Deep Generative Models

Lecture 2

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Recap of previous lecture

We are given i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^n \in \mathbb{R}^m$ from unknown distribution $\pi(\mathbf{x})$.

Goal

We would like to learn a distribution $\pi(\mathbf{x})$ for

- evaluating $\pi(\mathbf{x})$ for new samples (how likely to get object $\mathbf{x}$?);
- sampling from $\pi(\mathbf{x})$ (to get new objects $\mathbf{x} \sim \pi(\mathbf{x})$).

Instead of searching true $\pi(\mathbf{x})$ over all probability distributions, learn function approximation $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

Divergence

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

Divergence minimization task

$$\min_{\boldsymbol{\theta}} D(\pi||p).$$

Recap of previous lecture

Forward KL

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

Reverse KL

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

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 minimization of the Monte-Carlo estimate of forward KL.

Recap of previous lecture

Likelihood as product of conditionals

Let $\mathbf{x} = (x_1, \dots, x_m)$, $\mathbf{x}_{1:j} = (x_1, \dots, x_j)$. 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 problem for autoregressive model

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

Sampling

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

New generated object is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m)$.

Outline

1. Autoregressive models (continued)

2. Normalizing flows (NF)

3. Forward and Reverse KL for NF

4. NF examples
   Linear normalizing flows
   Gaussian autoregressive NF

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Autoregressive models: MLP

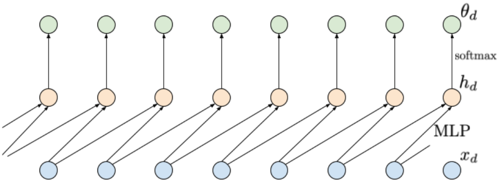
For large j the conditional distribution $p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$ could be infeasible. Moreover, the history $\mathbf{x}_{1:j-1}$ has non-fixed length.

Markov assumption

$$p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}) = p(x_j|\mathbf{x}_{j-d:j-1}, \boldsymbol{\theta}), \quad d \text{ is a fixed model parameter.}$$

Example

- $d = 2$;
- $x_j \in \{0, 255\}$;
- $\mathbf{h}_j = \text{MLP}_{\boldsymbol{\theta}}(x_{j-1}, x_{j-2})$;
- $\boldsymbol{\pi}_j = \text{softmax}(\mathbf{h}_j)$;
- $p(x_j|x_{j-1}, x_{j-2}, \boldsymbol{\theta}) = \text{Categorical}(\boldsymbol{\pi}_j)$.



Is it possible to model continuous distributions instead of discrete one?

image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

Autoregressive models: PixelCNN

Goal

Model a distribution $\pi(\mathbf{x})$ of natural images.

Solution

Autoregressive model on 2D pixels

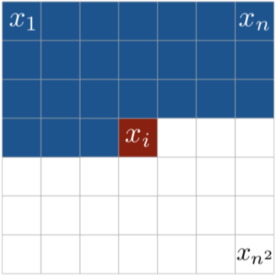
$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{\text{width}\times\text{height}} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}).$$

- We need to introduce the ordering of image pixels.
- The convolution should be **masked** to make them causal.
- The image has RGB channels, these dependencies could be addressed.

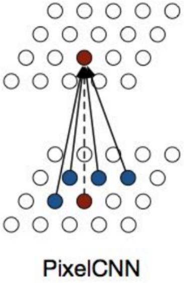
Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

Autoregressive models: PixelCNN

Raster ordering

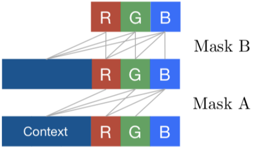


Dependencies between pixels



Mask for the convolution kernel

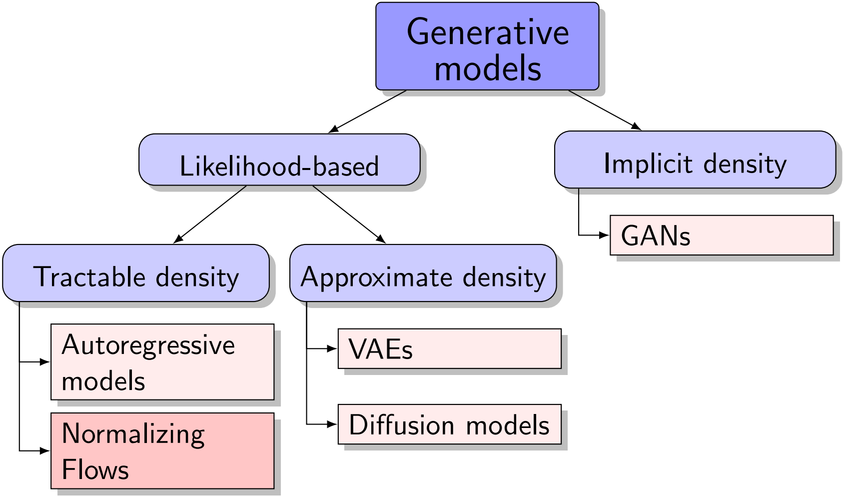
1	1	1
1	0	0
0	0	0



Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

Outline

Generative models zoo



Normalizing flows prerequisites

Jacobian matrix

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

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

Change of variable theorem (CoV)

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

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

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

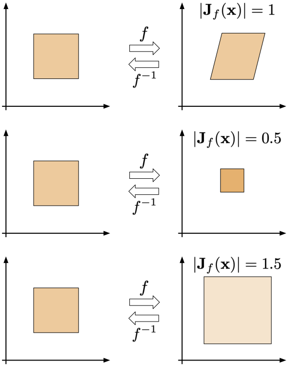
Jacobian determinant

Inverse function theorem

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



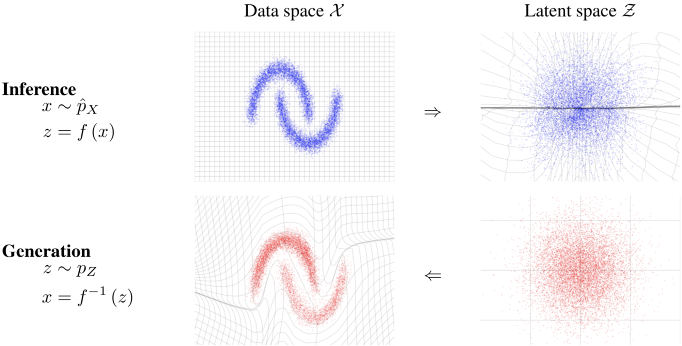
https://jmtomczak.github.io/blog/3/3_flows.html

Fitting normalizing flows

MLE problem

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

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



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

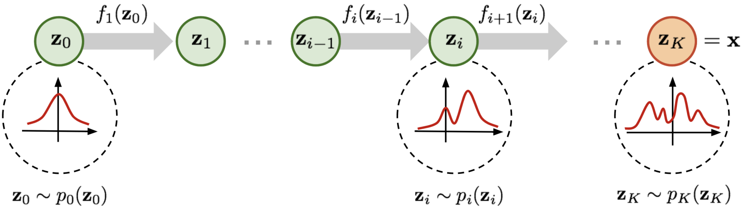
Composition of normalizing flows

Theorem

If $\{\mathbf{f}_k\}_{k=1}^K$ satisfy conditions of the change of variable theorem, then $\mathbf{z} = \mathbf{f}(\mathbf{x}) = \mathbf{f}_K \circ \cdots \circ \mathbf{f}_1(\mathbf{x})$ also satisfies it.

$$p(\mathbf{x}) = p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \dots \frac{\partial \mathbf{f}_1}{\partial \mathbf{x}} \right) \right| =$$

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



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

Normalizing flows (NF)

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

Definition

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

- **Normalizing** means that NF 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

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

Log likelihood

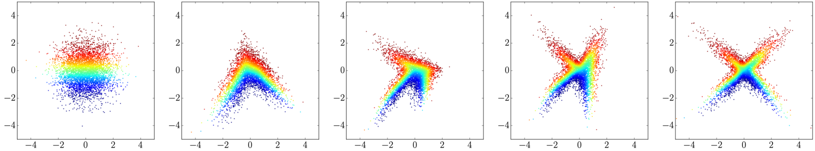
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_K \circ \cdots \circ \mathbf{f}_1(\mathbf{x})) + \sum_{k=1}^{K} \log|\det(\mathbf{J}_{\mathbf{f}_k})|,$$

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 of a 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 is the complexity of the determinant computation?

What do we need?

- efficient computation of the Jacobian matrix $\mathbf{J}_{\mathbf{f}} = \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})}{\partial \mathbf{x}}$;
- efficient inversion of $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$.

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

Outline

Forward KL vs Reverse KL

Forward KL $\equiv$ MLE

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

Forward KL for NF model

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

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

- We need to be able to compute $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ 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 $\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}) = \mathbf{f}_{\boldsymbol{\theta}}^{-1}(\mathbf{z})$ until we want to sample from the NF.

Forward KL vs Reverse KL

Reverse KL

$$KL(p||\pi) = \int p(\mathbf{x}|\boldsymbol{\theta}) \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x})} d\mathbf{x}$$
$$= \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \left[\log p(\mathbf{x}|\boldsymbol{\theta}) - \log \pi(\mathbf{x}) \right] \to \min_{\boldsymbol{\theta}}$$

Reverse KL for NF model (LOTUS trick)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{z}) + \log |\det(\mathbf{J_f})| = \log p(\mathbf{z}) - \log |\det(\mathbf{J_g})|$$

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

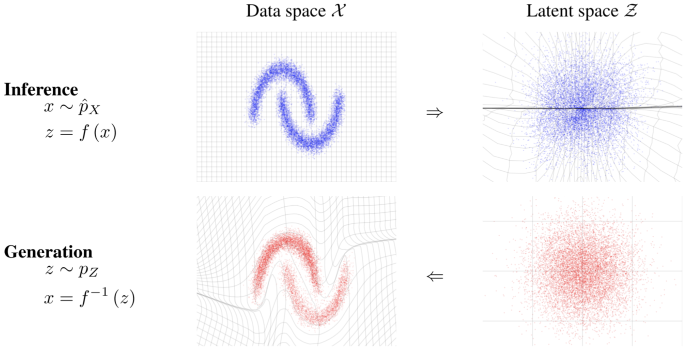
- We need to be able to compute $\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$ and its Jacobian.
- We need to be able to sample from the density $p(\mathbf{z})$ (do not need to evaluate it) and to evaluate(!) $\pi(\mathbf{x})$.
- We don't need to think about computing the function $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$.

Normalizing flows KL duality

Theorem

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

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



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

Normalizing flows KL duality

Theorem

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

Proof

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

$$\log p(\mathbf{z}|\boldsymbol{\theta}) = \log \pi(\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})) + \log|\det(\mathbf{J}_\mathbf{g})|;$$
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) + \log|\det(\mathbf{J}_\mathbf{f})|.$$

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

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

Summary

- PixelCNN model use masked causal convolutions (1D or 2D) to get autoregressive model.
- 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.