

Machine Learning for Graphs and Sequential Data Exercise Sheet 01

Normalizing Flows

Problem 1:

(a) We consider the following transformations:

- $f(\mathbf{z}) = \begin{bmatrix} 10z_1 + 1 \\ \cos(z_1)z_2 \\ \sin(z_1z_2) \end{bmatrix}$ from \mathbb{R}^3 to $\mathbb{R} \times \mathbb{R} \times [-1, 1]$.
- $f(\mathbf{z}) = \begin{bmatrix} z_1^3 \\ e^{z_1}z_2^5 \\ e^{-z_1-z_2}z_3^7 \end{bmatrix}$ from \mathbb{R}^3 to \mathbb{R}^3 .

Are these transformations invertible ?

(b) We consider the transformation $f(\mathbf{z}) = \begin{bmatrix} \sin(z_1) \\ \cos(z_2) \end{bmatrix}$ from $[a, b] \times [c, d]$ to $[-1, 1]^2$. Under what conditions on a, b, c, d is this transformation invertible ?

(c) We consider the transformation $f(\mathbf{z}) = \mathbf{A}\mathbf{z} + \mathbf{b}$ from \mathbb{R}^2 to \mathbb{R}^2 , where $\mathbf{A} \in \mathbb{R}^{2 \times 2}$ and $\mathbf{b} \in \mathbb{R}^2$. Under what conditions on \mathbf{A} and \mathbf{b} is this transformation invertible ?

Problem 2: We consider the following forward transformation $f(\mathbf{z}) = \begin{bmatrix} z_1 \\ e^{z_1}z_2 \\ |1 + z_2|z_3 + \sin(z_1) \end{bmatrix} = \mathbf{x}$ from \mathbb{R}^3 to \mathbb{R}^3 . We assume a uniform base distribution $p_1(\mathbf{z}) = U([0, 2]^3)$. Evaluate the density $p_2(\mathbf{x})$ at the two points $\mathbf{x}^{(1)} = \begin{bmatrix} 1 \\ 2e \\ 3 + \sin(1) \end{bmatrix}$ and $\mathbf{x}^{(2)} = \begin{bmatrix} 2 \\ e^2 \\ 6 + \sin(2) \end{bmatrix}$.

Problem 3: 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 $p_2(x^{(1)})$.

Problem 4: We consider the forward transformation $x = f(z) = az + b$ from \mathbb{R} to \mathbb{R} where $a, b \in \mathbb{R}$ are learnable parameters. We assume a Gaussian base distribution $p_1(z) = \mathcal{N}(0, 1)$. We observed three points $x^{(1)} = 0, x^{(2)} = 1, x^{(3)} = 2$. Compute the maximum likelihood estimate of the parameters a, b .
