

Deep Generative Models

Lecture 4

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Recap of previous lecture

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) - \log \frac{q(\mathbf{z}|\mathbf{x}, \phi)}{p(\mathbf{z})} \right] \rightarrow \max_{\phi, \theta}.$$

M-step: $\nabla_{\theta} \mathcal{L}(\phi, \theta)$, Monte Carlo estimation

$$\begin{aligned} \nabla_{\theta} \mathcal{L}(\phi, \theta) &= \int q(\mathbf{z}|\mathbf{x}, \phi) \nabla_{\theta} \log p(\mathbf{x}|\mathbf{z}, \theta) d\mathbf{z} \approx \\ &\approx \nabla_{\theta} \log p(\mathbf{x}|\mathbf{z}^*, \theta), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x}, \phi). \end{aligned}$$

E-step: $\nabla_{\phi} \mathcal{L}(\phi, \theta)$, reparametrization trick

$$\begin{aligned} \nabla_{\phi} \mathcal{L}(\phi, \theta) &= \int r(\epsilon) \nabla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon, \phi), \theta) d\epsilon - \nabla_{\phi} \text{KL} \\ &\approx \nabla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon^*, \phi), \theta) - \nabla_{\phi} \text{KL} \end{aligned}$$

Variational assumption

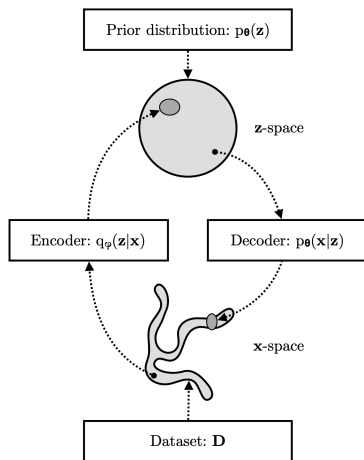
$$r(\epsilon) = \mathcal{N}(0, \mathbf{I}); \quad q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mu_{\phi}(\mathbf{x}), \sigma_{\phi}^2(\mathbf{x})).$$

$$\mathbf{z} = g(\mathbf{x}, \epsilon, \phi) = \sigma_{\phi}(\mathbf{x}) \cdot \epsilon + \mu_{\phi}(\mathbf{x}).$$

Recap of previous lecture

Variational autoencoder (VAE)

- ▶ VAE learns stochastic mapping between \mathbf{x} -space, from $\pi(\mathbf{x})$, and a latent \mathbf{z} -space, with simple distribution.
- ▶ The generative model learns distribution $p(\mathbf{x}, \mathbf{z} | \theta) = p(\mathbf{z})p(\mathbf{x} | \mathbf{z}, \theta)$, with a prior distribution $p(\mathbf{z})$, and a stochastic decoder $p(\mathbf{x} | \mathbf{z}, \theta)$.
- ▶ The stochastic encoder $q(\mathbf{z} | \mathbf{x}, \phi)$ (inference model), approximates the true but intractable posterior $p(\mathbf{z} | \mathbf{x}, \theta)$.



Recap of previous lecture

Decoder weakening

- ▶ Powerful decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ makes the model expressive, but posterior collapse is possible.
- ▶ PixelVAE model uses the autoregressive PixelCNN model with small number of layers to limit receptive field.

KL annealing

$$\mathcal{L}(\phi, \boldsymbol{\theta}, \beta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \beta \cdot KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z}))$$

Start training with $\beta = 0$, increase it until $\beta = 1$ during training.

Free bits

Ensure the use of less than λ bits of information:

$$\mathcal{L}(\phi, \boldsymbol{\theta}, \lambda) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \max(\lambda, KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z}))).$$

This results in $KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z})) \geq \lambda$.

Recap of previous lecture

VAE objective

$$\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x}, \phi)} \rightarrow \max_{q, \boldsymbol{\theta}}$$

IWAE objective

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x}, \phi)} \log \left(\frac{1}{K} \sum_{k=1}^K \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x}, \phi)} \right) \rightarrow \max_{\phi, \boldsymbol{\theta}}.$$

Theorem

1. $\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}_M(q, \boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta})$, for $K \geq M$;
 2. $\log p(\mathbf{x}|\boldsymbol{\theta}) = \lim_{K \rightarrow \infty} \mathcal{L}_K(q, \boldsymbol{\theta})$ if $\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x}, \phi)}$ is bounded.
- ▶ IWAE makes the variational bound tighter and extends the class of variational distributions.
 - ▶ Gradient signal becomes really small, training is complicated.
 - ▶ IWAE is a standard quality measure for VAE models.

Outline

1. Normalizing flows (NF)
2. Forward and Reverse KL for NF
3. Linear flows

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Likelihood-based models so far...

Autoregressive models

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

- ▶ tractable likelihood,
- ▶ no inferred latent factors.

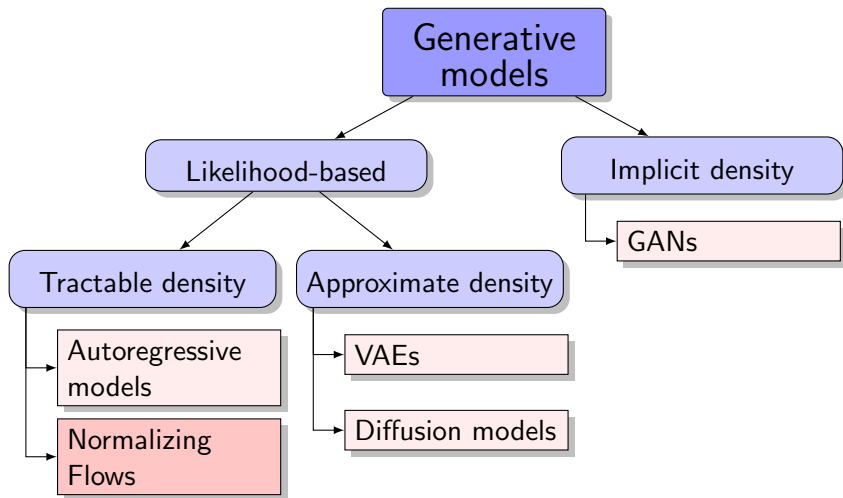
Latent variable models

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

- ▶ latent feature representation,
- ▶ intractable likelihood.

How to build model with latent variables and tractable likelihood?

Generative models zoo



Normalizing flows prerequisites

Jacobian matrix

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

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

Change of variable theorem (CoV)

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

$$\begin{aligned} p(\mathbf{x}) &= p(\mathbf{z}) |\det(\mathbf{J}_f)| = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| \\ p(\mathbf{z}) &= p(\mathbf{x}) |\det(\mathbf{J}_g)| = p(\mathbf{x}) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = p(g(\mathbf{z})) \left| \det \left(\frac{\partial g(\mathbf{z})}{\partial \mathbf{z}} \right) \right|. \end{aligned}$$

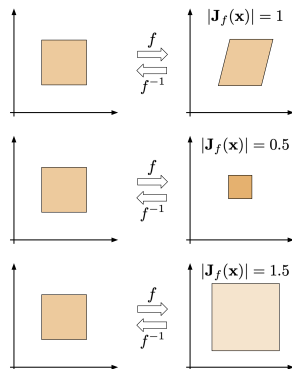
Jacobian determinant

Inverse function theorem

If function f is invertible and Jacobian matrix is continuous and non-singular, then

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

- ▶ \mathbf{x} and \mathbf{z} have the same dimensionality (\mathbb{R}^m).
- ▶ $f(\mathbf{x}, \boldsymbol{\theta})$ could be parametric function.
- ▶ Determinant of Jacobian matrix $\mathbf{J} = \frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}}$ shows how the volume changes under the transformation.

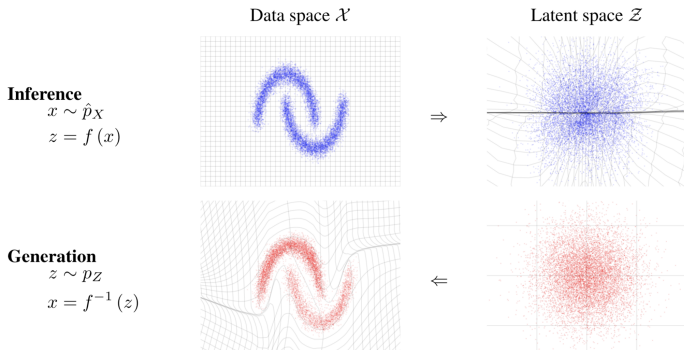


Fitting normalizing flows

MLE problem

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

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

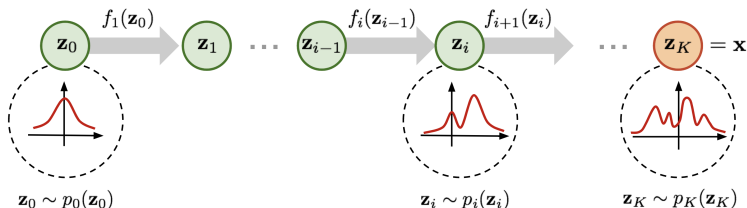


Composition of normalizing flows

Theorem

Diffeomorphisms are **composable** (If $\{f_k\}_{k=1}^K$ satisfy conditions of the change of variable theorem, then $\mathbf{z} = f(\mathbf{x}) = f_K \circ \dots \circ f_1(\mathbf{x})$ also satisfies it).

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



Normalizing flows (NF)

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

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 $\pi(\mathbf{x})$ and normalizes them into samples from the 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

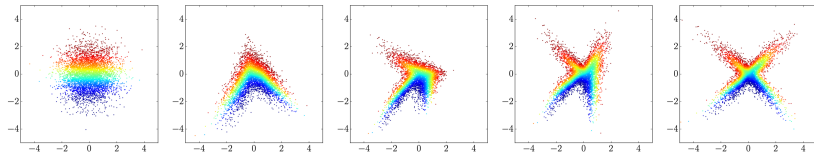
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f_K \circ \dots \circ f_1(\mathbf{x})) + \sum_{k=1}^K \log |\det(\mathbf{J}_{f_k})|,$$

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

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

Normalizing flows

Example of a 4-step flow



Flow log likelihood

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

What is the complexity of the determinant computation?

What we need:

- ▶ efficient computation of the Jacobian matrix $\mathbf{J}_f = \frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}}$;
- ▶ efficient inversion of $f(\mathbf{x}, \boldsymbol{\theta})$;
- ▶ loss function to minimize.

Outline

1. Normalizing flows (NF)
2. Forward and Reverse KL for NF
3. Linear flows

Forward KL vs Reverse KL

Forward KL \equiv MLE

$$\begin{aligned} KL(\pi||p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\boldsymbol{\theta})} d\mathbf{x} \\ &= -\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\boldsymbol{\theta}) + \text{const} \rightarrow \min_{\boldsymbol{\theta}} \end{aligned}$$

Forward KL for NF model

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

- ▶ We need to be able to compute $f(\mathbf{x}, \boldsymbol{\theta})$ and its Jacobian.
- ▶ We need to be able to compute the density $p(\mathbf{z})$.
- ▶ We don't need to think about computing the function $g(\mathbf{z}, \boldsymbol{\theta}) = f^{-1}(\mathbf{z}, \boldsymbol{\theta})$ until we want to sample from the flow.

Forward KL vs Reverse KL

Reverse KL

$$\begin{aligned} KL(p||\pi) &= \int p(\mathbf{x}|\boldsymbol{\theta}) \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x})} d\mathbf{x} \\ &= \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} [\log p(\mathbf{x}|\boldsymbol{\theta}) - \log \pi(\mathbf{x})] \rightarrow \min_{\boldsymbol{\theta}} \end{aligned}$$

Reverse KL for NF model (LOTUS trick)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{z}) + \log |\det(\mathbf{J}_f)| = \log p(\mathbf{z}) - \log |\det(\mathbf{J}_g)|$$

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

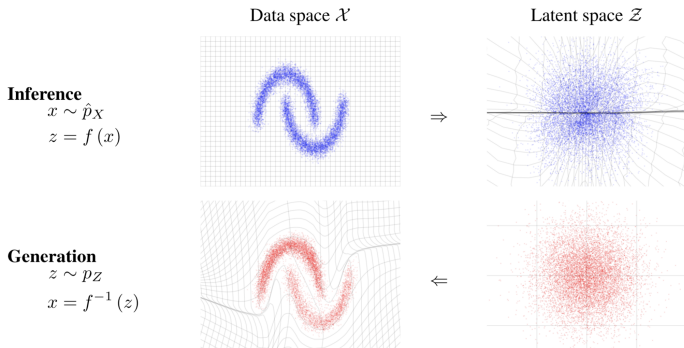
- ▶ We need to be able to compute $g(\mathbf{z}, \boldsymbol{\theta})$ and its Jacobian.
- ▶ We need to be able to sample from the density $p(\mathbf{z})$ (do not need to evaluate it) and to evaluate(!) $\pi(\mathbf{x})$.
- ▶ We don't need to think about computing the function $f(\mathbf{x}, \boldsymbol{\theta})$.

Flow KL duality

Theorem

Fitting NF model $p(\mathbf{x}|\theta)$ to the target distribution $\pi(\mathbf{x})$ using forward KL (MLE) is equivalent to fitting the induced distribution $p(\mathbf{z}|\theta)$ to the base $p(\mathbf{z})$ using reverse KL:

$$\arg \min_{\theta} KL(\pi(\mathbf{x})||p(\mathbf{x}|\theta)) = \arg \min_{\theta} KL(p(\mathbf{z}|\theta)||p(\mathbf{z})).$$



Flow KL duality

Theorem

$$\arg \min_{\theta} KL(\pi(\mathbf{x})||p(\mathbf{x}|\theta)) = \arg \min_{\theta} KL(p(\mathbf{z}|\theta)||p(\mathbf{z})).$$

Proof

$$\blacktriangleright \mathbf{z} \sim p(\mathbf{z}), \mathbf{x} = g(\mathbf{z}, \theta), \mathbf{x} \sim p(\mathbf{x}|\theta);$$

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

$$\log p(\mathbf{z}|\theta) = \log \pi(g(\mathbf{z}, \theta)) + \log |\det(\mathbf{J}_g)|;$$

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

$$\begin{aligned} KL(p(\mathbf{z}|\theta)||p(\mathbf{z})) &= \mathbb{E}_{p(\mathbf{z}|\theta)} [\log p(\mathbf{z}|\theta) - \log p(\mathbf{z})] = \\ &= \mathbb{E}_{p(\mathbf{z}|\theta)} [\log \pi(g(\mathbf{z}, \theta)) + \log |\det(\mathbf{J}_g)| - \log p(\mathbf{z})] = \\ &= \mathbb{E}_{\pi(\mathbf{x})} [\log \pi(\mathbf{x}) - \log |\det(\mathbf{J}_f)| - \log p(f(\mathbf{x}, \theta))] = \\ &= \mathbb{E}_{\pi(\mathbf{x})} [\log \pi(\mathbf{x}) - \log p(\mathbf{x}|\theta)] = KL(\pi(\mathbf{x})||p(\mathbf{x}|\theta)). \end{aligned}$$

Outline

1. Normalizing flows (NF)
2. Forward and Reverse KL for NF
3. Linear flows

Jacobian structure

Normalizing flows log-likelihood

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

The main challenge is a determinant of the Jacobian matrix.

What is the $\det(\mathbf{J})$ in the following cases?

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

1. Let \mathbf{z} be a permutation of \mathbf{x} .
2. Let z_j depend only on x_j .

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

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

Linear flows

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

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.

Invertible 1x1 conv

$\mathbf{W} \in \mathbb{R}^{c \times c}$ - kernel of 1x1 convolution with c input and c output channels. The computational complexity of computing or differentiating $\det(\mathbf{W})$ is $O(c^3)$. Cost to compute $\det(\mathbf{W})$ is $O(c^3)$. It should be invertible.

Linear flows

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

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, \mathbf{U} is upper triangular with positive diagonal.

► QR-decomposition

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

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

Decomposition should be done only once in the beginning. Next, we fit decomposed matrices ($\mathbf{P}/\mathbf{L}/\mathbf{U}$ or \mathbf{Q}/\mathbf{R}).

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

Hoogeboom E., et al. Emerging convolutions for generative normalizing flows, 2019

Summary

- ▶ Change of variable theorem allows to get the density function of the random variable under the invertible transformation.
- ▶ Normalizing flows transform a simple base distribution to a complex one via a sequence of invertible transformations with tractable Jacobian.
- ▶ Normalizing flows have a tractable likelihood that is given by the change of variable theorem.
- ▶ We fit normalizing flows using forward or reverse KL minimization.
- ▶ Linear flows try to parametrize set of invertible matrices via matrix decompositions.