Deep Generative Models

Lecture 2

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

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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

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

Reverse KL Divergence

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

Maximum Likelihood Estimation (MLE)

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

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

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

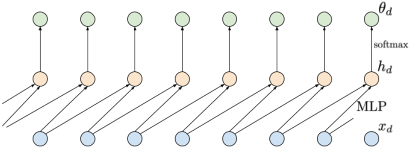
Sampling

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

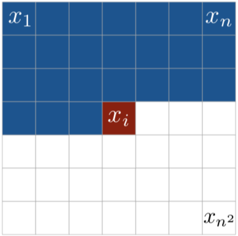
The generated sample is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_m)$.

Recap of Previous Lecture

Autoregressive MLP



Autoregressive Transformer



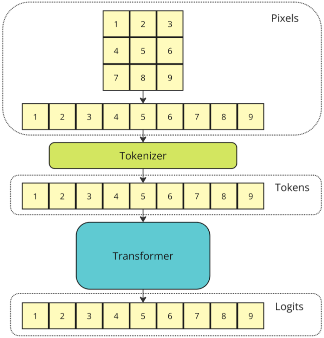


Image credit: https://jmtomczak.github.io/blog/2/2_ARM.html
Chen M. et al. Generative Pretraining from Pixels, 2020

Outline

1. Normalizing Flows (NF)

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

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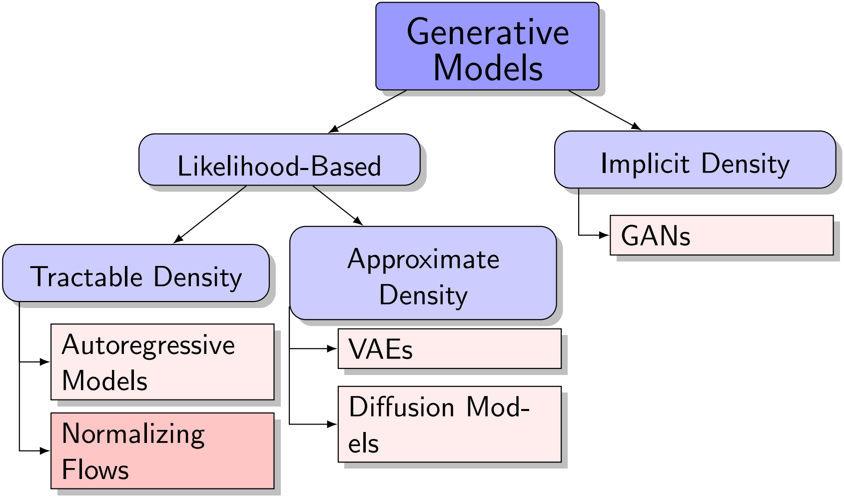
Generative Models Zoo



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

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

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Jacobian Determinant

Inverse Function Theorem

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

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

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- $\mathbf{x}$ and $\mathbf{z}$ reside in the same space ($\mathbb{R}^m$).
- $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ is a parameterized transformation.

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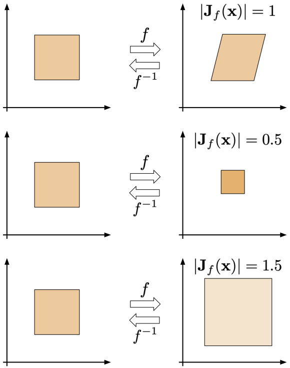
- $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ is a parameterized transformation.
- The determinant of the Jacobian $\mathbf{J} = \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})}{\partial \mathbf{x}}$ quantifies how the volume is changed by the transformation.



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Fitting Normalizing Flows

MLE Problem

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

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

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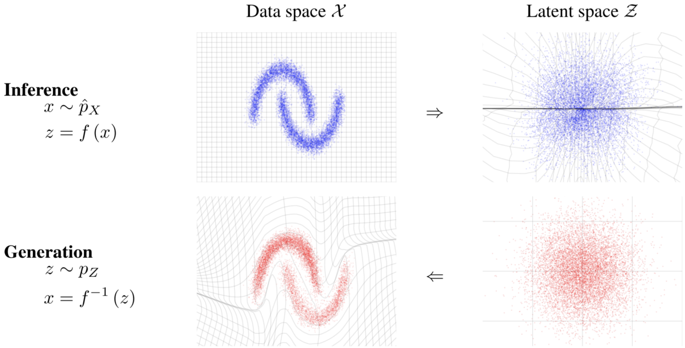

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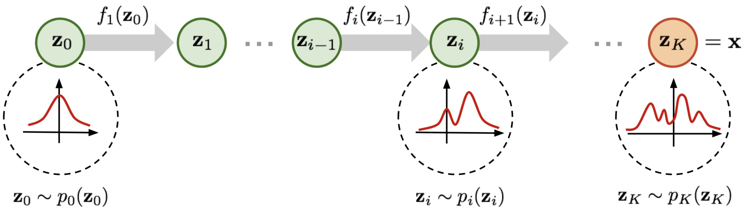
Composition of Normalizing Flows



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

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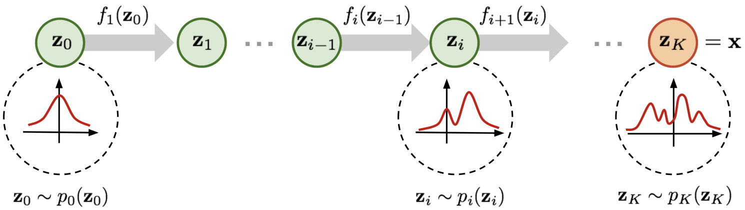

Theorem

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.

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

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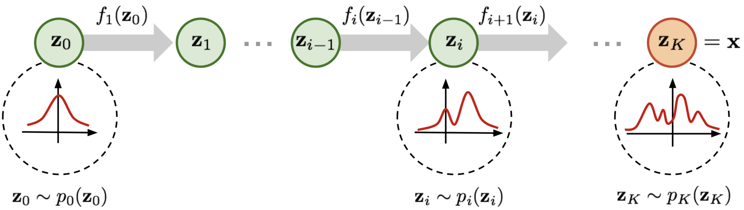

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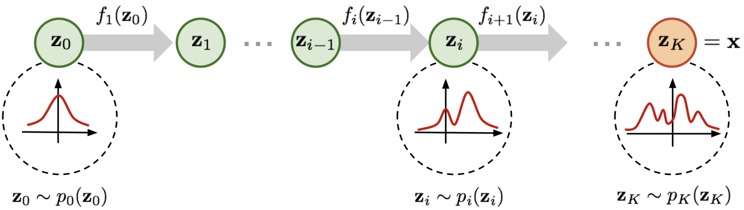

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Normalizing Flows (NF)

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

Definition

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- **Normalizing** refers to mapping samples from $\pi(\mathbf{x})$ to a base distribution $p(\mathbf{z})$.
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$$\mathbf{z} = \mathbf{f}_K \circ \ldots \circ \mathbf{f}_1(\mathbf{x}); \quad \mathbf{x} = \mathbf{f}_1^{-1} \circ \ldots \circ \mathbf{f}_K^{-1}(\mathbf{z}) = \mathbf{g}_1 \circ \ldots \circ \mathbf{g}_K(\mathbf{z})$$

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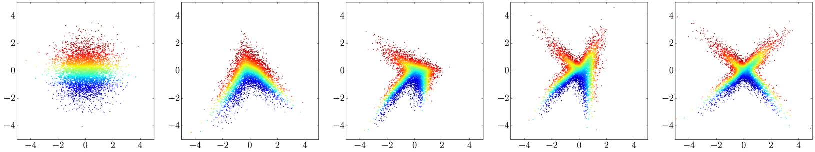
Note: Here we consider only **continuous** random variables.

Normalizing Flows

Example: 4-Step NF



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

Normalizing Flows

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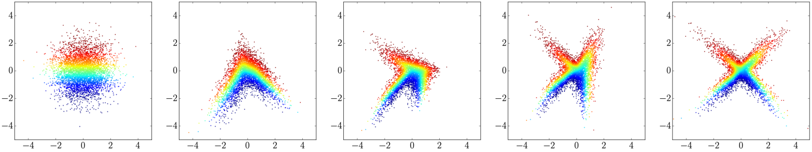

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What's the computational complexity of evaluating this determinant?

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

Normalizing Flows

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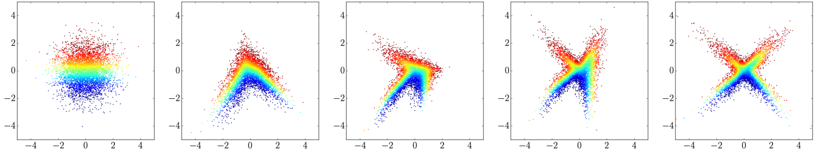

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Requirements

- 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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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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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

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

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

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

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Invertibility

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

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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.

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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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- **QR Decomposition:**

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

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

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- **QR Decomposition:**

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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
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Outline

1. Normalizing Flows (NF)

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

Gaussian Autoregressive Model

Consider the autoregressive model:

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

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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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- The Jacobian matrix of this transformation is triangular.

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Gaussian Autoregressive NF

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

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

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

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To generate samples, apply $\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$ sequentially;
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Forward KL for NFs

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

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

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

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

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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.

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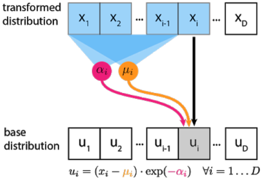

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Inverse Transformation: $\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$

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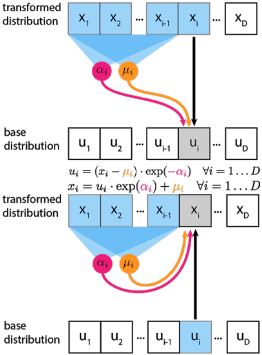

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Outline

1. Normalizing Flows (NF)

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

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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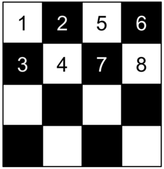
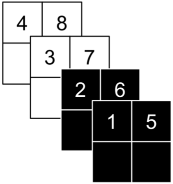
Image Partitioning





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

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

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

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

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

Jacobian

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

Gaussian AR NF

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

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

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

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

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