{\text{data}} \| p_{\boldsymbol{\theta}})$$

Recap of Previous Lecture

Forward KL Divergence

$$\mathrm{KL}(p_{\text{data}} \| p_{\boldsymbol{\theta}}) = \int \pi(\mathbf{x}) \log \frac{p_{\text{data}}(\mathbf{x})}{p_{\boldsymbol{\theta}}(\mathbf{x})} d\mathbf{x} \to \min_{\boldsymbol{\theta}}$$

Reverse KL Divergence

$$\mathrm{KL}(p_{\boldsymbol{\theta}} \| p_{\text{data}}) = \int p_{\boldsymbol{\theta}}(\mathbf{x}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x})}{p_{\text{data}}(\mathbf{x})} d\mathbf{x} \to \min_{\boldsymbol{\theta}}$$

Maximum Likelihood Estimation (MLE)

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

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

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

MLE for Autoregressive Models

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

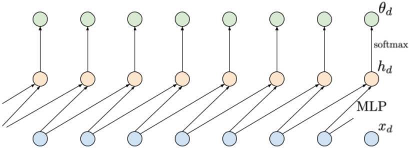
Sampling

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

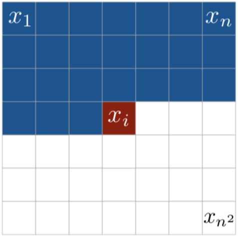
The generated sample is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_m)$.

Recap of Previous Lecture

Autoregressive MLP



Autoregressive Transformer



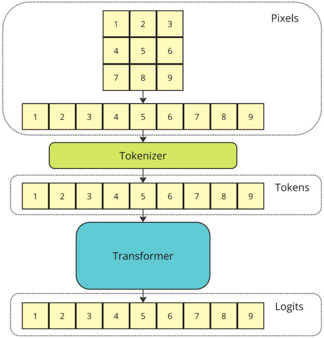


Image credit: https://jmtomczak.github.io/blog/2/2_ARM.html
Chen M. et al. Generative Pretraining from Pixels, 2020

Outline

1. Normalizing Flows (NF)

2. NF Examples
   Linear Normalizing Flows
   Gaussian Autoregressive NF
   Coupling Layer (RealNVP)

3. Latent Variable Models (LVM)

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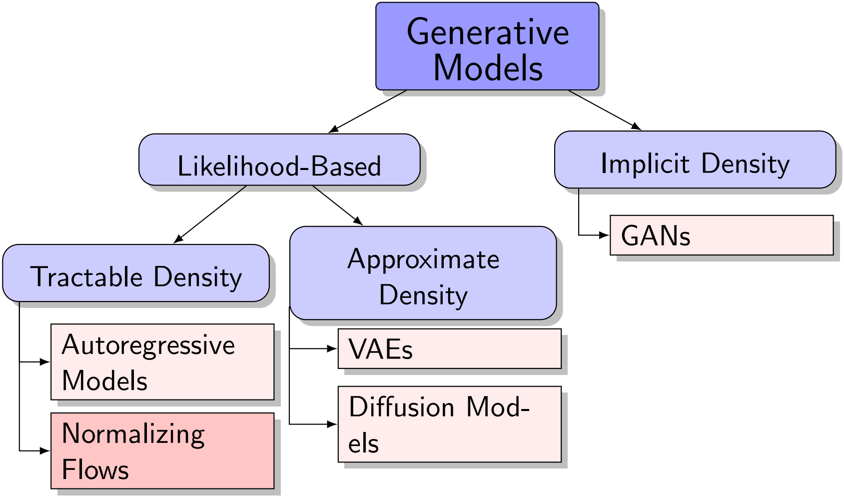
Generative Models Zoo



Normalizing Flows: Prerequisites

Jacobian Matrix

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

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

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Change of Variables Theorem (CoV)

Let $\mathbf{x} \in \mathbb{R}^m$ be a random vector with density $p(\mathbf{x})$, and let $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ be a C^1-diffeomorphism ($\mathbf{f}$ and $\mathbf{f}^{-1}$ are continuously differentiable mappings). If $\mathbf{z} = \mathbf{f}(\mathbf{x})$, then

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

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$$p(\mathbf{z}) = p(\mathbf{x}) |\det(\mathbf{J}_{\mathbf{f}^{-1}})| = p(\mathbf{x}) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = p(\mathbf{f}^{-1}(\mathbf{z})) \left| \det \left(\frac{\partial \mathbf{f}^{-1}(\mathbf{z})}{\partial \mathbf{z}} \right) \right|$$

Jacobian Determinant

Inverse Function Theorem

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

$$\mathbf{J}_{\mathbf{f}^{-1}} = \mathbf{J}_{\mathbf{f}}^{-1};$$

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- $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ is a parameterized transformation.

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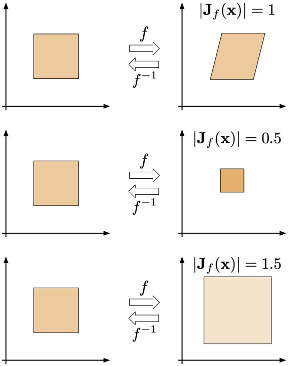
- $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ is a parameterized transformation.
- The determinant of the Jacobian $\mathbf{J} = \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})}{\partial \mathbf{x}}$ quantifies how the volume is changed by the transformation.



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Fitting Normalizing Flows

MLE Problem

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

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

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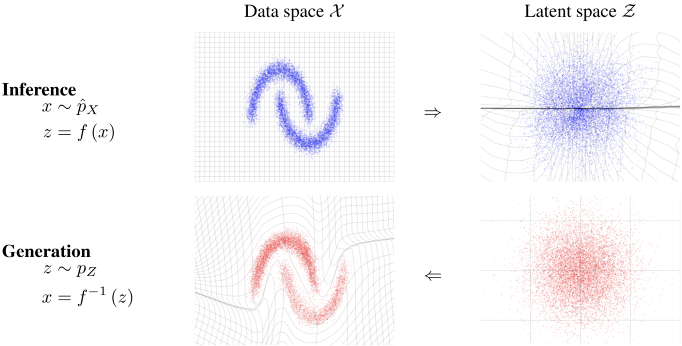

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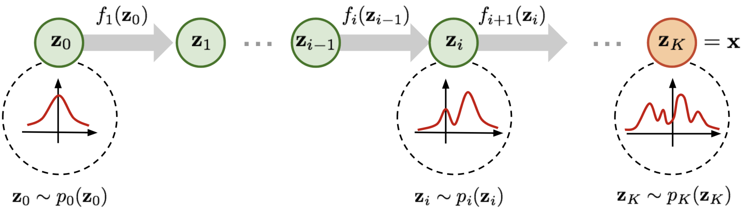
Composition of Normalizing Flows



https://lilianweng.github.io/lil-log/2018/10/13/flow-based-deep-generative-models.html

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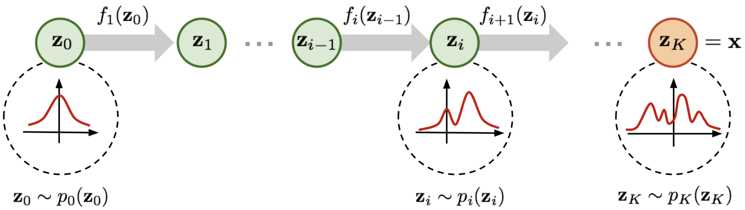

Theorem

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

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

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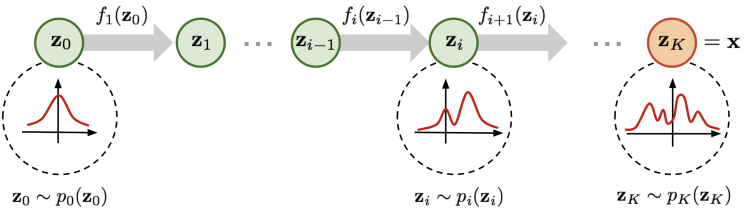

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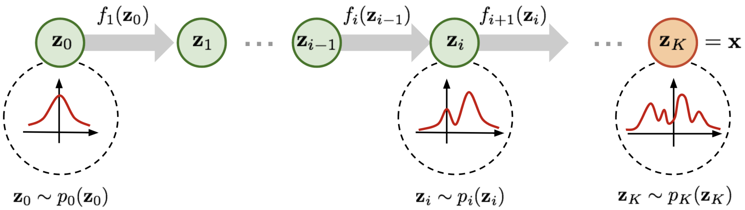

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$$= p(\mathbf{f}(\mathbf{x})) \prod_{k=1}^{K} \left| \det \left(\frac{\partial \mathbf{f}_k}{\partial \mathbf{f}_{k-1}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \prod_{k=1}^{K} |\det(\mathbf{J}_{\mathbf{f}_k})|$$

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Normalizing Flows (NF)

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

Definition

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- **Normalizing** refers to mapping samples from $p_{\text{data}}(\mathbf{x})$ 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.

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

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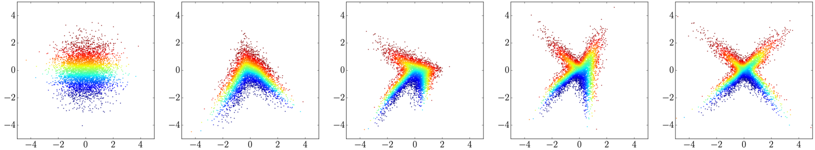
Note: Here we consider only **continuous** random variables.

Normalizing Flows

Example: 4-Step NF



Papamakarios G. et al. Normalizing Flows for Probabilistic Modeling and Inference, 2019

Normalizing Flows

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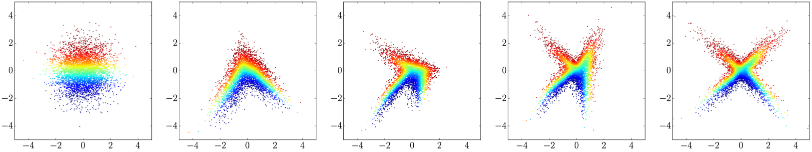

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What's the computational complexity of evaluating this determinant?

Papamakarios G. et al. Normalizing Flows for Probabilistic Modeling and Inference, 2019

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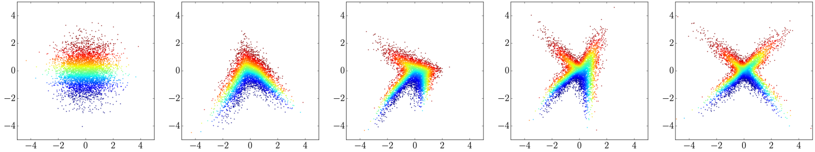

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Requirements

- 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 $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$

Papamakarios G. et al. Normalizing Flows for Probabilistic Modeling and Inference, 2019

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Jacobian Structure

Normalizing Flows Log-Likelihood

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The principal computational challenge is evaluating the Jacobian determinant.

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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 $\mathbf{x}$.

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

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

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

Linear Normalizing Flows

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

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

Papamakarios G. et al. Normalizing Flows for Probabilistic Modeling and Inference, 2019

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

Invertibility

- Diagonal matrix: $O(m)$.
- Triangular matrix: $O(m^2)$.
- Directly parameterizing all invertible matrices in a continuous way is infeasible
  (there is not surjective function from $\mathbb{R}^{m^2}$ to the set of all invertible matrices of size $m \times m$).

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

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

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

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- **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

Outline

Gaussian Autoregressive Model

Consider the autoregressive model:

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

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

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Sampling

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

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Inverse Transformation

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

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- This gives an C^1-**diffeomorphism** from $p(\mathbf{z})$ to $p_{\boldsymbol{\theta}}(\mathbf{x})$ (assume that $\sigma_j \neq 0$).

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- This model is called an autoregressive (AR) NF with base distribution $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.

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Sampling

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

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

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- 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.

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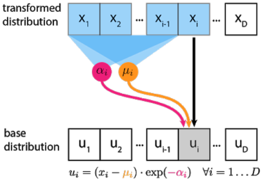
Gaussian Autoregressive NF

Forward Transformation: $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$

$$\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$$

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



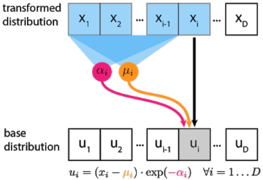
Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Gaussian Autoregressive NF

Forward Transformation: $\mathbf{f}_\theta(\mathbf{x})$

$$\mathbf{z} = \mathbf{f}_\theta(\mathbf{x})$$

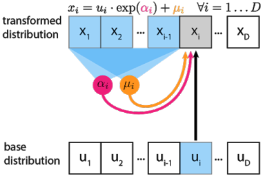
$$z_j = \frac{x_j - \mu_{j,\theta}(\mathbf{x}_{1:j-1})}{\sigma_{j,\theta}(\mathbf{x}_{1:j-1})}$$



Inverse Transformation: $\mathbf{f}_\theta^{-1}(\mathbf{z})$

$$\mathbf{x} = \mathbf{f}_\theta^{-1}(\mathbf{z})$$

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



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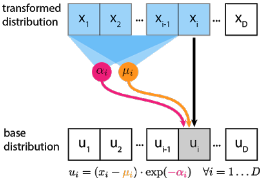

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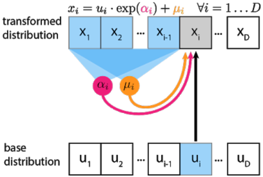

- Sampling must be done sequentially, but density estimation can be parallelized.
- The forward KL divergence is a natural objective for training.

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

Outline

RealNVP

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

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

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

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Coupling Layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1 \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}_1) + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}_1) \end{cases}$$

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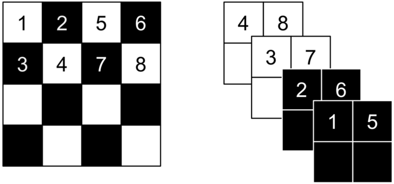
Image Partitioning



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

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

RealNVP

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

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

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Jacobian

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

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Gaussian AR NF

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

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

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

Outline

Bayesian Framework

Bayes' Theorem

$$p(\boldsymbol{\theta}|\mathbf{x}) = \frac{p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

- $\mathbf{x}$: observed variables;
- $\boldsymbol{\theta}$: unknown latent variables/parameters;
- $p_{\boldsymbol{\theta}}(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$: likelihood;
- $p(\mathbf{x}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$: evidence;
- $p(\boldsymbol{\theta})$: prior distribution;
- $p(\boldsymbol{\theta}|\mathbf{x})$: posterior distribution.

Bayesian Framework

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- $p(\boldsymbol{\theta})$: prior distribution;
- $p(\boldsymbol{\theta}|\mathbf{x})$: posterior distribution.

Interpretation

- We begin with unknown variables $\boldsymbol{\theta}$ and a prior belief $p(\boldsymbol{\theta})$.
- Once data $\mathbf{x}$ is observed, the posterior $p(\boldsymbol{\theta}|\mathbf{x})$ incorporates both prior beliefs and evidence from the data.

Bayesian Framework

Consider the case where the unobserved variables $\boldsymbol{\theta}$ are model parameters (i.e., $\boldsymbol{\theta}$ are random variables).

- $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$: observed samples;
- $p(\boldsymbol{\theta})$: prior distribution.

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$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

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If the evidence $p(\mathbf{X})$ is intractable (due to high-dimensional integration), the posterior cannot be computed exactly.

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If the evidence $p(\mathbf{X})$ is intractable (due to high-dimensional integration), the posterior cannot be computed exactly.

Maximum a Posteriori (MAP) Estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}) = \arg\max_{\boldsymbol{\theta}}(\log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}))$$

Latent Variable Models (LVM)

Maximum Likelihood Extimation (MLE) Problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p_{\boldsymbol{\theta}}(\mathbf{x}_i) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\mathbf{x}_i).$$

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Maximum Likelihood Extimation (MLE) Problem

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The distribution $p_{\boldsymbol{\theta}}(\mathbf{x})$ can be highly complex and often intractable (just like the true data distribution $p_{\text{data}}(\mathbf{x})$).

Latent Variable Models (LVM)

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Extended Probabilistic Model

Introduce a latent variable $\mathbf{z}$ for each observed sample $\mathbf{x}$:

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Motivation

Both $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ and $p(\mathbf{z})$ are usually much simpler than $p_{\boldsymbol{\theta}}(\mathbf{x})$.

Summary

- The CoV 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.
- 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.
- The Bayesian framework generalizes nearly all standard machine learning methods.