`normflows`: A PyTorch Package for Normalizing Flows

Vincent Stimper[1,2,@]**, David Liu**[1]**, Andrew Campbell**[1]**, Vincent Berenz**[2]**, Lukas Ryll**[1]**,
Bernhard Schölkopf**[2]**, José Miguel Hernández-Lobato**[1]

[1]University of Cambridge, Cambridge, United Kingdom
[2]Max Planck Institute for Intelligent Systems, Tübingen, Germany
[@]Corresponding author: `vstimper@tue.mpg.de`

Summary

Normalizing flows model probability distributions through an expressive tractable density [Tabak and Vanden-Eijnden, 2010, Tabak and Turner, 2013, Rezende and Mohamed, 2015]. They transform a simple base distribution, such as a Gaussian, through a sequence of invertible functions, which are referred to as layers. These layers typically use neural networks to become very expressive. Flows are ubiquitous in machine learning and have been applied to image generation [Kingma and Dhariwal, 2018, Grcić et al., 2021], text modeling [Wang and Wang, 2019], variational inference [Rezende and Mohamed, 2015], approximating Boltzmann distributions [Noé et al., 2019], and many other problems [Kobyzev et al., 2021, Papamakarios et al., 2021].

Here, we present `normflows`, a Python package for normalizing flows. It allows to build normalizing flow models from a suite of base distributions, flow layers, and neural networks. The package is implemented in the popular deep learning framework PyTorch [Paszke et al., 2019], which simplifies the integration of flows in larger machine learning models or pipelines. It supports most of the common normalizing flow architectures, such as Real NVP [Dinh et al., 2017], Glow [Kingma and Dhariwal, 2018], Masked Autoregressive Flows [Papamakarios et al., 2017], Neural Spline Flows [Müller et al., 2019, Durkan et al., 2019], Residual Flows [Chen et al., 2019], and many more. The package can be easily installed via `pip` and the code is publicly available on GitHub[1].

Statement of need

`normflows` focuses on flows that are composed of discrete transformations, as opposed to continuous normalizing flows [Chen et al., 2018, Papamakarios et al., 2021]. There are several other packages implementing discrete normalizing flows, such as TensorFlow Probability [Dillon et al., 2017] for TensorFlow, `distrax` [Babuschkin et al., 2020] for JAX, and `nflows` [Durkan et al., 2020] and `FrEIA` [Ardizzone et al., 2018-2022] for PyTorch. However, none of them support the two popular flow architectures, residual and autoregressive flows, within a single package, while we do so.

Moreover, `normflows` stands out by providing tools that are often used when approximating Boltzmann distributions. First, sampling layers needed for Stochastic Normalizing Flows [Wu et al., 2020, Nielsen et al., 2020] are included. Second, Neural Spline Flows on circular coordinates are supported [Rezende et al., 2020], which can be combined with standard coordinates on bounded or unbounded intervals. They are needed when modeling the internal coordinates of molecules consisting of angles
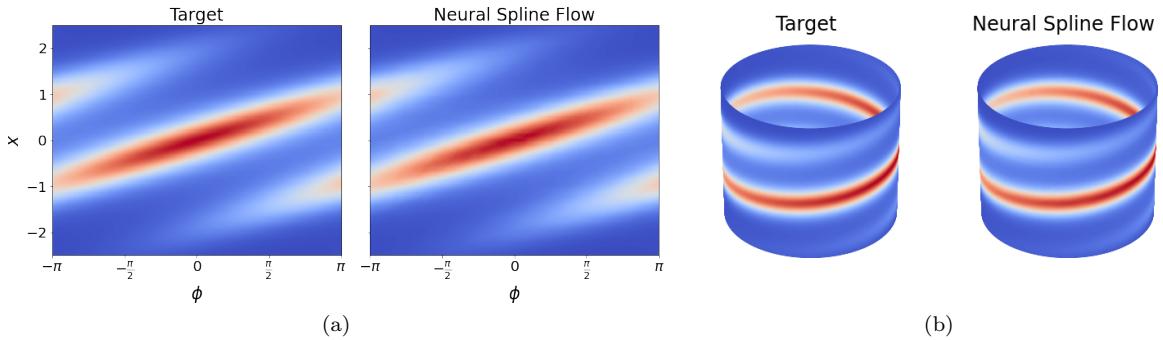
---

[1]https://github.com/VincentStimper/normalizing-flows

Figure 1: Target density defined on a cylinder surface, having an unbounded coordinate x and a circular coordinate ϕ. A Neural Spline Flow is fit to it, being almost indistinguishable from the target. (a) shows the densities in 2D and (b) is a visualization on the cylinder surface.

and lengths [Midgley et al., 2023]. Furthermore, there is an extension for `normflows` that adds Boltzmann distributions as targets as well as flow layers converting between Cartesian and internal coordinates [Stimper et al., 2023].

Our package has already been used in several scientific projects and publications [Campbell et al., 2021, Stimper et al., 2022, Midgley et al., 2023]. Due to its modular nature, `normflows` can be easily extended to house new flow layers, base distributions, or other tools. For instance, Stimper et al. [2022] extends the package by adding resampled base distributions, which overcome an architectural weakness of normalizing flows and make them more expressive.

Examples

In the GitHub repository of our package[1], we provide various examples illustrating how to use it. We show how to build a flow model from a base distribution, a list of flow layers, and, optionally, a target distribution. They can be trained by computing a loss through the respective methods provided and minimizing it with the standard PyTorch optimizers. We show how to approximate simple 2D distributions, but, moreover, apply flows to images through the multiscale architecture [Dinh et al., 2017], which `normflows` provides as well. Furthermore, there is an example of how to build a variational autoencoder with normalizing flows as well.

Here, we want to illustrate a strength of `normflows`, i.e. that it can deal with combinations of standard and circular coordinates. Therefore, we consider a distribution of two random variables, x and ϕ. x follows a Gaussian distribution with density $p(x) = \mathcal{N}(x|0,1)$ and ϕ has a circular von Mises distribution such that $p(\phi|x) = \mathcal{M}(\phi|\mu(x),1)$ with $\mu(x) = 3x$. We train a Neural Spline Flow with an unbound and a circular coordinate to approximate the target distribution $p(x,\phi) = p(x)p(\phi|x)$ by minimizing the reverse Kullback-Leibler divergence. As shown in Figure 1, the density of the flow is almost indistinguishable from the target.

Acknowledgements

and spotting bugs.

References

Lynton Ardizzone, Till Bungert, Felix Draxler, Ullrich Köthe, Jakob Kruse, Robert Schmier, and Peter Sorrenson. Framework for Easily Invertible Architectures (FrEIA), 2018-2022. URL https://github.com/vislearn/FrEIA.

Igor Babuschkin, Kate Baumli, Alison Bell, Surya Bhupatiraju, Jake Bruce, Peter Buchlovsky, David Budden, Trevor Cai, Aidan Clark, Ivo Danihelka, Claudio Fantacci, Jonathan Godwin, Chris Jones, Ross Hemsley, Tom Hennigan, Matteo Hessel, Shaobo Hou, Steven Kapturowski, Thomas Keck, Iurii Kemaev, Michael King, Markus Kunesch, Lena Martens, Hamza Merzic, Vladimir Mikulik, Tamara Norman, John Quan, George Papamakarios, Roman Ring, Francisco Ruiz, Alvaro Sanchez, Rosalia Schneider, Eren Sezener, Stephen Spencer, Srivatsan Srinivasan, Luyu Wang, Wojciech Stokowiec, and Fabio Viola. The DeepMind JAX Ecosystem, 2020.

Andrew Campbell, Wenlong Chen, Vincent Stimper, Jose Miguel Hernandez-Lobato, and Yichuan Zhang. A gradient based strategy for Hamiltonian Monte Carlo hyperparameter optimization. In *Proceedings of the 38th International Conference on Machine Learning*, pages 1238–1248. PMLR, 2021.

Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural Ordinary Differential Equations. In *Advances in Neural Information Processing Systems*, volume 31, 2018.

Ricky T. Q. Chen, Jens Behrmann, David K Duvenaud, and Joern-Henrik Jacobsen. Residual flows for invertible generative modeling. In *Advances in Neural Information Processing Systems*, volume 32, 2019.

Joshua V. Dillon, Ian Langmore, Dustin Tran, Eugene Brevdo, Srinivas Vasudevan, Dave Moore, Brian Patton, Alex Alemi, Matt Hoffman, and Rif A. Saurous. TensorFlow Distributions. *arXiv preprint arXiv:1711.10604*, 2017.

Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using Real NVP. *International Conference on Learning Representations*, 2017.

Conor Durkan, Artur Bekasov, Iain Murray, and George Papamakarios. Neural spline flows. *Advances in Neural Information Processing Systems*, 32:7511–7522, 2019.

Conor Durkan, Artur Bekasov, Iain Murray, and George Papamakarios. nflows: normalizing flows in PyTorch. *Zenodo*, 2020. URL https://doi.org/10.5281/zenodo.4296287.

Matej Grcić, Ivan Grubišić, and Siniša Šegvić. Densely connected normalizing flows. In *Advances in Neural Information Processing Systems*, volume 34, 2021.

Diederik P Kingma and Prafulla Dhariwal. Glow: Generative flow with invertible 1x1 convolutions. In *Advances in Neural Information Processing Systems*, volume 31, 2018.

Ivan Kobyzev, Simon J.D. Prince, and Marcus A. Brubaker. Normalizing flows: An introduction and review of current methods. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 43(11):3964–3979, 2021. doi: 10.1109/TPAMI.2020.2992934.

Laurence Illing Midgley, Vincent Stimper, Gregor N. C. Simm, Bernhard Schölkopf, and José Miguel Hernández-Lobato. Flow Annealed Importance Sampling Bootstrap. *International Conference on Learning Representations*, 2023.

Thomas Müller, Brian McWilliams, Fabrice Rousselle, Markus Gross, and Jan Novák. Neural importance sampling. *ACM Transactions on Graphics (TOG)*, 38(5):1–19, 2019.

Didrik Nielsen, Priyank Jaini, Emiel Hoogeboom, Ole Winther, and Max Welling. SurVAE flows: Surjections to bridge the gap between VAEs and flows. *Advances in Neural Information Processing Systems 33*, 2020.

Frank Noé, Simon Olsson, Jonas Köhler, and Hao Wu. Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. *Science*, 365(6457), 2019.

George Papamakarios, Theo Pavlakou, and Iain Murray. Masked autoregressive flow for density estimation. In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, NIPS'17, pages 2335–2344, Red Hook, NY, USA, December 2017. Curran Associates Inc.

George Papamakarios, Eric Nalisnick, Danilo Jimenez Rezende, Shakir Mohamed, and Balaji Lakshminarayanan. Normalizing flows for probabilistic modeling and inference. *Journal of Machine Learning Research*, 22(57):1–64, 2021.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library. In *Advances in Neural Information Processing Systems 32*, pages 8024–8035. 2019.

Danilo Rezende and Shakir Mohamed. Variational inference with normalizing flows. In *Proceedings of the 32nd International Conference on Machine Learning*, pages 1530–1538. PMLR, 2015.

Danilo Jimenez Rezende, George Papamakarios, Sébastien Racanière, Michael S. Albergo, Gurtej Kanwar, Phiala E. Shanahan, and Kyle Cranmer. Normalizing flows on tori and spheres. In *Proceedings of the 37th International Conference on Machine Learning*, volume 119, pages 8083–8092. PMLR, 2020.

Vincent Stimper, Bernhard Schölkopf, and José Miguel Hernández-Lobato. Resampling Base Distributions of Normalizing Flows. In *Proceedings of The 25th International Conference on Artificial Intelligence and Statistics*, volume 151, pages 4915–4936, 2022.

Vincent Stimper, Andrew Campbell, and José Miguel Hernández-Lobato. Implementing Boltzmann generators with normflows. *Zenodo*, 2023. URL https://doi.org/10.5281/zenodo.7565800.

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

Esteban G. Tabak and Eric Vanden-Eijnden. Density estimation by dual ascent of the log-likelihood. *Communications in Mathematical Sciences*, 8(1):217–233, 2010. ISSN 15396746, 19450796. doi: 10.4310/CMS.2010.v8.n1.a11.

Prince Zizhuang Wang and William Yang Wang. Riemannian normalizing flow on variational Wasserstein autoencoder for text modeling. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, 2019.

Hao Wu, Jonas Köhler, and Frank Noe. Stochastic normalizing flows. In *Advances in Neural Information Processing Systems*, volume 33, pages 5933–5944, 2020.