Appendix: On the expressivity of bi-Lipschitz normalizing flows

Alexandre Verine ALEXANDRE.VERINE@DAUPHINE.PSL.EU
Benjamin Negrevergne BENJAMIN.NEGREVERGNE@DAUPHINE.PSL.EU
Yann Chevaleyre YANN.CHEVALEYRE@DAUPHINE.PSL.EU
LAMSADE, Université Paris-Dauphine, PSL, Paris, France

Fabrice Rossi ROSSI@CEREMADE.DAUPHINE.FR
CEREMADE, Université Paris-Dauphine, PSL, Paris, France

Editors: Emtiyaz Khan and Mehmet Gönen

Appendix A. Proofs

A.1. Proof of theorem 6

By definition we have $\widehat{P}(A) = \int_A \hat{p}(\boldsymbol{x})d\boldsymbol{x}$, then with the change of variable formula we obtain :

$$\begin{aligned}\widehat{P}(A) &= \int_A |\mathrm{Jac}_F(\boldsymbol{x})| q(F(\boldsymbol{x}))d\boldsymbol{x} \\ &= \frac{1}{(2\pi)^{d/2}} \int_A |\mathrm{Jac}_F(\boldsymbol{x})| e^{-\|F(\boldsymbol{x})\|^2/2} d\boldsymbol{x}\end{aligned}$$

As F is L_1-Lipschitz we have $|\mathrm{Jac}_F(\boldsymbol{x})| \leq L_1^d$, then

$$\begin{aligned}\widehat{P}(A) &\leq \left(\frac{L_1}{\sqrt{2\pi}}\right)^d \int_A e^{-\|F(\boldsymbol{x})\|_2^2} d\boldsymbol{x} \\ &\leq \left(\frac{L_1}{\sqrt{2\pi}}\right)^d \int_A d\boldsymbol{x} \\ &\leq \left(\frac{L_1}{\sqrt{2\pi}}\right)^d \mathrm{vol}(A),\end{aligned}$$

and thus $TV(P^*, \widehat{P}) = \sup_A |P^*(A) - \widehat{P}(A)|$ implies

$$TV(P^*, \widehat{P}) \geq \sup_A \left(P^*(A) - \left(\frac{L_1}{\sqrt{2\pi}}\right)^d \mathrm{vol}(A) \right)$$

A.2. Proof of theorem 7

By definition of the TV distance, we have

$$\mathcal{D}_{\mathrm{TV}}(P^*, \widehat{P}) \geq \sup_{R,\boldsymbol{x}_0} |P^*(B_{R,\boldsymbol{x}_0}) - Q(F(B_{R,\boldsymbol{x}_0}))|,$$

where $B_{R,\boldsymbol{x}_0}$ is the ball of a radius R centered in $\boldsymbol{x}_0$.

Then, the idea is to show that the image of a ball B_R by a L_1-Lipschitz function is in a ball of radius $L_1 R$, and then use a reverse isoperimetric inequality the find an upper bound of the measure of a ball of a radius $L_1 R$.

Proof of $F(B_{R,\boldsymbol{x}_0}) \subset B_{L_1R,F(\boldsymbol{x}_0)}$

First of all, for every $\boldsymbol{z} \in F(B_{R,\boldsymbol{x}_0})$, there exist $\boldsymbol{x} \in B_R$ such that $F^{-1}(\boldsymbol{z}) = \boldsymbol{x}$, we have :

$$\begin{aligned} \|F(F^{-1}(\boldsymbol{z})) - F(\boldsymbol{x}_0)\| &= \|F(\boldsymbol{x}) - F(\boldsymbol{x}_0)\| \\ &\leq L_1\|\boldsymbol{x} - \boldsymbol{x}_0\| \\ &\leq L_1 R \end{aligned}$$

Upper bound of $Q(B_{L_1R})$ This bound is extracted from the work of Ball (1993) on the Reverse Isoperimetric Inequality. First of all, it can be easily establish that $Q(B_{L_1R}(F(\boldsymbol{x}_0)))$ is at a maximum when $F(\boldsymbol{x}_0) = 0$. From now on, we will only consider B_{L_1R} the ball centered on 0. Therefore the objective is to find an upper bound on :

$$\begin{aligned} Q(B_{L_1R}) &= \int_{\|\boldsymbol{z}\|<L_1R} q(\boldsymbol{z}) d\boldsymbol{z} \\ &= \int_{\|\boldsymbol{z}\|<L_1R} \frac{1}{(\sqrt{2\pi})^d} e^{-\|\boldsymbol{z}\|^2/2} d\boldsymbol{z} \end{aligned}$$

We can use the polar coordinates system to get another expression of the Gaussian measure with $S_{d-1}(r) = \frac{2\pi^{d/2} r^{d-1}}{Q(d/2)}$ being the volume of the hypersphere :

$$\begin{aligned} Q(B_{L_1R}) &= \frac{1}{(2\pi)^{d/2}} \int_0^{L_1R} S_{d-1}(r) e^{-r^2/2} dr \\ &= \frac{2}{2^{d/2}\Gamma(d/2)} \int_0^{L_1R} r^{d-1} e^{-r^2/2} dr \end{aligned}$$

However $r^{d-1}e^{-r^2/2}$ has a maximum value reached for $r = \sqrt{d-1}$, we can have an upper bound :

$$\begin{aligned} Q(B_{L_1R}) &\leq \frac{2}{2^{d/2}\Gamma(d/2)} \sqrt{d-1}^{d-1} e^{-\frac{d-1}{2}} \int_0^{L_1R} dr \\ &\leq \frac{\sqrt{2}L_1R}{\Gamma(d/2)} \left(\frac{d-1}{2e}\right)^{\frac{d-1}{2}} \end{aligned}$$

Then, with the Stirling approximation of the Gamma function:

$$\begin{aligned} \frac{1}{2}\Gamma(d/2) = \frac{1}{d}\Gamma(d/2+1) \\ &\geq \frac{\sqrt{\pi}\sqrt{d}}{d}(d/2)^{d/2} e^{-d/2} \\ &\geq \frac{\sqrt{\pi}}{2^{d/2}} d^{\frac{d-1}{2}} e^{-\frac{d}{2}} \end{aligned}$$

We obtain:

$$\begin{aligned} Q(B_{L_1R}) &\leq \frac{2}{2^{d/2}\Gamma(d/2)} (d-1)^{\frac{d-1}{2}} e^{-\frac{d-1}{2}} \\ &\leq \frac{L_1R\sqrt{e}}{\sqrt{\pi}} \left(\frac{d-1}{d}\right)^{\frac{d-1}{2}} \end{aligned}$$

Using the bound

$$\frac{1}{\sqrt{e}} < \left(\frac{d-1}{d}\right)^{\frac{d-1}{2}},$$

we have

$$Q(B_{L_1R}) < \frac{L_1R}{\sqrt{\pi}}$$

Lower Bound of the TV As soon as we have an upper bound on $Q(B_{L_1R})$, we have :

$$\begin{aligned}\mathcal{D}_{\mathrm{TV}}(P^*, \widehat{P}) &\geq \sup_{R,\boldsymbol{x}_0} \left(P^*(B_{R,\boldsymbol{x}_0}) - Q(F(B_{R,\boldsymbol{x}_0}))\right) \\ &\geq \sup_{R,\boldsymbol{x}_0} \left(P^*(B_{R,\boldsymbol{x}_0}) - Q(B_{L_1R,\boldsymbol{x}_0})\right) \\ &\geq \sup_{R,\boldsymbol{x}_0} \left(P^*(B_{R,\boldsymbol{x}_0}) - \frac{L_1R}{\sqrt{\pi}}\right)\end{aligned}$$

A.3. Proof of Theorem 8

Value of $Q(B_{R,0})$ By construction

$$Q(B_{R,0}) = \mathbb{P}\left(\|\boldsymbol{z}\|^2 \leq R^2\right),$$

when $\boldsymbol{z}$ follows the standard Gaussian distribution in $\mathbb{R}^d$. This quantity can be computed using the cumulative distribution function of the chi-square distribution, i.e.

$$Q(B_{R,0}) = \frac{\gamma\left(\frac{d}{2}, \frac{R^2}{2}\right)}{\Gamma\left(\frac{d}{2}\right)},$$

where γ is the lower incomplete gamma function given by

$$\gamma(x, k) = \int_0^x t^{k-1} e^{-t} dt.$$

Lower Bound of the TV Since we have the closed form of the measure over a ball we can write :

$$\begin{aligned}\mathcal{D}_{\mathrm{TV}}(P^*, \widehat{P}) &\geq \sup_{R,\boldsymbol{x}_0} \left(P^*(B_{R,\boldsymbol{x}_0}) - Q(F(B_{R,\boldsymbol{x}_0}))\right) \\ &\geq \sup_{R,\boldsymbol{x}_0} \left(P^*(B_{R,\boldsymbol{x}_0}) - Q(B_{L_1R,\boldsymbol{x}_0})\right) \\ &\geq \sup_{R,\boldsymbol{x}_0} \left(P^*(B_{R,\boldsymbol{x}_0}) - \frac{\gamma\left(\frac{d}{2}, \frac{L_1^2R^2}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}\right)\end{aligned}$$

A.4. Proof of theorem 9

In this section, we denote $B_R = B_{R,F^{-1}(0)}$. As F^{-1} is L_2-Lipschitz, $F^{-1}(B_{R/L_2,0}) \subset B_R$ and thus

$$\widehat{P}(B_R) \geq \widehat{P}(F^{-1}(B_R)) = Q(B_{R/L_2,0}).$$

Therefore, by analogy with the proof of Theorem 8:

$$\begin{aligned}
\mathcal{D}_{\text{TV}}(P^*, \widehat{P}) &\geq \sup_R \left(Q(F(B_R)) - P^*(B_R)\right) \\
&\geq \sup_R \left(Q(B_{R/L_2}) - P^*(B_R)\right) \\
&\geq \sup_R \left(\frac{\gamma\left(\frac{d}{2}, \frac{R^2}{2L_2^2}\right)}{\Gamma\left(\frac{d}{2}\right)} - P^*(B_R)\right)
\end{aligned}$$

A.5. Proof of Corollary 10

Since M_1 and M_2 are separated by a distance D the ball centered on $F^{-1}(0)$ has a radius at least as big as D that we might call B_D to simplify the notation. Therefore :

$$\begin{array}{rcl}
\bar{\alpha} &=& \widehat{P}(M_1) + \widehat{P}(M_2) \\
&=& 1 - \widehat{P}(\overline{M_2 \cup M_1}) \\
&\leq& 1 - \widehat{P}(B_D) \\
&\leq& 1 - Q(F(B_D)) \\
&\leq& 1 - Q(B_{D/L_2})) \\
&\leq& 1 - \frac{\gamma(\frac{d}{2}, \frac{D^2}{2L_2^2})}{\Gamma(\frac{d}{2})}
\end{array}$$

And since $P^*(B_D) = 0$:

$$\begin{array}{rcl}
\mathcal{D}_{\text{TV}}(P^*, \widehat{P}) &\geq& |\widehat{P}(B_D) - P^*(B_D)| \\
&\geq& \widehat{P}(B_D(F^{-1}(0)) \\
&\geq& \frac{\gamma(\frac{d}{2}, \frac{D^2}{2L_2^2})}{\Gamma(\frac{d}{2})}
\end{array}$$

A.6. Bounds for learned variance

For a given variance σ^2 and the corresponding covariance matrix $\sigma^2 I$, the Gaussian measure of a ball $Q_\sigma(B_R)$ of radius R associated can be written as :

$$\begin{array}{rcl}
Q_\sigma(B_R) &=& \int_{\|\boldsymbol{z}\|<L_1 R} q_\sigma(\boldsymbol{z}) d\boldsymbol{z} \\
&=& \int_{\|\boldsymbol{z}\|<R} \frac{1}{(\sqrt{2\pi})^d \sigma^d} e^{-\|\boldsymbol{z}\|^2/2\sigma^2} d\boldsymbol{z}
\end{array}$$

Then, with the proper change of variable $z' = z/\sigma$, we have :

$$\begin{array}{rcl}
Q_\sigma(B_R) &=& \int_{\|\sigma \boldsymbol{z}'\|<R} \frac{1}{(\sqrt{2\pi})^d \sigma^d} e^{-\|\boldsymbol{z}\|^2/2} \left|\sigma I\right| d\boldsymbol{z}' \\
&=& \int_{\|\boldsymbol{z}\|<\frac{R}{\sigma}} \frac{1}{(\sqrt{2\pi})^d} e^{-\|\boldsymbol{z}\|^2/2} d\boldsymbol{z} \\
&=& Q(B_{R/\sigma})
\end{array}$$

Hence the two bounds become :

$$\mathcal{D}_{\text{TV}}(P^*, \widehat{P}) \geq \sup_{R, \boldsymbol{x}_0} \left(P^*(B_{R,\boldsymbol{x}_0}) - \frac{\gamma(\frac{d}{2}, \frac{L_1^2 R^2}{2\sigma^2})}{\Gamma(\frac{d}{2})}\right),$$

and

$$\mathcal{D}_{\mathrm{TV}}(P^*, \widehat{P}) \geq \sup_R \left(\frac{\gamma(\frac{d}{2}, \frac{\sigma^2 R^2}{2L_2^2})}{\Gamma(\frac{d}{2})} - P^*(B_{R,F^{-1}(0)}) \right).$$

Appendix B. 2D datsets

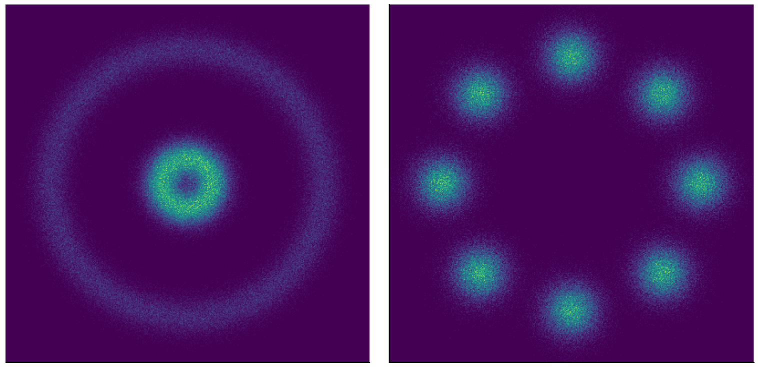

Figure B.1: 2D Dataset : *Circles* (left) and *8 Gaussians* (right).

Appendix C. Inverse image of the center of the Gaussian latent distribution

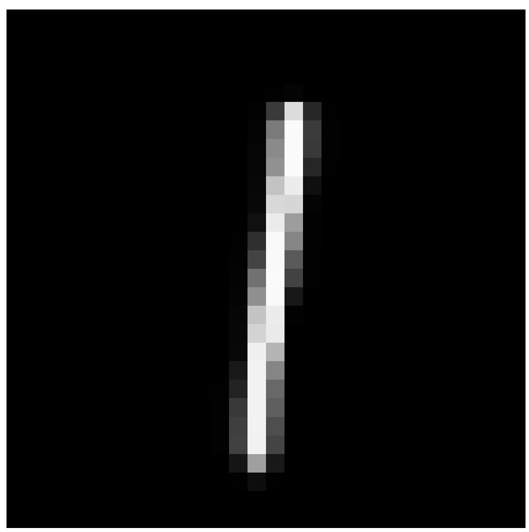

Figure C.2: Image of $F^{-1}(0)$ for *MNIST* of the Residual Flow of Chen et al. (2020)

Figure C.3: Image of $F^{-1}(0)$ for *CIFAR10* of the Residual Flow of Chen et al. (2020)