

# 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

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

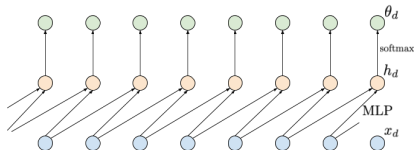
## Sampling

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

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

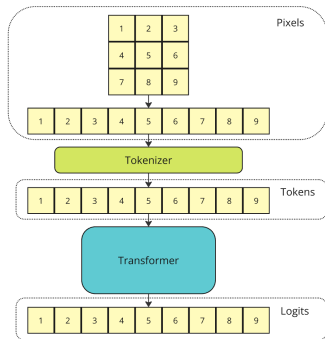
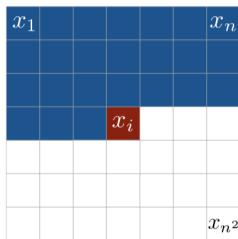


Image credit: [https://jmtomczak.github.io/blog/2/2\\_ARM.html](https://jmtomczak.github.io/blog/2/2_ARM.html)  
Chen M. et al. Generative Pretraining from Pixels, 2020

# Outline

## 1. Normalizing Flows (NF)

## 2. NF Examples

- Linear Normalizing Flows

- Gaussian Autoregressive NF

- Coupling Layer (RealNVP)

# Outline

## 1. Normalizing Flows (NF)

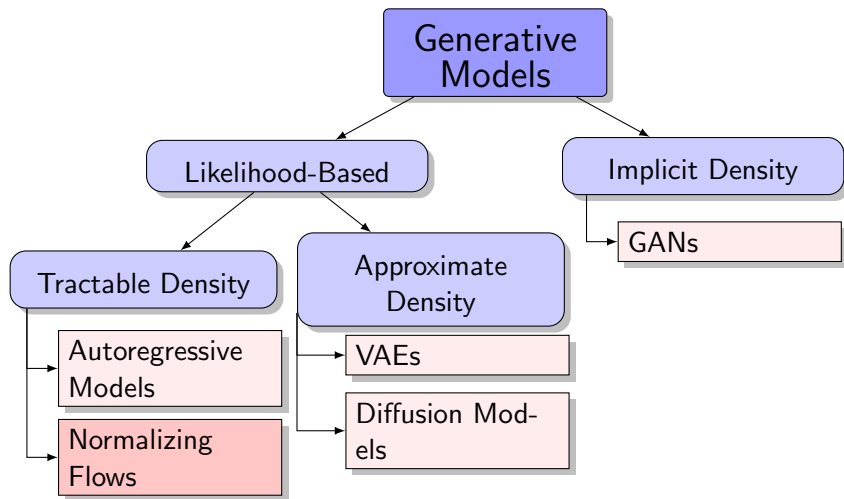
## 2. NF Examples

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

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

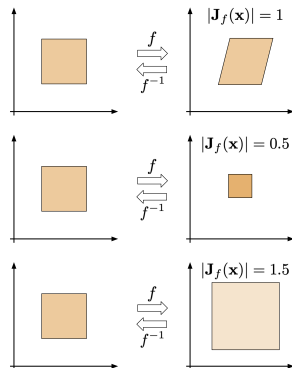
# Jacobian Determinant

## 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.

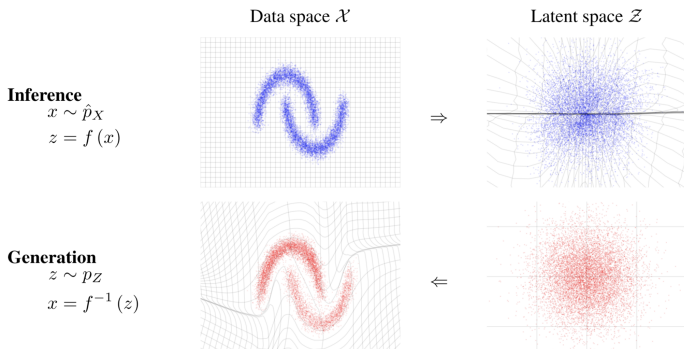


# Fitting Normalizing Flows

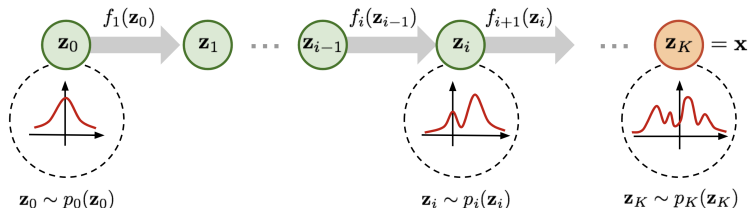
## MLE Problem

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

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



# 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

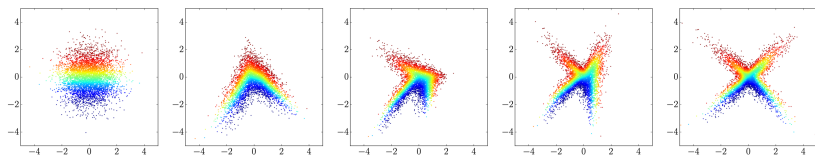
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_K \circ \dots \circ \mathbf{f}_1(\mathbf{x})) + \sum_{k=1}^K \log |\det(\mathbf{J}_{\mathbf{f}_k})|$$

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

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

# Outline

## 1. Normalizing Flows (NF)

## 2. NF Examples

- Linear Normalizing Flows

- Gaussian Autoregressive NF

- Coupling Layer (RealNVP)

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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

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

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

## Invertibility

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

## Invertible $1 \times 1$ Convolution

$\mathbf{W} \in \mathbb{R}^{c \times c}$  acts as the kernel of a  $1 \times 1$  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.

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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

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

- ▶ 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.

# Gaussian Autoregressive NF

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

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

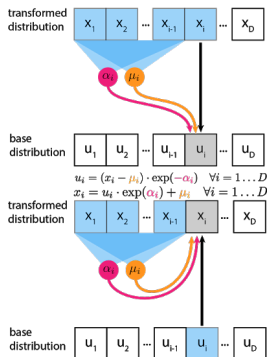
- ▶ Sampling must be done sequentially, but density estimation can be parallelized.
- ▶ The forward KL divergence is a natural objective for training.

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

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

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

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



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# RealNVP

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

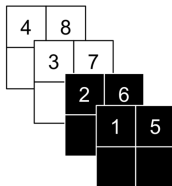
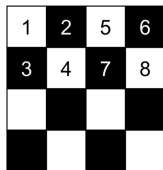
$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}]$$

## 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

$$\begin{aligned} \mathbf{x} = \mathbf{g}_{\theta}(\mathbf{z}) &\Rightarrow \mathbf{x}_j = \sigma_{j,\theta}(\mathbf{x}_{1:j-1}) \cdot \mathbf{z}_j + \mu_{j,\theta}(\mathbf{x}_{1:j-1}) \\ \mathbf{z} = \mathbf{f}_{\theta}(\mathbf{x}) &\Rightarrow \mathbf{z}_j = (\mathbf{x}_j - \mu_{j,\theta}(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_{j,\theta}(\mathbf{x}_{1:j-1})}. \end{aligned}$$

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

## Glow: Coupling Layers + Linear Flows ( $1 \times 1$ Convolutions)



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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.