Deep Generative Models

Lecture 6

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AI Masters

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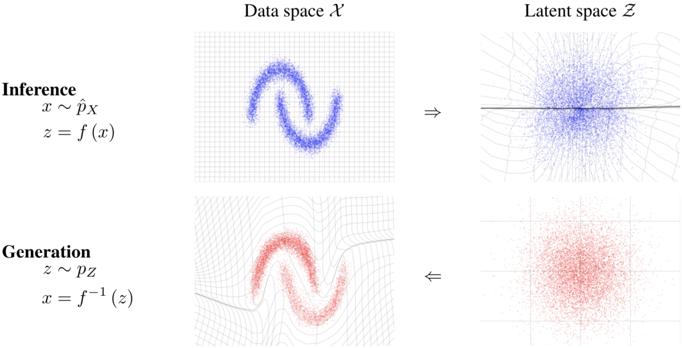
Recap of previous lecture

MLE problem

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

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f(\mathbf{x}, \boldsymbol{\theta})) + \log |\det(\mathbf{J}_f)| \to \max_{\boldsymbol{\theta}}$$



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

Recap of previous lecture

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

Definition

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

- **Normalizing** means that the inverse flow takes samples from $p(\mathbf{x})$ and normalizes them into samples from density $p(\mathbf{z})$.
- **Flow** refers to the trajectory followed by samples from $p(\mathbf{z})$ as they are transformed by the sequence of transformations

$$\mathbf{z} = f_K \circ \dots \circ f_1(\mathbf{x}); \quad \mathbf{x} = f_1^{-1} \circ \dots \circ f_K^{-1}(\mathbf{z}) = g_1 \circ \dots \circ g_K(\mathbf{z})$$

Log likelihood

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

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

Recap of previous lecture

Forward KL for flow model

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

Reverse KL for flow model

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

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;
- $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta})$, $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$;
- $\mathbf{x} \sim \pi(\mathbf{x})$, $\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta})$, $\mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta})$;

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

Recap of previous lecture

Flow log-likelihood

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

The main challenge is a determinant of the Jacobian.

Residual flows: planar/Sylvester

$$g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{u}\, \sigma(\mathbf{w}^T \mathbf{z} + b); \quad g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{A}\, \sigma(\mathbf{B}\mathbf{z} + \mathbf{b}).$$

Matrix determinant lemma for calculating the Jacobian.

Linear flows

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

Matrix decompositions (LU or QR helps to parametrize matrix $\mathbf{W}$ and reduce the cost of computing the $det(\mathbf{J})$).

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015
Berg R. et al. Sylvester normalizing flows for variational inference, 2018
Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018

Outline

1. RealNVP: coupling layer

Autoregressive flows

$$x_j = \tau(z_j, c(\mathbf{z}_{1:j-1})) \quad \Leftrightarrow \quad z_j = \tau^{-1}(x_j, c(\mathbf{z}_{1:j-1}))$$

- $\tau(\cdot, \cdot)$ – coupling law (invertible by first argument, differentiable).
- $c(\cdot)$ – coupling function (do not need to be invertible, could be neural network).

Coupling law $\tau(\cdot, \cdot)$

- $\tau(x, c) = x + c$ – additive;
- $\tau(x, c) = x \odot c_1 + c_2$ – affine.

What is the Jacobian for the additive/affine coupling law?

Jacobian

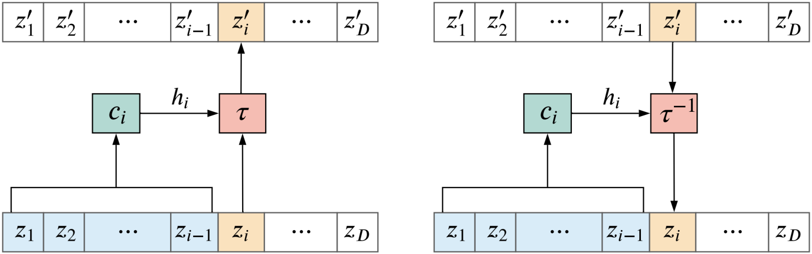
$$\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}}\right) = \prod_{j=1}^{m} \frac{\partial x_j}{\partial z_j} = \prod_{j=1}^{m} \frac{\partial \tau(z_j, c(\mathbf{z}_{1:j-1}))}{\partial z_j}$$

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

Autoregressive flows

Forward and inverse transforms

$$x_j = \tau(z_j, c(\mathbf{z}_{1:j-1})) \quad \Leftrightarrow \quad z_j = \tau^{-1}(x_j, c(\mathbf{z}_{1:j-1}))$$



- Forward transform is **not sequential**.
- Inverse transform is **sequential**.

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

Outline

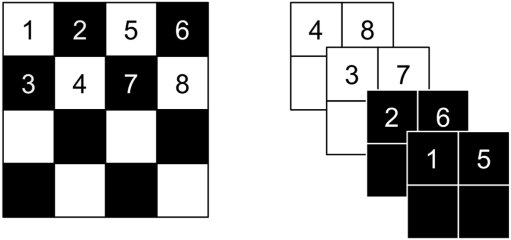
1. RealNVP: coupling layer

RealNVP

Coupling layer

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \tau(\mathbf{x}_{d:m}, c(\mathbf{x}_{1:d})); \end{cases} \quad \Leftrightarrow \quad \begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \tau^{-1}(\mathbf{z}_{d:m}, c(\mathbf{z}_{1:d})). \end{cases}$$

Image partitioning



Checkerboard ordering uses masking, channelwise ordering uses splitting.

Dinh L., Krueger D., Bengio Y. NICE: Non-linear Independent Components Estimation, 2014

RealNVP

Affine coupling law

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \mathbf{x}_{d:m} \odot c_1(\mathbf{x}_{1:d}, \boldsymbol{\theta}) + c_2(\mathbf{x}_{1:d}, \boldsymbol{\theta}). \end{cases}$$

$$\begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = (\mathbf{z}_{d:m} - c_2(\mathbf{z}_{1:d}, \boldsymbol{\theta})) \cdot \frac{1}{c_1(\mathbf{z}_{1:d}, \boldsymbol{\theta})}. \end{cases}$$

Jacobian

$$\det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) = \det \begin{pmatrix} \mathbf{I}_d & 0_{d \times m-d} \\ \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{1:d}} & \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}} \end{pmatrix} = \prod_{j=1}^{m-d} c_1(\mathbf{x}_{1:d}, \boldsymbol{\theta})_j.$$

Non-Volume Preserving (the determinant of Jacobian $\neq 1$).

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

AF vs IAF vs RealNVP

MADE/AF

$$\mathbf{x} = \boldsymbol{\sigma}(\mathbf{x}) \odot \mathbf{z} + \boldsymbol{\mu}(\mathbf{x}).$$

Estimating the density $p(\mathbf{x}|\boldsymbol{\theta})$ - 1 pass, sampling - m passes.

IAF

$$\mathbf{x} = \tilde{\boldsymbol{\sigma}}(\mathbf{z}) \odot \mathbf{z} + \tilde{\boldsymbol{\mu}}(\mathbf{z}).$$

Estimating the density $p(\mathbf{x}|\boldsymbol{\theta})$ - m passes, sampling - 1 pass.

RealNVP

$$\begin{cases} \mathbf{x}_{1:d} & = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} & = \mathbf{z}_{d:m} \odot c_1(\mathbf{z}_{1:d}, \boldsymbol{\theta}) + c_2(\mathbf{z}_{1:d}, \boldsymbol{\theta}). \end{cases}$$

Estimating the density $p(\mathbf{x}|\boldsymbol{\theta})$ - 1 pass, sampling - 1 pass.

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

AF vs IAF vs RealNVP

RealNVP

$$\begin{cases} \mathbf{x}_{1:d} &= \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} &= \mathbf{z}_{d:m} \odot c_1(\mathbf{z}_{1:d}, \boldsymbol{\theta}) + c_2(\mathbf{z}_{1:d}, \boldsymbol{\theta}). \end{cases}$$

- Calculating the density $p(\mathbf{x}|\boldsymbol{\theta})$ - 1 pass.
- Sampling - 1 pass.

RealNVP is a special case of AF and IAF:

AF

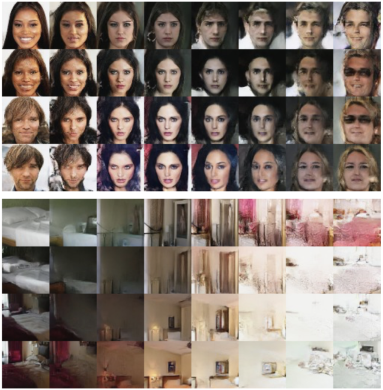
$$\begin{cases} \mu_j = 0, \sigma_j = 1, \, j = 1, \dots, d; \\ \mu_j, \sigma_j \text{ -- functions of } \mathbf{x}_{1:d}, \, j = d+1, \dots, m. \end{cases}$$

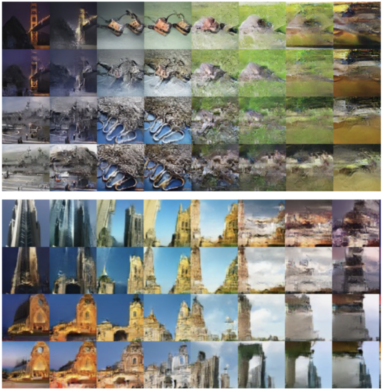
IAF

$$\begin{cases} \tilde{\mu}_j = 0, \tilde{\sigma}_j = 1, \, j = 1, \dots, d; \\ \tilde{\mu}_j, \tilde{\sigma}_j \text{ -- functions of } \mathbf{z}_{1:d}, \, j = d+1, \dots, m. \end{cases}$$

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

RealNVP samples





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

Linear flows

RealNVP

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \tau(\mathbf{x}_{d:m}, c(\mathbf{x}_{1:d})); \end{cases} \quad \Leftrightarrow \quad \begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \tau^{-1}(\mathbf{z}_{d:m}, c(\mathbf{z}_{1:d})). \end{cases}$$

- First step is a **split** operator which decouples a variable into 2 subparts: $\mathbf{x}_1$ and $\mathbf{x}_2$ (usualy channel-wise).
- We should **permute** components between different layers.

$$\mathbf{z} = \mathbf{W}\mathbf{x}, \quad \mathbf{W} \in \mathbb{R}^{m \times m}$$

In general, we need $O(m^3)$ to invert matrix.

Invertibility

- Diagonal matrix $O(m)$.
- Triangular matrix $O(m^2)$.
- It is impossible to parametrize all invertible matrices.

Glow samples

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

Summary

- Gaussian autoregressive model is an autoregressive flow with triangular Jacobian.
- Inverse autoregressive flow is able to sample fast, but the inference is slow.
- AF/IAF is a special case of autoregressive flows.
- The RealNVP is an effective type of flow (special case of AR flows) that uses coupling layer.