Normalizing Flows

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Abstract

Notes on normalizing flows.

1 Introduction

Simple distributions (e.g., Gaussian) are often used as likelihood distributions. However, the true distribution is often far from this simple distribution and this results in issues such as blurry reconstructions in the case of images. Latent variable models such as VAEs often set the prior distribution $p(\mathbf{z})$ to a factorial multivariate Gaussian distribution. Such a simplistic assumption hampers the model in multiple ways. For instance, this does not allow a multi-modal latent space distribution. Normalizing Flows allow transformation of samples from a simple distribution (subsequently denoted by q_0) to samples from a complex distribution by applying a series of invertible flows.

1.1 Distribution of a Simple Transformation of a RV

Before jumping into normalizing flows, let's consider a simple univariate distribution $p(x) = 2x$ with support $x \in [0, 1]$. Define a function $y = f(x) = x^2$. Note that $f(x)$ is monotonically increasing in $[0, 1]$. What is the PDF of the variable y?

We can compute $p(y)$ using the CDFs as follows.

$$F_Y(y) = P(Y \leq y) \tag{1}$$
$$= P(X^2 \leq y) \tag{2}$$
$$= P(X \leq \sqrt{y}) \tag{3}$$
$$= F_X(\sqrt{y}) \tag{4}$$

Now, $p(y) = F_Y'(y) = \frac{dF_X(\sqrt{y})}{dy}$ where

$$F_X(\sqrt{y}) = \int_0^{\sqrt{y}} p(x)dx \tag{5}$$

$$= \left[2\frac{x^2}{2}\right]_0^{\sqrt{y}} \tag{6}$$

$$= y \tag{7}$$

differentiating w.r.t. y we get $\frac{d(y)}{dy} = 1$ which means that $p(y) = \mathcal{U}(0,1)$.

1.2 Change of Variables

The method described above can be extended to multivariate distributions $q_0(\mathbf{z})$ and smooth invertible mappings $f : \mathbb{R}^d \Rightarrow \mathbb{R}^d$. Samples $\mathbf{z} \sim q_0(\mathbf{z})$ can be transformed using f to give $\mathbf{y} = f(\mathbf{z})$. The PDF of $\mathbf{y}$ is given by

$$q_1(\mathbf{y}) = q_0(\mathbf{z}) \left|\det \frac{\partial f^{-1}}{\partial \mathbf{y}}\right| = q_0(\mathbf{z}) \left|\det \frac{\partial f}{\partial \mathbf{z}}\right|^{-1} \tag{8}$$

where the second equality comes from the inverse-function theorem.

Rezende et. al. proposed two different families of invertible transformations: planar flow and radial flow.

2 Planar Flow

Planar flows use functions of form

$$f(\mathbf{z}) = \mathbf{z} + \mathbf{u}h(\mathbf{w}^\top \mathbf{z} + b) \tag{9}$$

where $\mathbf{u}, \mathbf{w} \in \mathbb{R}^d$, $b \in \mathbb{R}$, and h is an element-wise non-linearity such as tanh. The Jacobian is then given by

$$\frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} = \mathbf{I} + \mathbf{u}h'(\mathbf{w}^\top \mathbf{z} + b)\mathbf{w}^\top$$

Now, using the matrix determinant lemma

$$\det \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} = (1 + h'(\mathbf{w}^\top \mathbf{z} + b)\mathbf{w}^\top \mathbf{I}^{-1}\mathbf{u}) \det(\mathbf{I}) \tag{10}$$

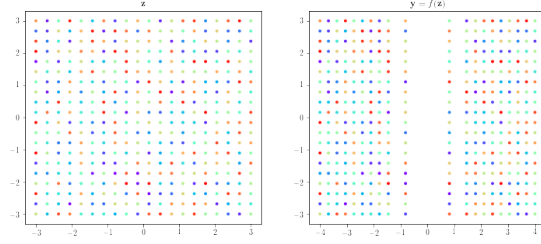$$= (1 + h'(\mathbf{w}^\top \mathbf{z} + b)\mathbf{w}^\top \mathbf{u}) \tag{11}$$

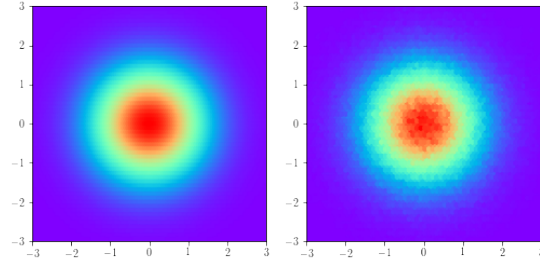Figure 1: Applying planar flow to uniformly spaced points

Figure 2: Analytic and empirical density $q_0(\mathbf{z})$

2.1 Example

Let's look at a specific example for $\mathbf{z} \in \mathbb{R}^2$. We will apply a planar flow to $\mathbf{z}$ to get $\mathbf{y} = f(\mathbf{z})$.

$$q_0(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})$$
$$\mathbf{w} = \begin{bmatrix} 5 & 0 \end{bmatrix}^\top$$
$$\mathbf{u} = \begin{bmatrix} 1 & 0 \end{bmatrix}^\top$$
$$b = 0$$
$$h(\mathbf{x}) = \tanh(\mathbf{x})$$

The determinant of the Jacobian can be computed using Eq. (11) and the analytic PDF $q_1(\mathbf{y})$ can then be computed using Eq. (8). The effect of the flow on uniformly space points is shown in Figure 1. The analytic density $q_0(\mathbf{z})$ and the corresponding empirical density plotted as a 2D histogram of samples from $q_0(\mathbf{z})$ is shown in Figure 2. The analytic density $q_1(\mathbf{y})$ computed using Eq. (8) and the corresponding empirical density plotted as a 2D histogram of variables $\mathbf{y}$ obtained by applying f to samples from $q_0(\mathbf{z})$ is shown in Figure 3.
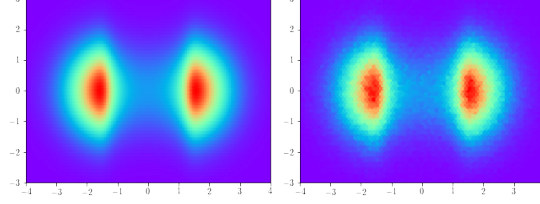
Figure 3: Analytic and empirical density $q_1(\mathbf{y})$ after applying planar flow

3 Radial Flow

Radial flows use functions of the form

$$f(\mathbf{z}) = \mathbf{z} + \beta h(\alpha, r)(\mathbf{z} - \mathbf{z}_0)$$

where $\alpha \in \mathbb{R}^+$, $\beta \in \mathbb{R}$, $h(\alpha, r) = (\alpha + r)^{-1}$ and $r = ||\mathbf{z} - \mathbf{z}_0||$.
The Jacobian is then given by

$$\frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} = \mathbf{I} + \beta \left((\mathbf{z} - \mathbf{z}_0)h'(\alpha, r)\frac{\partial r}{\partial \mathbf{z}} + h(\alpha, r)\mathbf{I} \right)$$

$$= (1 + \beta h(\alpha, r))\mathbf{I} + \beta h'(\alpha, r)(\mathbf{z} - \mathbf{z}_0)\frac{(\mathbf{z} - \mathbf{z}_0)^\top}{||\mathbf{z} - \mathbf{z}_0||}$$

Let $\gamma = (1 + \beta h(\alpha, r))$. Again, using the matrix determinant lemma

$$\det \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} = \left(1 + \beta h'(\alpha, r)\frac{(\mathbf{z} - \mathbf{z}_0)^\top}{||\mathbf{z} - \mathbf{z}_0||}\frac{\mathbf{I}}{\gamma}(\mathbf{z} - \mathbf{z}_0) \right) \det(\gamma \mathbf{I}) \tag{12}$$

$$= \left(\frac{1 + \beta h(\alpha, r) + \beta h'(\alpha, r)||\mathbf{z} - \mathbf{z}_0||}{(1 + \beta h(\alpha, r))} \right) (1 + \beta h(\alpha, r))^d \tag{13}$$

$$= (1 + \beta h(\alpha, r) + \beta h'(\alpha, r)r) (1 + \beta h(\alpha, r))^{d-1} \tag{14}$$

3.1 Example

Let's look at a specific example for $\mathbf{z} \in \mathbb{R}^2$. We will apply a radial flow to $\mathbf{z}$ to get $\mathbf{y} = f(\mathbf{z})$.

$$q_0(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I}) \tag{15}$$

$$\mathbf{z}_0 = \begin{bmatrix} 1 & 0 \end{bmatrix}^\top \tag{16}$$

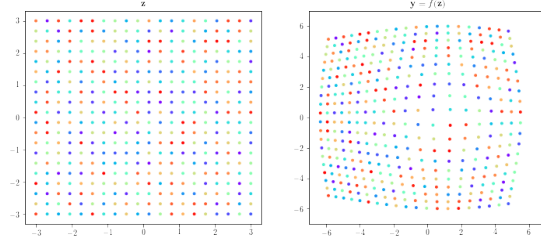$$\alpha = 2 \tag{17}$$

$$\beta = 5 \tag{18}$$

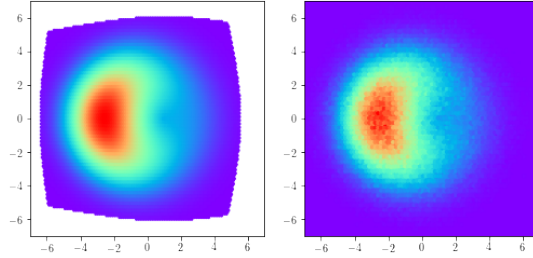Figure 4: Applying radial flow to uniformly spaced points

Figure 5: Analytic and empirical density $q_1(\mathbf{y})$ after applying radial flow

The determinant of the Jacobian can be computed using Eq. (14) and the analytic PDF $q_1(\mathbf{y})$ can then be computed using Eq. (8). The effect of the flow on uniformly space points is shown in Figure 4. The analytic density $q_0(\mathbf{z})$ and the corresponding empirical density plotted as a 2D histogram of samples from $q_0(\mathbf{z})$ is shown in Figure 2. The analytic density $q_1(\mathbf{y})$ computed using Eq. (8) and the corresponding empirical density plotted as a 2D histogram of variables $\mathbf{y}$ obtained by applying f to samples from $q_0(\mathbf{z})$ is shown in Figure 5.