A RAD APPROACH TO DEEP MIXTURE MODELS

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ABSTRACT

Flow based models such as Real NVP are an extremely powerful approach to density estimation. However, existing flow based models are restricted to transforming continuous densities over a continuous input space into similarly continuous distributions over continuous latent variables. This makes them poorly suited for modeling and representing discrete structures in data distributions, for example class membership or discrete symmetries. To address this difficulty, we present a normalizing flow architecture which relies on domain partitioning using locally invertible functions, and possesses both real and discrete valued latent variables. This Real and Discrete (RAD) approach retains the desirable normalizing flow properties of exact sampling, exact inference, and analytically computable probabilities, while at the same time allowing simultaneous modeling of both continuous and discrete structure in a data distribution.

1 INTRODUCTION

Latent generative models are one of the prevailing approaches for building expressive and tractable generative models. The generative process for a sample $x$ can be expressed as

$$z \sim p_Z(z),$$

$$x = g(z),$$

where $z$ is a noise vector, and $g$ a parametric generator network (typically a deep neural network). This paradigm has several incarnations, including variational autoencoders (Kingma & Welling, 2014; Rezende et al., 2014), generative adversarial networks (Goodfellow et al., 2014), and flow based models (Baird et al., 2005; Tabak & Turner, 2013; Dinh et al., 2015, 2017; Kingma & Dhariwal, 2018; Chen et al., 2018; Grathwohl et al., 2019).

The training process and model architecture for many existing latent generative models, and for all published flow based models, assumes a unimodal smooth distribution over latent variables $z$. Given the parametrization of $g$ as a neural network, the mapping to $x$ is a continuous function. This imposed structure makes it challenging to model data distributions with discrete structure – for instance, multi-modal distributions, distributions with holes, distributions with discrete symmetries, or distributions that lie on a union of manifolds (as may approximately be true for natural images, see Tenenbaum et al., 2000). Indeed, such cases require the model to learn a generator whose input Jacobian has highly varying or infinite magnitude to separate the initial noise source into different clusters. Such variations imply a challenging optimization problem due to large changes in curvature. This shortcoming can be critical as several problems of interest are hypothesized to follow a clustering structure, i.e. the distributions is concentrated along several disjoint connected sets (Eghbal-zadeh et al., 2018).

A standard way to address this issue has been to use mixture models (Yeung et al., 2017; Richardson & Weiss, 2018; Eghbal-zadeh et al., 2018) or structured priors (Johnson et al., 2016). In order to efficiently parametrize the model, mixture models are often formulated as discrete latent variable models (Hinton & Salakhutdinov, 2006; Courville et al., 2011; Mnih & Gregor, 2014; van den Oord...
et al., 2017), some of which can be expressed as a deep mixture model (Tang et al., 2012; Van den Oord & Schrauwen, 2014; van den Oord & Dambre, 2015). Although the resulting exponential number of mixture components with depth in deep mixture models is an advantage in terms of expressivity, it is an impediment to inference, evaluation, and training of such models, often requiring as a result the use of approximate methods like hard-EM or variational inference (Neal & Hinton, 1998).

In this paper we combine piecewise invertible functions, with discrete auxiliary variables selecting which invertible function applies, to describe a deep mixture model. This framework enables a probabilistic model’s latent space to have both real and discrete valued units, and to capture both continuous and discrete structure in the data distribution. It achieves this added capability while preserving the exact inference, exact sampling, exact evaluation of log-likelihood, and efficient training that make standard flow based models desirable.

## 2 Model definition

We aim to learn a parametrized distribution $p_X(x)$ on the continuous input domain $\mathbb{R}^d$ by maximizing log-likelihood. The major obstacle to training an expressive probabilistic model is typically efficiently evaluating log-likelihood.

### 2.1 Partitioning

If we consider a mixture model with a large number $|K|$ of components, the likelihood takes the form

$$p_X(x) = \sum_{k=1}^{|K|} p_K(k) p_{X|K}(x | k).$$

In general, evaluating the likelihood requires computing probabilities for all $|K|$ components. However, following a strategy similar to Rainforth et al. (2018), if we partition the domain $\mathbb{R}^d$ into disjoint subsets $A_k$ for $1 \leq k \leq |K|$ such that $\forall i \neq j, A_i \cap A_j = \emptyset$ and $\bigcup_{k=1}^{|K|} A_k = \mathbb{R}^d$, constrain the support of $p_{X|K}(x | k)$ to $A_k$ (i.e. $\forall x \notin A_k, p_{X|K}(x | k) = 0$), and define a set identification function $f_K(x)$ such that $\forall x \in \mathbb{R}^d, x \in A_{f_K(x)}$, we can write the likelihood as

$$p_X(x) = p_K(f_K(x)) p_{X|K}(x | f_K(x)).$$

This transforms the problem of summation to a search problem $x \mapsto f_K(x)$. This can be seen as the inferential converse of a stratified sampling strategy (Rubinstein & Kroese, 2016).

### 2.2 Change of variable formula

The proposed approach will be a direct extension of flow based models (Rippel & Adams, 2013; Dinh et al., 2015, 2017; Kingma & Dhariwal, 2018). Flow based models enable log-likelihood
(a) An example of a trimodal distribution $p_X$, sinusoidal distribution. The different modes are colored in red, green, and blue.

(b) The resulting unimodal distribution $p_Z$, corresponding to the distribution of any of the initial modes in $p_X$.

(c) An example $f_Z(x)$ of a piecewise invertible function aiming at transforming $p_Z$ into a unimodal distribution. The red, green, and blue zones corresponds to the different modes in input space.

Figure 2: Example of a trimodal distribution (2a) turned into a unimodal distribution (2b) using a piecewise invertible function (2c). Note that the initial distribution $p_X$ correspond to an unfolding of $p_{f_{Z}}(x)$ as $p_{X}(x) = \frac{1}{3}(p_{Z}(-3x) + p_{Z}(3x - \frac{2}{3}) + p_{Z}(3x + \frac{2}{3}))$.

Evaluating by relying on the change of variable formula

$$p_X(x) = p_Z(f_Z(x)) \left| \frac{\partial f_Z}{\partial x^T}(x) \right|,$$

with $f_Z$ a parametrized bijective function from $\mathbb{R}^d$ onto $\mathbb{R}^d$ and $\left| \frac{\partial f_Z}{\partial x^T} \right|$ the absolute value of the determinant of its Jacobian.

As also proposed in Falorsi et al. (2019), we relax the constraint that $f_Z$ be bijective, and instead have it be surjective onto $\mathbb{R}^d$ and piecewise invertible. That is, we require $f_{Z|A_k}(x)$ to be an invertible function, where $f_{Z|A_k}(x)$ indicates $f_Z(x)$ restricted to the domain $A_k$. Given a distribution $p_{Z,K}(z,k) = p_{K|Z}(k|z)p_{Z}(z)$ such that $\forall(z,k), z \notin f_Z(A_k) \Rightarrow p_{Z,K} = 0$, we can define the following generative process:

$$z, k \sim p_{Z,K}(z,k)$$
$$x = (f_{Z|A_k})^{-1}(z).$$

If we use the set identification function $f_K$ associated with $A_k$, the distribution corresponding to this stochastic inversion can be defined by a change of variable formula

$$p_X(x) = \sum_{k=1}^{K} p_{Z,K}(f_Z(x),k) \left| \frac{\partial f_{Z|A_k}}{\partial x^T} \right|$$
$$= p_{Z,K}(f_Z(x),f_K(x)) \left| \frac{\partial f_Z}{\partial x^T} \right|.$$

Because of the use of both Real and Discrete stochastic variables, we call this class of model RAD. The particular parametrization we use on is depicted in Figure 2. We rely on piecewise invertible functions that allow us to define a mixture model of repeated symmetrical patterns, following a
Figure 3: Stochastic computational graph in a deep RAD mixture model of $\prod_{l=1}^{3} |K^{(l)}|$ components.

(a) An example of a distribution $p_X$ (sinusoidal) with many modes.
(b) A simple absolute value function $z = |x|$ transforms $p_X$ into $p_Z = U([0,1])$.
(c) The gating network $p_{K|Z}$ allowing us to recover the distribution $p_X$ from $U([0,1])$, here taking the form $p_X > 0 | Z$ and $p_X < 0 | Z$.

Figure 4: Illustration of the expressive power the gating distribution $p_{K|Z}$ provides. By capturing the structure in a sine wave in $p_{K|Z}$, the function $z, k \mapsto x$ can take on an extremely simple form, corresponding only to a linear function with respect to $z$.

method of folding the input space. Note that in this instance the function $f_K$ is implicitly defined by $f_Z$, as the discrete latent corresponds to which invertible component of the piecewise function $x$ falls on.

So far, we have defined a mixture of $|K|$ components with disjoint support. However, if we factorize $p_{Z,K}$ as $p_Z \cdot p_{K|Z}$, we can apply another piecewise invertible map to $Z$ to define $p_Z$ as another mixture model. Recursively applying this method results in a deep mixture model (see Figure 3).

Another advantage of such factorization is in the gating network $p_{K|Z}$, as also designated in [van den Oord & Dambre, 2015]. It provides a more constrained but less sample wasteful approach than rejection sampling (Bauer & Mnih, 2019) by taking into account the untransformed sample $z$ before selecting the mixture component $k$. This allows the model to exploit the distribution $p_Z$ in different regions $A_k$ in more complex ways than repeating it as a pattern as illustrated in Figure 4.

The function from the input to the discrete variables, $f_K (x)$, contains discontinuities. This presents the danger of introducing discontinuities into $\log p_X (x)$, making optimization more difficult. However, by carefully imposing boundary conditions on the gating network, we are able to exactly counteract the effect of discontinuities in $f_K$, and cause $\log p_X (x)$ to remain continuous with respect to the parameters. This is discussed in detail in Appendix A.
3 Experiments

3.1 Problems

We conduct a brief comparison on six two-dimensional toy problems with Real NVP to demonstrate the potential gain in expressivity RAD models can enable. Synthetic datasets of 10,000 points each are constructed following the manifold hypothesis and/or the clustering hypothesis. We designate these problems as: grid Gaussian mixture, ring Gaussian mixture, two moons, two circles, spiral, and many moons (see Figure 5).

3.2 Architecture

For the RAD model implementation, we use the piecewise linear activations defined in Appendix A in a coupling layer architecture [Dinh et al., 2015, 2017] for $f_Z$ where, instead of a conditional linear transformation, the conditioning variable $x_1$ determines the parameters of the piecewise linear activation on $x_2$ to obtain $z_2$ and $k_2$, with $z_1 = x_1$ (see Figure 6). For the gating network $p_{K|Z}$, the gating logit neural network $s(z)$ take as input $z = (z_1, z_2)$. We compare with a Real NVP model using only affine coupling layers. $p_Z$ is a standard Gaussian distribution.

As both these models can easily approximately solve these generative modeling tasks provided enough capacity, we study these model in a relatively low capacity regime, where we can showcase the potential expressivity RAD may provide. Each of these models uses six coupling layers, and each coupling layer uses a one-hidden-layer rectified network with a tanh output activation scaled by a scalar parameter as described in [Dinh et al., 2017]. For RAD, the logit network $s(·)$ also uses a one-hidden-layer rectified neural network, but with linear output. In order to fairly compare with respect to number of parameters, we provide Real NVP seven times more hidden units per
hidden layer than RAD, which uses 8 hidden units per hidden layer. For each level, \( p_{K\mid Z} \) and \( f_Z \) are trained using stochastic gradient ascent with ADAM (Kingma & Ba, 2015) on the log-likelihood with a batch size of 500 for 50,000 steps.

3.3 RESULTS

In each of these problems, RAD is consistently able to obtain higher log-likelihood than REAL NVP.

|                      | RAD  | REAL NVP |
|----------------------|------|----------|
| Grid Gaussian mixture| −1.20| −2.26    |
| Ring Gaussian mixture| 3.57 | 1.85     |
| Two moons            | −1.21| −1.48    |
| Two circles          | −1.81| −2.17    |
| Spiral               | 0.29 | −0.36    |
| Many moons           | −0.83| −1.50    |

3.3.1 SAMPLING AND GAUSSIANIZATION

We plot the samples (Figure 7) of the described RAD and REAL NVP models trained on these problems. In the described low capacity regime, REAL NVP fails by attributing probability mass over spaces where the data distribution has low density. This is consistent with the mode covering behavior of maximum likelihood. However, the particular inductive bias of REAL NVP is to prefer modeling the data as one connected manifold. This results in the unwanted probability mass being distributed along the space between clusters.

Flow-based models often follow the principle of Gaussianization (Chen & Gopinath, 2001), i.e., transforming the data distribution into a Gaussian. The inversion of that process on a Gaussian distribution would therefore approximate the data distribution. We plot in Figure 8 the inferred Gaussianized variables \( z^{(5)} \) for both models trained on the ring Gaussian mixture problem. The Gaussianization from REAL NVP leaves some area of the standard Gaussian distribution unpopulated. These unattended areas correspond to unwanted regions of probability mass in the input space. RAD suffers significantly less from this problem.

An interesting feature is that RAD seems also to outperform REAL NVP on the spiral dataset. One hypothesis is that the model successfully exploits some non-linear symmetries in this problem.
Figure 8: Comparison of the Gaussianization process for RAD and REAL NVP on the ring Gaussian mixture problem. Both plots show the image of data samples in the latent $z$ variables, with level sets of the standard normal distribution plotted for reference. REAL NVP leaves some area of this Gaussian unpopulated, an effect which is not visually apparent for RAD.

Figure 9: Comparison of the inference process for RAD and REAL NVP on the two moons problem. Each pane shows input samples embedded in different networks layers, progressing from left to right from earlier to later network layers. The points are colored according to their original position in the input space. In RAD several points which were far apart in the input space become neighbors in $z^{(5)}$. This is not the case for REAL NVP.

3.3.2 Folding

We take a deeper look at the Gaussianization process involved in both models. In Figure 9 we plot the inference process of $z^{(5)}$ from $x$ for both models trained on the two moons problem. As a result of a folding process similar to that in Montufar et al. (2014), several points which were far apart in the input space become neighbors in $z^{(5)}$ in the case of RAD.

We further explore this folding process using the visualization described in Figure 10. We verify that the non-linear folding process induced by RAD plays at least two roles: bridging gaps in the distribution of probability mass, and exploiting symmetries in the data.

We observe that in the case of the ring Gaussian mixture (Figure 11a), RAD effectively uses foldings in order to bridge the different modes of the distribution into a single mode, primarily in the last layers of the transformation. We contrast this with REAL NVP (Figure 11b) which struggles to combine these modes under the standard Gaussian distribution using bijections.

In the spiral problem (Figure 12), RAD decomposes the spiral into three different lines to bridge (Figure 12a) instead of unrolling the manifold fully, which REAL NVP struggles to do (Figure 12b).

In both cases, the points remain generally well separated by labels, even after being pushed through a RAD layer (Figure 11a and 12a). This enables the model to maximize the conditional log-probability $\log(p_{K|z})$. 
Figure 10: Understanding the folding process, and understanding other visualizations of the folding process.

4 CONCLUSION

We introduced an approach to tractably evaluate and train deep mixture models using piecewise invertible maps as a folding mechanism. This allows exact inference, exact generation, and exact evaluation of log-likelihood, avoiding many issues in previous discrete variables models. This method can easily be combined with other flow based architectural components, allowing flow based models to better model datasets with discrete as well as continuous structure.

ACKNOWLEDGEMENTS

The authors would like to thank Kyle Kastner, Johanna Hansen, Harm De Vries, Ben Poole, Prajit Ramachandran, Dustin Tran, David Grangier, George J. Tucker, Matt D. Hoffman, Daniel Duckworth, Anna Huang, Arvind Neelakantan, Dale Schuurmans, Graham Taylor, Bart van Merrienböjer, Daniel Duckworth, Vincent Dumoulin, Marc G. Bellemare, and Ross Goroshin for valuable discussion and feedbacks.

REFERENCES

Leemon Baird, David Smalenberger, and Shawn Ingkiriwang. One-step neural network inversion with pdf learning and emulation. In International Joint Conference on Neural Networks, volume 2, pp. 966–971. IEEE, 2005.

Matthias Bauer and Andriy Mnih. Resampled priors for variational autoencoders. In Proceedings of the twenty-second international conference on artificial intelligence and statistics, 2019.

Scott Shaobing Chen and Ramesh A Gopinath. Gaussianization. In Advances in neural information processing systems, pp. 423–429, 2001.

Tian Qi Chen, Yulia Rubanova, Jesse Bettencourt, and David K Duvenaud. Neural ordinary differential equations. In Advances in Neural Information Processing Systems, pp. 6572–6583, 2018.

Aaron Courville, James Bergstra, and Yoshua Bengio. A spike and slab restricted boltzmann machine. In Proceedings of the fourteenth international conference on artificial intelligence and statistics, pp. 233–241, 2011.

Laurent Dinh, David Krueger, and Yoshua Bengio. Nice: Non-linear independent components estimation. In International Conference on Learning Representations: Workshop Track, 2015.
(a) RAD folding strategy on the ring Gaussian mixture problem. The top rows correspond to each RAD layer’s input points, and the bottom rows to its output points, as shown in [10]. The labels tend to be well separated in output space as well.

(b) REAL NVP inference strategy on the ring Gaussian mixture problem. The points are colored according to their original position in the input space.

Figure 11: RAD and REAL NVP inference processes on the ring Gaussian mixture problem. Each column correspond to a RAD or affine coupling layer. RAD effectively uses foldings in order to bridge the multiple modes of the distribution into a single mode, primarily in the last layers of the transformation, whereas REAL NVP struggles to bring together these modes under the standard Gaussian distribution using continuous bijections.

(a) RAD folding strategy on the spiral problem. The top rows correspond to each RAD layer’s input points, and the bottom rows to its output points, as shown in [10].

(b) REAL NVP inference strategy on the spiral problem. The points are colored according to their original position in the input space.

Figure 12: RAD and REAL NVP inference processes on the spiral problem. Each column correspond to a RAD or affine coupling layer. Instead of unrolling the manifold as REAL NVP tries to, RAD uses a more successful strategy of decomposing the spiral into three different lines that it later bridges.
Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using real nvp. In *International Conference on Learning Representations*, 2017.

Hamid Eghbal-zadeh, Werner Zellinger, and Gerhard Widmer. Mixture density generative adversarial networks. *Neural Information Processing Systems: Bayesian Deep Learning Workshop*, 2018.

Luca Falorsi, Pim de Haan, Tim R. Davidson, and Patrick Forr. Reparameterizing distributions on lie groups. In *Proceedings of the twenty-second international conference on artificial intelligence and statistics*, 2019.

Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. In *Advances in Neural Information Processing Systems*, pp. 2672–2680, 2014.

Will Grathwohl, Dami Choi, Yuhuai Wu, Geoffrey Roeder, and David Duvenaud. Backpropagation through the void: Optimizing control variates for black-box gradient estimation. In *International Conference on Learning Representations*, 2018.

Will Grathwohl, Ricky TQ Chen, Jesse Betterncourt, Ilya Sutskever, and David Duvenaud. Ffjord: Free-form continuous dynamics for scalable reversible generative models. 2019.

Geoffrey E Hinton and Ruslan R Salakhutdinov. Reducing the dimensionality of data with neural networks. *Science*, 313(5786):504–507, 2006.

Eric Jang, Shixiang Gu, and Ben Poole. Categorical reparameterization with gumbel-softmax. In *International Conference on Learning Representations*, 2017.

Matthew Johnson, David K Duvenaud, Alex Wiltschko, Ryan P Adams, and Sandeep R Datta. Composing graphical models with neural networks for structured representations and fast inference. In *Advances in neural information processing systems*, pp. 2946–2954, 2016.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *International Conference on Learning Representations*, 2015.

Diederik P Kingma and Max Welling. Auto-encoding variational bayes. In *International Conference on Learning Representations*, 2014.

Durk P Kingma and Prafulla Dhariwal. Glow: Generative flow with invertible 1x1 convolutions. In *Advances in Neural Information Processing Systems*, pp. 10236–10245, 2018.

Chris J Maddison, Andriy Mnih, and Yee Whye Teh. The concrete distribution: A continuous relaxation of discrete random variables. In *International Conference on Learning Representations*, 2017.

Andriy Mnih and Karol Gregor. Neural variational inference and learning in belief networks. In *International Conference on Machine Learning*, 2014.

Guido F Montufar, Razvan Pascanu, Kyunghyun Cho, and Yoshua Bengio. On the number of linear regions of deep neural networks. In *Advances in neural information processing systems*, pp. 2924–2932, 2014.

Radford M Neal and Geoffrey E Hinton. A view of the em algorithm that justifies incremental, sparse, and other variants. In *Learning in graphical models*, pp. 355–368. Springer, 1998.

Tom Rainforth, Yuan Zhou, Xiaoyu Lu, Yee Whye Teh, Frank Wood, Hongseok Yang, and Jan-Willem van de Meent. Inference trees: Adaptive inference with exploration. *arXiv preprint arXiv:1806.09550*, 2018.

Danilo Jimenez Rezende, Shakir Mohamed, and Daan Wierstra. Stochastic backpropagation and approximate inference in deep generative models. In *International Conference on Machine Learning*, 2014.

Eitan Richardson and Yair Weiss. On gans and gmms. In *Advances in Neural Information Processing Systems*, pp. 5852–5863, 2018.
Oren Rippel and Ryan Prescott Adams. High-dimensional probability estimation with deep density models. *arXiv preprint arXiv:1302.5125*, 2013.

Jason Tyler Rolfe. Discrete variational autoencoders. In *International Conference on Learning Representations*, 2017.

Reuven Y Rubinstein and Dirk P Kroese. *Simulation and the Monte Carlo method*, volume 10. John Wiley & Sons, 2016.

EG Tabak and Cristina V Turner. A family of nonparametric density estimation algorithms. *Communications on Pure and Applied Mathematics*, 66(2):145–164, 2013.

Yichuan Tang, Ruslan Salakhutdinov, and Geoffrey Hinton. Deep mixtures of factor analysers. In *International Conference on Machine Learning*, 2012.

Joshua B Tenenbaum, Vin De Silva, and John C Langford. A global geometric framework for nonlinear dimensionality reduction. *science*, 290(5500):2319–2323, 2000.

George Tucker, Andriy Mnih, Chris J Maddison, John Lawson, and Jascha Sohl-Dickstein. Rebar: Low-variance, unbiased gradient estimates for discrete latent variable models. In *Advances in Neural Information Processing Systems*, pp. 2627–2636, 2017.

Aäron van den Oord and Joni Dambre. Locally-connected transformations for deep gmms. In *International Conference on Machine Learning (ICML): Deep Learning Workshop*, pp. 1–8, 2015.

Aaron Van den Oord and Benjamin Schrauwen. Factoring variations in natural images with deep gaussian mixture models. In *Advances in Neural Information Processing Systems*, pp. 3518–3526, 2014.

Aaron van den Oord, Oriol Vinyals, et al. Neural discrete representation learning. In *Advances in Neural Information Processing Systems*, pp. 6306–6315, 2017.

Serena Yeung, Anitha Kannan, Yann Dauphin, and Li Fei-Fei. Tackling over-pruning in variational autoencoders. *arXiv preprint arXiv:1706.03643*, 2017.
β > or \( f \) everywhere, the log-likelihood is unfortunately discontinuous. Let’s decompose the log-likelihood on the negative log-likelihood. Although the model enables the computation of a gradient almost everywhere, the log-likelihood is unfortunately discontinuous. Let’s decompose the log-likelihood

\[
\log(p_X(x)) = \log(p_Z(f_Z(x))) + \log(p_{K|Z}(f_K(x) | f_Z(x))) + \log\left(\left| \frac{\partial f_Z}{\partial f_T} \right| (x) \right).
\]

There are two sources of discontinuity in this expression: \( f_K \) is a function with discrete values (therefore discontinuous) and \( \frac{\partial f_Z}{\partial f_T} \) is discontinuous because of the transition between the subsets \( \mathcal{A}_k \), leading to the expression of interest

\[
\log(p_{K|Z}(f_K(x) | f_Z(x))) + \log\left(\left| \frac{\partial f_Z}{\partial f_T} \right| (x) \right),
\]

which takes a role similar to the log-Jacobian determinant, a pseudo log-Jacobian determinant.

Let’s build from now on the simple scalar case and a piecewise linear function

\[
f_Z(x) = \begin{cases} 
\alpha_1(x + \beta) + \alpha_2 \beta, & \text{if } x \leq -\beta \\
\alpha_3(x - \beta) - \alpha_2 \beta, & \text{if } x \geq \beta \\
-\alpha_2 x, & \text{if } |x| \leq \beta
\end{cases}
\]

or \( f_Z(x) = \alpha_1 \min(x + \beta, 0) + \alpha_3 \max(x - \beta, 0) - \alpha_2 \min(\max(x, -\beta), \beta) \) (with \( \alpha_k > 0 \) and \( \beta \geq 0 \), see figure 13a), then \( \mathcal{A}_1 = ]-\infty, -\beta[, \mathcal{A}_2 = [-\beta, \beta], \mathcal{A}_3 = ]\beta, +\infty[ \) and \( f_K(x) = 1(x > -\beta) + 1(x > \beta) \).

In this case, \( s(z) = \{\log(p_{K|Z}(k | z))\}_{k \in \mathcal{N}} + C \mathbf{1}_{|K|} \) can be seen as a vector valued function.

We can attempt at parametrizing the model such that the pseudo log-Jacobian determinant becomes continuous with respect to \( \beta \) by expressing the boundary condition at \( x = \beta \)

\[
\log(p_{K|Z}(f_K(\beta^-) | f_Z(\beta^-))) + \log\left(|f_Z'| (\beta^-)\right) \\
= \log(p_{K|Z}(f_K(\beta^+) | f_Z(\beta^+))) + \log\left(|f_Z'| (\beta^+)\right) \\
\Rightarrow s(-\alpha_2 \beta) + \log(\alpha_2) = s(-\alpha_2 \beta) + \log(\alpha_3).
\]

If we define \( \Omega_{2,3} = \begin{bmatrix} 0 & 0 & 0 \\
0 & 0 & \Omega \end{bmatrix} \) and \( \Omega_{1,2} = \begin{bmatrix} \Omega & 0 & 0 \\
0 & 0 & 0 \end{bmatrix} \), with \( \Omega = \frac{1}{2} \begin{bmatrix} -1 & 1 & 1 \\
1 & -1 & -1 \end{bmatrix} \), then this boundary condition can be enforced, together with a similar one at \( x = -\beta \), by replacing the

\[
\Omega = \frac{1}{2} \begin{bmatrix} -1 & 1 & 1 \\
1 & -1 & -1 \end{bmatrix}.
\]
function $s$ with

$$
\beta s(z) + \frac{\beta}{2} \left( 1 + \cos \left( \frac{(z\alpha_2^{-1} - \beta)\pi}{2\beta} \right) \right) s(z) \cdot \Omega_{2,3}
$$

$$
- (\log(\alpha_1), \log(\alpha_2), \log(\alpha_3)) + \frac{\beta}{2} \left( 1 + \cos \left( \frac{(z\alpha_2^{-1} + \beta)\pi}{2\beta} \right) \right) s(z) \cdot \Omega_{1,2}.
$$

Another type of boundary condition can be found at between the non-invertible area and the invertible area $z = \alpha_2\beta$, as $\forall z > \alpha_2\beta, p_{k|z}(3 \mid z) = 1$, therefore

$$
\log \left( p_{k|z}(3 \mid f_Z((1 + \alpha_3^{-1}\alpha_2)\beta)) \right) + \log \left( |f_Z'| \left( \left( (1 + \alpha_3^{-1}\alpha_2)\beta \right)^+ \right) \right) = \log \left( |f_Z'| \left( \left( (1 + \alpha_3^{-1}\alpha_2)\beta \right)^- \right) \right).
$$

Since the condition $\forall k < 3, p_{k|z}(k \mid z) \rightarrow 0$ when $z \rightarrow (\alpha_2\beta)^-$ will lead to an infinite loss barrier at $x = -\beta$, another way to enforce this boundary condition is by adding linear pieces (Figure [13b]):

$$
f_Z(x) =
\begin{cases}
\alpha_1(x + \beta) + \alpha_2\beta, & \text{if } x \in [-(1 + \alpha_1^{-1}\alpha_2)\beta, -\beta]\\
\alpha_3(x - \beta) - \alpha_2\beta, & \text{if } x \in [\beta, (1 + \alpha_1^{-1}\alpha_2)\beta]\\
\alpha_1 \cdot p_{k|z}(1 \mid -\alpha_2\beta)(x + (1 + \alpha_1^{-1}\alpha_2)\beta) - \alpha_2\beta, & \text{if } x < -(1 + \alpha_1^{-1}\alpha_2)\beta\\
\alpha_3 \cdot p_{k|z}(3 \mid \alpha_2\beta)(x - (1 + \alpha_3^{-1}\alpha_2)\beta) + \alpha_2\beta, & \text{if } x > (1 + \alpha_3^{-1}\alpha_2)\beta\\
-\alpha_2 x, & \text{if } |x| < \beta
\end{cases}
$$

$$
= \alpha_1 \min(x + \beta, 0) + \alpha_3 \max(x - \beta, 0) - \alpha_2 \min(\max(x, -\beta), \beta)
$$

$$
- \alpha_1(1 - p_{k|z}(1 \mid -\alpha_2\beta)) \min(x + (1 + \alpha_1^{-1}\alpha_2)\beta, 0)
$$

$$
- \alpha_3(1 - p_{k|z}(3 \mid \alpha_2\beta)) \max(x - (1 + \alpha_3^{-1}\alpha_2)\beta, 0).
$$

The inverse is defined as

$$
\forall z \in \mathbb{R}, x =
\begin{cases}
\alpha_1^{-1}(p_{k|z}(1 \mid -\alpha_2\beta))^{-1}(z + \alpha_2\beta) - \beta, & \text{if } z \leq -\alpha_2\beta\\
\alpha_3^{-1}(p_{k|z}(3 \mid \alpha_2\beta))^{-1}(z - \alpha_2\beta) + \beta, & \text{if } z \geq \alpha_2\beta\\
\alpha_1^{-1}(z - \alpha_2\beta) - \beta, & \text{if } x \in \mathbb{A}_1\\
\alpha_2^{-1}z, & \text{if } x \in \mathbb{A}_2\\
\alpha_3^{-1}(z + \alpha_2\beta) + \beta, & \text{if } x \in \mathbb{A}_3
\end{cases}
$$

In order to know the values of $s$ at the boundaries $\pm\alpha_2\beta$, we can use the logit function

$$
\beta (a_s z + b_s) + \frac{\beta}{2} \left( 1 + \cos \left( \frac{(z\alpha_2^{-1} - \beta)\pi}{2\beta} \right) \right) (a_s z + b_s) \cdot \Omega_{2,3}
$$

$$
- (\log(\alpha_1), \log(\alpha_2), \log(\alpha_3)) + \frac{\beta}{2} \left( 1 + \cos \left( \frac{(z\alpha_2^{-1} + \beta)\pi}{2\beta} \right) \right) (a_s z + b_s) \cdot \Omega_{1,2}
$$

$$
+ \frac{\beta}{2} \left( 1 + \cos \left( \frac{z\pi}{\alpha_2\beta} \right) \right) s(z),
$$

where $(a_s, b_s) \in (\mathbb{R}^3)^2$.

Given those constraints, the model can then be reliably learned through gradient descent methods. Note that the resulting tractability of the model results from the fact that the discrete variables $k$ is only interfaced during inference with the distribution $p_{k|z}$, unlike discrete variational autoencoders approaches (Mnih & Gregor, 2014; van den Oord et al., 2017) where it is fed to a deep neural network. Similar to Rolfe (2017), the learning of discrete variables is achieved by relying on the the continuous component of the model, and, as opposed as other approaches (Jang et al., 2017; Maddison et al., 2017; Grathwohl et al., 2018; Tucker et al., 2017), this gradient signal extracted is exact and closed form.
We plot the remaining inference processes of RAD and REAL NVP on the remaining problems not plotted previously: grid Gaussian mixture (Figure 14), two circles (Figure 15), two moons (Figure 16), and many moons (Figure 17). We also compare the final results of the Gaussianization processes on both models on the different toy problems in Figure 18.

B INFEERENCE PROCESSES
(a) **RAD** folding strategy on the two moons problem. The top rows correspond to a **RAD** layer input points, and the bottom rows to its output points, as shown in [10].

(b) **REAL** NVP inference strategy on the two moons problem. The points are colored according to their original position in the input space.

Figure 16: **RAD** and **REAL** NVP inference process on the two moons problem. Each column correspond to a **RAD** or affine coupling layer.

(a) **RAD** folding strategy on the many moons problem. The top rows correspond to a **RAD** layer input points, and the bottom rows to its output points, as shown in [10].

(b) **REAL** NVP inference strategy on the many moons problem. The points are colored according to their original position in the input space.

Figure 17: **RAD** and **REAL** NVP inference process on the many moons problem. Each column correspond to a **RAD** or affine coupling layer.
Figure 18: Comparison of the Gaussianization from the trained REAL NVP (top row) (a-f) and RAD (bottom row) (g-l). REAL NVP fails in a low capacity setting by leaving unpopulated areas where the standard Gaussian attributes probability mass. Here, these spaces as often ones separating clusters, showing the failure in modeling the data as one manifold.