Recap Normalizing Flows

Learn complex distribution by mapping from a simple distribution, e.g., Standard Normal

$\Rightarrow$ Change of variable:

$p_1(z)$; $p_2(x)$; $f^{-1}(x) = z$

$$\underline{p_2(x)} = p_1(\underline{f^{-1}(x)}) \cdot \underbrace{\left| \det\left(\frac{\partial f^{-1}(x)}{\partial x} \right) \right|}_{\text{re-normalization}}$$

Main Challenge:

find expression $f(z)$ that is invertible and differentiable

$\swarrow$

Stacking transformations $f_n \circ \ldots \circ f_1$

where it is know that the stacked transformation is invertible and differentiable if each f_i is

Reverse:

$$p_2(x) = p_1(f^{-1}(x)) \, \underline{\left| \det\left(\frac{\partial f^{-1}(x)}{\partial x} \right) \right|}$$

$\hookrightarrow$ Forward: realize $\underline{f^{-1}(x) = z}$ and $\left| \det\left(\frac{\partial f^{-1}(x)}{\partial x} \right) \right| = \frac{1}{\det\left(\frac{\partial f(z)}{\partial z} \right)}$

$$\Rightarrow \quad p_2(x) = \underline{p_1(z)} \cdot \underline{\left| \det\left(\frac{\partial f(z)}{\partial z} \right) \right|^{-1}}$$

Advanced Machine Learning – Deep Generative Models Exercise Sheet 01

Normalizing Flows

Problem 1: Consider the following transformation $f : \mathbb{R}^3 \to \mathbb{R}^3$

$$f(\boldsymbol{z}) = \begin{bmatrix} 2z_1 \\ e^{z_1} z_2 \\ e^{-z_1-z_2} z_3 \end{bmatrix}.$$

Prove or disprove whether the transformation f is invertible.

To compute the inverse $f^{-1}(\boldsymbol{x})$ we need to solve the following system of (non-linear) equations for $\boldsymbol{z}$

$$\begin{cases} x_1 &= 2z_1 \\ x_2 &= e^{z_1} z_2 \\ x_3 &= e^{-z_1-z_2} z_3 \end{cases}.$$

The solution to this is

$$\begin{cases} z_1 &= \frac{1}{2}x_1 \\ z_2 &= e^{-\frac{1}{2}x_1} x_2 \\ z_3 &= e^{\frac{1}{2}x_1 + e^{-\frac{1}{2}x_1} x_2} x_3 \end{cases}.$$

The solution is unique and well-defined for any $\boldsymbol{x} = (x_1, x_2, x_3)^T \in \mathbb{R}^3$. Therefore, the function f is invertible.

Problem 2: Consider the following transformation $f : \mathbb{R}^2 \to \mathbb{R}^2$:

$$f(\boldsymbol{z}) = \begin{bmatrix} z_1^2 z_2 \\ z_2^3 \end{bmatrix}.$$

Prove or disprove whether the transformation f is invertible.

To prove that a transformation is not invertible, it is sufficient to find to points $\boldsymbol{z}^{(1)} \neq \boldsymbol{z}^{(2)}$ such that $f(\boldsymbol{z}^{(1)}) = f(\boldsymbol{z}^{(2)})$. This would mean that the transformation f is not one-to-one, and therefore not bijective (=not invertible). or any $a, b \in \mathbb{R}$ with $[a,0]^T; [b,0]^T \to \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

For example, consider $\boldsymbol{z}^{(1)} = [1, 0]^T$ and $\boldsymbol{z}^{(2)} = [-1, 0]^T$. Both points get mapped to the same value $[0, 0]$, therefore the transformation f is not invertible.

Problem 3: Consider the tranformation $f(\boldsymbol{z}) = \boldsymbol{A}\boldsymbol{z} + \boldsymbol{b}$ from $\mathbb{R}^2$ to $\mathbb{R}^2$, where $\boldsymbol{A} \in \mathbb{R}^{2\times 2}$ and $\boldsymbol{b} \in \mathbb{R}^2$. Under what conditions on $\boldsymbol{A}$ and $\boldsymbol{b}$ is this tranformation invertible? Justify your answer.

The Jacobian determinant of a linear transformation f is:

$$\det \frac{\partial f(\boldsymbol{z})}{\partial \boldsymbol{z}} = \det \boldsymbol{A}^T = \det \boldsymbol{A}$$

We can compute the determinant of a matrix $\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \in \mathbb{R}^{2\times 2}$ in closed form:

$$\det \boldsymbol{A} = a_{11}a_{22} - a_{21}a_{12}$$

The necessary and sufficient condition for f to be invertible is $a_{11}a_{22} - a_{21}a_{12} \neq 0$. There is no condition on $\boldsymbol{b}$. as a shift does not change the volume

Problem 4: We consider the following forward tranformation $f \colon \mathbb{R}^3 \to \mathbb{R}^3$

$$\boldsymbol{x} = f(\boldsymbol{z}) = \begin{bmatrix} z_1 \\ e^{z_1} z_2 \\ \sqrt[3]{e^{-z_1} z_3 + z_1^2} \end{bmatrix}.$$

We assume a uniform base distribution $p_1(\boldsymbol{z}) = U([0,2]^3)$. Evaluate the density $p_2(\boldsymbol{x})$ at the points $\boldsymbol{x}^{(1)} = \begin{bmatrix} 0 \\ 1 \\ \frac{1}{3} \end{bmatrix}$ and $\boldsymbol{x}^{(2)} = \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}$.

Our goal is to perform density estimation. This can be done using the change of variables formula as

Reverse

$$p_2(\boldsymbol{x}) = p_1(f^{-1}(\boldsymbol{x})) \left| \det \frac{\partial f^{-1}(\boldsymbol{x})}{\partial \boldsymbol{x}} \right|.$$

For this we need to

1. compute the inverse transformation $f^{-1}(\boldsymbol{x})$,
2. the Jacobian determinant $\det \frac{\partial f^{-1}(\boldsymbol{x})}{\partial \boldsymbol{x}}$.

To obtain the inverse we need to solve a system of (non-linear) equations for $\boldsymbol{z}$

$$\begin{cases} x_1 = z_1 \\ x_2 = e^{z_1} z_2 \\ x_3 = \sqrt[3]{e^{-z_1} z_3 + z_1^2} \end{cases}$$

$$\begin{cases} z_1 = x_1 \\ z_2 = x_2 e^{-x_1} \\ z_3 = (x_3^3 - x_1^2) e^{x_1} \end{cases}$$

That is, we can compute the inverse transformation $f^{-1}(\boldsymbol{x})$ as

$$f^{-1}(\boldsymbol{x}) = \begin{bmatrix} x_1 \\ x_2 e^{-x_1} \\ (x_3^3 - x_1^2) e^{x_1} \end{bmatrix}.$$

Second, we compute the Jacobian determinant. We notice that the Jacobian is triangular. Hence, we only need the diagonal entries to compute its determinant:

$$\left|\det \frac{\partial f^{-1}(\boldsymbol{x})}{\partial \boldsymbol{x}}\right| = \begin{vmatrix} 1 & 0 & 0 \\ * & e^{-x_1} & 0 \\ * & * & 3x_3^2 e^{x_1} \end{vmatrix} = 3x_3^2. \quad = \cancel{1 \cdot e^{-x}} \cdot 3x_3^2 \cancel{e^{x_1}}$$

Third, we compute the inverse of $\boldsymbol{x}^{(1)} = \begin{bmatrix} 0 \\ 1 \\ \frac{1}{3} \end{bmatrix}$ and $\boldsymbol{x}^{(2)} = \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}$:

$$f^{-1}(x^{(1)}) = \begin{bmatrix} 0 \\ 1 \cdot e^{-1} \\ ((\frac{1}{3})^3 - 0) \cdot 1 \end{bmatrix}$$

$$f^{-1}(\boldsymbol{x}^{(1)}) = \begin{bmatrix} 0 \\ 1 \\ \frac{1}{27} \end{bmatrix} = \boldsymbol{z}^{(1)}$$

$$f^{-1}(x^{(2)}) = \begin{bmatrix} -1 \\ 2 \cdot e \\ (1-1) \cdot e^{-1} \end{bmatrix}$$

$$f^{-1}(\boldsymbol{x}^{(2)}) = \begin{bmatrix} -1 \\ 2e \\ 0 \end{bmatrix} = \boldsymbol{z}^{(2)}$$

Finally, we use the change of variables formula. Since $f^{-1}(\boldsymbol{x}^{(1)}) \in [0,2]^3$, we have $p_1(f^{-1}(\boldsymbol{x}^{(1)})) = \frac{1}{2^3}$:

as for any point in $[0,2]^3$

$$\begin{aligned} p_2(\boldsymbol{x}^{(1)}) &= p_1(f^{-1}(\boldsymbol{x}^{(1)})) \left|\det \frac{\partial f^{-1}(\boldsymbol{x}^{(1)})}{\partial \boldsymbol{x}}\right| \\ &= \frac{1}{2^3} \cdot 3 \cdot \frac{1}{9} = \frac{1}{24} \end{aligned}$$

Since $f^{-1}(\boldsymbol{x}^{(2)}) \notin [0,2]^2$, we have $p_1(f^{-1}(\boldsymbol{x}^{(2)})) = 0$:

$$\begin{aligned} p_2(\boldsymbol{x}^{(2)}) &= p_1(f^{-1}(\boldsymbol{x}^{(2)})) \left|\det \frac{\partial f^{-1}(\boldsymbol{x}^{(2)})}{\partial \boldsymbol{x}}\right| \\ &= 0 \end{aligned}$$

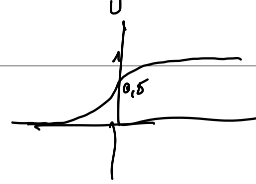
Problem 5: We consider the following forward transformation $x = f(z) = \sum_{k=1}^{K} \sigma(kz)$ from $\mathbb{R}$ to $(0, K)$ with $\sigma(z) = \frac{1}{1+e^{-z}}$. We assume a Gaussian base distribution $p_1(z) = \mathcal{N}(0,1)$. We sampled one point from the base distribution $z^{(1)} = 0$. Compute the corresponding sample $x^{(1)}$ from the transformed distribution and evaluate its density $p_2(x^{(1)})$.

To compute the sampled value $x^{(1)}$, we need to compute the forward transformation of $z^{(1)}$:

$$f(z^{(1)}) = \sum_{k=1}^{K} \underbrace{\sigma(k \times 0)}_{\frac{1}{2}} = \frac{K}{2}.$$

(Remember that $\sigma(0) = \frac{1}{2}$)

Sigmoid



To evaluate the density, we need first the Jacobian determinant:

$$\begin{aligned}\left|\det \frac{\partial f(z)}{\partial z}\right| &= f'(z) \\ &= \sum_{k=1}^{K} \sigma'(kz) \\ &= \sum_{k=1}^{K} k\sigma(kz)(1-\sigma(kz))\end{aligned}$$

Using the chain rule

$$\frac{\partial \sigma(kz)}{\partial z} = \frac{\partial \sigma(kz)}{\partial kz} \cdot \frac{\partial kz}{\partial z}$$

$$= \underbrace{(1-\sigma(kz))\cdot\sigma(kz)}_{\frac{\partial \sigma(x)}{\partial x}} \cdot k$$

Using the change of variables formula, we obtain:

$$\begin{aligned}p_2(x^{(1)}) &= p_1(z^{(1)}) \left|\det \frac{\partial f(z^{(1)})}{\partial z}\right|^{-1} \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{\sum_{k=1}^{K} k\underbrace{\sigma(k \times 0)}_{\frac{1}{2}}(1-\underbrace{\sigma(k \times 0)}_{\frac{1}{2}})} \\ &= \frac{1}{\sqrt{2\pi}} \frac{4}{\sum_{k=1}^{K} k} \\ &= \frac{1}{\sqrt{2\pi}} \frac{8}{K(K+1)}.\end{aligned}$$

$$p_1(0) = \frac{1}{1\cdot\sqrt{2\pi}} \cdot e^{-\frac{1}{2}\left(\frac{0-0}{1}\right)^2}$$