

# sbi reloaded: a toolkit for simulation-based inference workflows

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## ABSTRACT

Scientists and engineers use simulators to model empirically observed phenomena. However, tuning the parameters of a simulator to ensure its outputs match observed data presents a significant challenge. Simulation-based inference (SBI) addresses this by enabling Bayesian inference for simulators, identifying parameters that match observed data and align with prior knowledge. Unlike traditional Bayesian inference, SBI only needs access to simulations from the model and does not require evaluations of the likelihood function. In addition, SBI algorithms do not require gradients through the simulator, allow for massive parallelization of simulations, and can perform inference for different observations without further simulations or training, thereby amortizing inference. Over the past years, we have developed, maintained, and extended sbi, a PyTorch-based package<sup>4</sup> that implements Bayesian SBI algorithms based on neural networks. The sbi toolkit implements a wide range of inference methods, neural network architectures, sampling methods, and diagnostic tools. In addition, it provides well-tested default settings, but also offers flexibility to fully customize every step of the simulation-based inference workflow. Taken together, the sbi toolkit enables scientists and engineers to apply state-of-the-art SBI methods to black-box simulators, opening up new possibilities for aligning simulations with empirically observed data.

## 1 Statement of need

Bayesian inference is a principled approach for determining parameters consistent with empirical observations: Given a prior over parameters, a forward-model (defining the likelihood), and observations, it returns a posterior distribution. The posterior distribution captures the entire space of parameters that are compatible with the observations and the prior

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<sup>4</sup>sbi is available at [github.com/sbi-dev/sbi](https://github.com/sbi-dev/sbi) under the Apache 2.0 license.

and it quantifies parameter uncertainty. When the forward-model is given by a stochastic simulator, Bayesian inference can be challenging: (1) the forward-model can be slow to evaluate, making algorithms that rely on sequential evaluations of the likelihood (such as Markov-Chain Monte-Carlo, MCMC) impractical, (2) the simulator can be non-differentiable, prohibiting the use of gradient-based MCMC or variational inference (VI) methods, and (3) likelihood-evaluations can be intractable, meaning that we can only generate samples from the model, but not evaluate their likelihoods.

Recently, simulation-based inference (SBI) algorithms based on neural networks have been developed to overcome these limitations [1–3]. Unlike classical methods from Approximate Bayesian Computation (ABC [4]), these methods use neural networks to learn the relationship between parameters and simulation outputs. Neural SBI algorithms (1) allow for massive parallelization of simulations (in contrast to sequential evaluations in MCMC methods), (2) do not require gradients through the simulator, and (3) do not require evaluations of the likelihood, but only samples from the simulator. Finally, many of these algorithms allow for *amortized* inference, that is, after a large upfront cost of simulating data for the training phase, they can return the posterior distribution for any observation without requiring further simulations or retraining.

To aid in the effective application of these algorithms to a wide range of problems, we developed the `sbi` toolkit. `sbi` implements a variety of state-of-the-art SBI algorithms, offering both high-level interfaces, extensive documentation and tutorials for practitioners, as well as low-level interfaces for experienced users and SBI researchers (giving full control over simulations, the training loop, and the sampling procedure). Since the original release of the `sbi` package [5], the community of contributors has expanded significantly, resulting in a large number of improvements that have made `sbi` more flexible, performant, and reliable. `sbi` now supports a wider range of amortized and sequential inference methods, neural network architectures (including normalizing flows, flow and score matching, and various embedding network architectures), samplers (including MCMC, variational inference, importance sampling, and rejection sampling), diagnostic tools, visualization tools, and a comprehensive set of tutorials on how to use these features.

The `sbi` package is already used extensively by the machine learning research community [6–18] but has also fostered the application of SBI in various research fields [19–37].

## 2 Description

`sbi` is a flexible and extensive toolkit for running simulation-based Bayesian inference workflows. `sbi` supports any kind of (offline) simulator and prior, a wide range of inference methods, neural networks, and samplers, as well as diagnostic methods and analysis tools (Fig. 1).

Simulator & prior	Method classes	Neural networks	Training	Sampling	Diagnostics	Analysis
<ul style="list-style-type: none"> <li>• Use pre-simulated data or...</li> <li>• ...use utilities for parallel simulation</li> <li>• Combine independent priors</li> <li>• Build truncated priors</li> </ul>	<ul style="list-style-type: none"> <li>• Neural Posterior Estimation (NPE)</li> <li>• Neural Likelihood Estimation (NLE)</li> <li>• Neural Ratio Estimation (NRE)</li> <li>• Amortized and sequential versions of all algorithms</li> </ul>	<ul style="list-style-type: none"> <li>• (Continuous) Normalizing flows</li> <li>• Score-matching</li> <li>• Flow-matching</li> <li>• Pre-configured or customizable embedding networks</li> </ul>	<ul style="list-style-type: none"> <li>• Preconfigured training loop with good defaults or...</li> <li>• ...complete access to the training loop for full flexibility</li> </ul>	<ul style="list-style-type: none"> <li>• MCMC (with parallel chains across data)</li> <li>• Variational inference</li> <li>• Importance sampling &amp; SIR</li> <li>• Rejection sampling</li> </ul>	<ul style="list-style-type: none"> <li>• Simulation-based calibration (SBC)</li> <li>• Expected coverage</li> <li>• Local C2ST</li> <li>• TARP</li> </ul>	<ul style="list-style-type: none"> <li>• Marginal plot</li> <li>• Conditional plot</li> <li>• Sensitivity analysis</li> </ul>

Figure 1: **Features of the `sbi` package.** Components that were added since the initial release described in Tejero-Cantero et al. [5] are marked in red.

A significant challenge in making SBI algorithms accessible to a broader community lies in accommodating diverse and complex simulators, as well as varying degrees of flexibility in each step of the inference process. To address this, `sbi` provides pre-configured defaults for all inference methods, but also allows full customization of every step in the process (including simulation, training, sampling, diagnostics and analysis).

**Simulator & prior:** The `sbi` toolkit requires only simulation parameters and simulated data as input and no direct access to the simulator itself. However, if the simulator can be provided as a Python callable, `sbi` can optionally parallelize running the simulations from a given prior using Joblib [38]. Additionally, `sbi` can automatically handle failed simulations or missing values, it supports both discrete and continuous parameters and observations (or mixtures thereof) and it provides utilities to flexibly define priors.

**Methods:** `sbi` implements a wide range of neural network-based SBI algorithms, among them Neural Posterior Estimation (NPE) with various conditional estimators, Neural Likelihood Estimation (NLE), and Neural Ratio Estimation (NRE). Each of these methods can be run either in an *amortized* mode, where the neural network is trained once on a set of pre-existing simulations results and then performs inference on *any* observation without further simulations or retraining, or in a *sequential* mode, where inference is focused on one observation to improve simulation efficiency with active learning.

**Neural networks and training:** `sbi` implements a wide variety of state-of-the-art conditional density estimators for NPE and NLE, including normalizing flows [39, 40] (via nflows and Zukō [41, 42]), diffusion models [43–45],

mixture density networks [46], and flow matching [47, 48] (via Zuko [42]), as well as ensembles of any of these networks. sbi also implements a large set of embedding networks that can automatically learn summary statistics of (potentially) high-dimensional simulation outputs (including multilayer perceptrons, convolutional networks, and permutation-invariant networks). The neural networks can be trained with a preconfigured training loop with established default values, but sbi also allows full access over the training loop when desired.

**Sampling:** For NLE and NRE, sbi implements a large range of samplers, including MCMC (with chains vectorized across observations), variational inference, rejection sampling, or importance sampling, as well as wrappers to use MCMC samplers from Pyro and PyMC [49, 50]. sbi can perform inference for single observations or for multiple i.i.d. observations, and can use importance sampling to correct for potential inaccuracies in the posterior if the likelihood is available.

**Diagnostics and analysis:** The sbi toolkit also implements a large set of diagnostic tools, such as simulation-based calibration (SBC) [51], expected coverage [6, 16], local C2ST [17], and TARP [52]. Additionally, sbi offers visualization tools, including marginal and conditional corner plots to visualize high-dimensional distributions, calibration plots, and wrappers for Arviz [53] diagnostic plots.

With sbi, our goal is to advance scientific discovery and computational engineering by making Bayesian inference accessible to a broad range of models, including those with inaccessible likelihoods, and to a broader range of users, including both machine learning researchers and domain practitioners. We have created an open architecture and embraced community-driven development practices to encourage collaboration with other machine learning researchers and applied scientists to join us in this long-term vision.

### 3 Related software

Simulation-based inference methods implemented in the sbi package require only access to simulated data, which can also be generated offline in other programming languages or frameworks. This sets sbi apart from toolboxes for traditional Bayesian inference, such as MCMC-based methods [49, 50, 54], which rely on likelihood evaluations, and from probabilistic programming languages (e.g., Pyro [49], NumPyro [55], Stan [54], or Turing.jl [56]), which typically require the simulator to be differentiable and implemented within their respective frameworks [57].

Since the original release of the sbi package, several other packages have emerged that implement neural network-based SBI algorithms. The Lampe [58] package offers neural posterior and neural ratio estimation, primarily targeting SBI researchers with a low-level API and full flexibility over the training loop<sup>5</sup>. The BayesFlow [59] package focuses on a set of amortized SBI algorithms based on posterior and likelihood estimation. The Swyft [60] package specializes in algorithms based on neural ratio estimation. The sbijax [61] package implements a set of inference methods in JAX.

### 4 Author contributions

This work represents a collaborative effort with contributions from a large and diverse team. Author contributions are categorized as follows: Jan Boelts and Michael Deistler are the current maintainers and lead developers of the sbi package and contributed equally to this work. Manuel Gloeckler, Álvaro Tejero-Cantero, Jan-Matthis Lueckmann, and Guy Moss have made substantial and sustained core contributions to the codebase and project direction. Peter Steinbach, Thomas Moreau, Fabio Muratore, Julia Linhart, and Conor Durkan have made major contributions to specific features or aspects of the package. All other authors listed have contributed to the sbi package through code, documentation, or discussions. Jakob H. Macke provided overall project supervision and guidance.

### Acknowledgements

This work has been supported by the German Federal Ministry of Education and Research (BMBF, projects ‘Simalesam’, FKZ 01IS21055 A-B and ‘DeepHumanVision’, FKZ: 031L0197B, and the Tübingen AI Center FKZ: 01IS18039A), the German Research Foundation (DFG) through Germany’s Excellence Strategy (EXC-Number 2064/1, PN 390727645) and SFB1233 (PN 276693517), SFB 1089 (PN 227953431), SPP 2041 ‘Computational Connectomics’, SPP 2298-2 (PN 543917411), the ‘Certification and Foundations of Safe Machine Learning Systems in Healthcare’ project funded by the Carl Zeiss Foundation, the Else Kröner Fresenius Stiftung (Project ClinbrAIn), and the European Union (ERC, “DeepCoMechTome”, ref. 101089288). CD was supported by the EPSRC Centre for Doctoral Training in Data Science, funded by the UK Engineering and Physical Sciences Research Council (grant EP/L016427/1) and the University of Edinburgh. BKM is part of the ELLIS PhD program, receiving travel support from the ELISE mobility program which has received funding from the European Union’s Horizon 2020 research and innovation programme under ELISE grant agreement No 951847. DSG is supported by Helmholtz AI. JL is a recipient of the Pierre-Aguilar Scholarship and thankful for the funding of the Capital Fund Management (CFM). ANK is supported by an FWO grant (G097022N). TG was supported by “Third Wave of AI”, funded by the Excellence Program of the Hessian Ministry of Higher

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<sup>5</sup>The development of the Lampe package has stopped in favor of the sbi package in July 2024

Education, Science, Research and Art. TM and PLCR were supported from a national grant managed by the French National Research Agency (Agence Nationale de la Recherche) attributed to the ExaDoST project of the NumPEX PEPR program, under the reference ANR-22-EXNU-0004.. PS is supported by the Helmholtz Association Initiative and Networking Fund through the Helmholtz AI platform grant. MD, MG, GM, JV, MP, SB, JKL, AS, ZS, JB are members of the International Max Planck Research School for Intelligent Systems (IMPRS-IS).

## References

- [1] George Papamakarios and Iain Murray. Fast  $\varepsilon$ -free inference of simulation models with bayesian conditional density estimation. *Advances in neural information processing systems*, 29, 2016. doi: 10.48550/arXiv.1605.06376.
- [2] George Papamakarios, David Sterratt, and Iain Murray. Sequential neural likelihood: Fast likelihood-free inference with autoregressive flows. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 837–848. PMLR, 2019. doi: 10.48550/arXiv.1805.07226.
- [3] Joeri Hermans, Volodimir Begy, and Gilles Louppe. Likelihood-free mcmc with amortized approximate ratio estimators. In *International Conference on Machine Learning*, pages 4239–4248. PMLR, 2020. doi: 10.48550/arXiv.1903.04057.
- [4] S. A. Sisson, Fan Y., and Beaumont M. A. Overview of abc. In *Handbook of Approximate Bayesian Computation*, Chapman & Hall/CRC Handbooks of Modern Statistical Methods, chapter 1. CRC Press, Taylor & Francis Group, 2018. ISBN 9781439881507. doi: 10.1201/9781315117195.
- [5] Alvaro Tejero-Cantero, Jan Boelts, Michael Deistler, Jan-Matthis Lueckmann, Conor Durkan, Pedro J. Goncalves, David S. Greenberg, and Jakob H. Macke. sbi: A toolkit for simulation-based inference. *Journal of Open Source Software*, 5(52):2505, 2020. doi: 10.21105/joss.02505.
- [6] Michael Deistler, Pedro J. Goncalves, and Jakob H. Macke. Truncated proposals for scalable and hassle-free simulation-based inference. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho, editors, *Advances in Neural Information Processing Systems*, 2022. doi: 10.48550/arXiv.2210.04815.
- [7] Manuel Glöckler, Michael Deistler, and Jakob H Macke. Variational methods for simulation-based inference. In *International Conference on Learning Representations*, 2022. doi: 10.48550/arXiv.2203.04176.
- [8] Fabio Muratore, Theo Gruner, Florian Wiese, Boris Belousov, Michael Gienger, and Jan Peters. Neural posterior domain randomization. In *Conference on Robot Learning*, pages 1532–1542. PMLR, 2022.
- [9] Manuel Gloeckler, Michael Deistler, and Jakob H Macke. Adversarial robustness of amortized bayesian inference. In *International Conference on Machine Learning*, pages 11493–11524. PMLR, 2023. doi: 10.48550/arXiv.2305.14984.
- [10] Joel Dyer, Patrick Cannon, J. Doyne Farmer, and Sebastian M Schmon. Calibrating agent-based models to microdata with graph neural networks. In *ICML 2022 Workshop AI for Agent-Based Modelling*, 2022. doi: 10.48550/arXiv.2206.07570.
- [11] Samuel Wiqvist, Jes Frellsen, and Umberto Picchini. Sequential neural posterior and likelihood approximation. *arXiv preprint arXiv:2102.06522*, 2021. doi: 10.48550/arXiv.2102.06522.
- [12] A Spurio Mancini, MM Docherty, MA Price, and JD McEwen. Bayesian model comparison for simulation-based inference. *RAS Techniques and Instruments*, 2(1):710–722, 2023. doi: 10.1093/rasti/rzad051.
- [13] Simon Dirmeier, Carlo Albert, and Fernando Perez-Cruz. Simulation-based inference using surjective sequential neural likelihood estimation. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2308.01054.
- [14] Richard Gao, Michael Deistler, and Jakob H Macke. Generalized bayesian inference for scientific simulators via amortized cost estimation. *Advances in Neural Information Processing Systems*, 36:80191–80219, 2023.
- [15] Manuel Gloeckler, Michael Deistler, Christian Dietrich Weilbach, Frank Wood, and Jakob H. Macke. All-in-one simulation-based inference. In *Forty-first International Conference on Machine Learning*, 2024. doi: 10.48550/arXiv.2404.09636.
- [16] Joeri Hermans, Arnaud Delaunoy, François Rozet, Antoine Wehenkel, and Gilles Louppe. A crisis in simulation-based inference? beware, your posterior approximations can be unfaithful. *Transactions on Machine Learning Research*, 2022.
- [17] Julia Linhart, Alexandre Gramfort, and Pedro Rodrigues. L-c2st: Local diagnostics for posterior approximations in simulation-based inference. *Advances in Neural Information Processing Systems*, 36, 2024. doi: 10.48550/arXiv.2306.03580.
- [18] Jan Boelts, Jan-Matthis Lueckmann, Richard Gao, and Jakob H Macke. Flexible and efficient simulation-based inference for models of decision-making. *eLife*, 11:e77220, 2022. doi: 10.7554/eLife.77220.
- [19] Lukas N Groschner, Jonatan G Malis, Birte Zuidinga, and Alexander Borst. A biophysical account of multiplication by a single neuron. *Nature*, 603(7899):119–123, 2022. doi: 10.1038/s41586-022-04428-3.

- [20] Vladyslav Bondarenko, Mikhail Nikolaev, Dimitri Kromm, Roman Belousov, Adrian Wolny, Marloes Blotenburg, Peter Zeller, Saba Rezakhani, Johannes Hugger, Virginie Uhlmann, et al. Embryo-uterine interaction coordinates mouse embryogenesis during implantation. *The EMBO Journal*, 42(17):e113280, 2023. doi: 10.15252/embj.2022113280.
- [21] Basile Confavreux, Poornima Ramesh, Pedro J Goncalves, Jakob H Macke, and Tim Vogels. Meta-learning families of plasticity rules in recurrent spiking networks using simulation-based inference. *Advances in Neural Information Processing Systems*, 36:13545–13558, 2023.
- [22] Dylan Myers-Joseph, Katharina A Wilmes, Marian Fernandez-Otero, Claudia Clopath, and Adil G Khan. Disinhibition by *vip* interneurons is orthogonal to cross-modal attentional modulation in primary visual cortex. *Neuron*, 112(4):628–645, 2024. doi: 10.1016/j.neuron.2023.11.006.
- [23] Grace Avecilla, Julie N Chuong, Fangfei Li, Gavin Sherlock, David Gresham, and Yoav Ram. Neural networks enable efficient and accurate simulation-based inference of evolutionary parameters from adaptation dynamics. *PLoS biology*, 20(5):e3001633, 2022. doi: 10.1371/journal.pbio.3001633.
- [24] Eric Lowet, Daniel J Sheehan, Ulises Chialva, Rodrigo De Oliveira Pena, Rebecca A Mount, Sheng Xiao, Samuel L Zhou, Hua-an Tseng, Howard Gritton, Sanaya Shroff, et al. Theta and gamma rhythmic coding through two spike output modes in the hippocampus during spatial navigation. *Cell reports*, 42(8), 2023. doi: 10.1016/j.celrep.2023.112906.
- [25] Yves Bernaerts, Michael Deistler, Pedro J Gonçalves, Jonas Beck, Marcel Stimberg, Federico Scala, Andreas S Tolias, Jakob Macke, Dmitry Kobak, and Philipp Berens. Combined statistical-mechanistic modeling links ion channel genes to physiology of cortical neuron types. *bioRxiv*, pages 2023–03, 2023. doi: 10.1101/2023.03.02.530774.
- [26] Siddharth Mishra-Sharma and Kyle Cranmer. Neural simulation-based inference approach for characterizing the galactic center  $\gamma$ -ray excess. *Physical Review D*, 105(6):063017, 2022. doi: 10.1103/PhysRevD.105.063017.
- [27] Joel Dyer, Patrick Cannon, J Doyne Farmer, and Sebastian Schmon. Black-box bayesian inference for economic agent-based models. *arXiv preprint arXiv:2202.00625*, 2022. doi: 10.48550/arXiv.2202.00625.
- [28] Meysam Hashemi, Anirudh N Vattikonda, Jayant Jha, Viktor Sip, Marmaduke M Woodman, Fabrice Bartolomei, and Viktor K Jirsa. Amortized bayesian inference on generative dynamical network models of epilepsy using deep neural density estimators. *Neural Networks*, 163:178–194, 2023. doi: 10.1016/j.neunet.2023.03.040.
- [29] ChangHoon Hahn and Peter Melchior. Accelerated bayesian sed modeling using amortized neural posterior estimation. *The Astrophysical Journal*, 938(1):11, 2022. doi: 10.3847/1538-4357/ac7b84.
- [30] Pablo Lemos, Liam Parker, ChangHoon Hahn, Shirley Ho, Michael Eickenberg, Jiamin Hou, Elena Massara, Chirag Modi, Azadeh Moradinezhad Dizgah, Bruno Régaldo-Saint Blanchard, et al. Field-level simulation-based inference of galaxy clustering with convolutional neural networks. *Physical Review D*, 109(8):083536, 2024. doi: 10.1103/physrevd.109.083536.
- [31] Michael Deistler, Jakob H Macke, and Pedro J Gonçalves. Energy-efficient network activity from disparate circuit parameters. *Proceedings of the National Academy of Sciences*, 119(44):e2207632119, 2022. doi: 10.1073/pnas.2207632119.
- [32] Nina Rößler, Tassilo Jungenitz, Albrecht Sigler, Alexander Bird, Martin Mittag, Jeong Seop Rhee, Thomas Deller, Hermann Cuntz, Nils Brose, Stephan W Schwarzacher, et al. Skewed distribution of spines is independent of presynaptic transmitter release and synaptic plasticity, and emerges early during adult neurogenesis. *Open Biology*, 13(8):230063, 2023. doi: 10.1098/rsob.230063.
- [33] Lars Dingeldein, Pilar Cossio, and Roberto Covino. Simulation-based inference of single-molecule force spectroscopy. *Machine Learning: Science and Technology*, 4(2):025009, 2023. doi: 10.1016/j.bjpt.2022.11.920.
- [34] Huaqing Jin, Parul Verma, Fei Jiang, Srikanth S Nagarajan, and Ashish Raj. Bayesian inference of a spectral graph model for brain oscillations. *NeuroImage*, 279:120278, 2023. doi: 10.1016/j.neuroimage.2023.120278.
- [35] Jan Boelts, Philipp Harth, Richard Gao, Daniel Udvari, Felipe Yáñez, Daniel Baum, Hans-Christian Hege, Marcel Oberlaender, and Jakob H Macke. Simulation-based inference for efficient identification of generative models in computational connectomics. *PLOS Computational Biology*, 19(9):e1011406, 2023. doi: 10.1101/2023.01.31.526269.
- [36] Richard Gao, Michael Deistler, Auguste Schulz, Pedro J Gonçalves, and Jakob H Macke. Deep inverse modeling reveals dynamic-dependent invariances in neural circuit mechanisms. *bioRxiv*, pages 2024–08, 2024. doi: 10.1101/2024.08.21.608969.
- [37] Xiaoyu Wang, Ryan P. Kelly, Adrienne L. Jenner, David J. Warne, and Christopher Drovandi. A comprehensive guide to simulation-based inference in computational biology, 2024.
- [38] Gael Varoquaux. joblib. <https://github.com/joblib/joblib>, 2008.
- [39] 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. doi: 10.48550/arXiv.1912.02762.

- [40] David Greenberg, Marcel Nonnenmacher, and Jakob Macke. Automatic posterior transformation for likelihood-free inference. In *International Conference on Machine Learning*, pages 2404–2414. PMLR, 2019. doi: 10.48550/arXiv.1905.07488.
- [41] Conor Durkan, Artur Bekasov, George Papamakarios, and Iain Murray. nflows: Normalizing flows in pytorch. <https://github.com/bayesiains/nflows>, 2019.
- [42] Francois Rozet. Zuko - normalizing flows in pytorch. <https://github.com/probabilists/zuko>, 2023.
- [43] Yang Song, Jascha Sohl-Dickstein, Diederik P Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations. In *International Conference on Learning Representations*, 2021. doi: 10.48550/arXiv.2011.13456.
- [44] Tomas Geffner, George Papamakarios, and Andriy Mnih. Compositional score modeling for simulation-based inference. In *International Conference on Machine Learning*, pages 11098–11116. PMLR, 2023. doi: 10.48550/arXiv.2209.14249.
- [45] Jack Simons, Louis Sharrock, Song Liu, and Mark Beaumont. Neural score estimation: Likelihood-free inference with conditional score based diffusion models. In *Fifth Symposium on Advances in Approximate Bayesian Inference*, 2023. doi: 10.48550/arXiv.2210.04872.
- [46] C M Bishop. Mixture density networks. *Technical Report. Aston University, Birmingham*, 1994.
- [47] Yaron Lipman, Ricky T. Q. Chen, Heli Ben-Hamu, Maximilian Nickel, and Matthew Le. Flow matching for generative modeling. In *The Eleventh International Conference on Learning Representations*, 2023. doi: 10.48550/arXiv.2210.02747.
- [48] Jonas Bernhard Wildberger, Maximilian Dax, Simon Buchholz, Stephen R Green, Jakob H. Macke, and Bernhard Schölkopf. Flow matching for scalable simulation-based inference. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023. doi: 10.48550/arXiv.2305.17161.
- [49] Eli Bingham, Jonathan P. Chen, Martin Jankowiak, Fritz Obermeyer, Neeraj Pradhan, Theofanis Karaletsos, Rohit Singh, Paul A. Szerlip, Paul Horsfall, and Noah D. Goodman. Pyro: Deep universal probabilistic programming. *J. Mach. Learn. Res.*, 20:28:1–28:6, 2019. doi: 10.48550/arXiv.1810.09538.
- [50] Oriol Abril-Pla, Virgile Andreani, Colin Carroll, Larry Dong, Christopher J Fonnesbeck, Maxim Kochurov, Ravin Kumar, Junpeng Lao, Christian C Luhmann, Osvaldo A Martin, et al. Pymc: a modern, and comprehensive probabilistic programming framework in python. *PeerJ Computer Science*, 9:e1516, 2023. doi: 10.7717/peerj-cs.1516.
- [51] Sean Talts, Michael Betancourt, Daniel Simpson, Aki Vehtari, and Andrew Gelman. Validating bayesian inference algorithms with simulation-based calibration. *arXiv preprint arXiv:1804.06788*, 2018. doi: 10.48550/arXiv.1804.06788.
- [52] Pablo Lemos, Adam Coogan, Yashar Hezaveh, and Laurence Perreault-Levasseur. Sampling-based accuracy testing of posterior estimators for general inference. In *International Conference on Machine Learning*, pages 19256–19273. PMLR, 2023. doi: 10.48550/arXiv.2302.03026.
- [53] Ravin Kumar, Colin Carroll, Ari Hartikainen, and Osvaldo Martin. Arviz a unified library for exploratory analysis of bayesian models in python. *Journal of Open Source Software*, 4(33):1143, 2019. doi: 10.21105/joss.01143.
- [54] Andrew Gelman, Daniel Lee, and Jiqiang Guo. Stan: A probabilistic programming language for bayesian inference and optimization. *Journal of Educational and Behavioral Statistics*, 40(5):530–543, 2015. doi: 10.3102/1076998615606113.
- [55] Du Phan, Neeraj Pradhan, and Martin Jankowiak. Composable effects for flexible and accelerated probabilistic programming in numpyro. *arXiv preprint arXiv:1912.11554*, 2019. doi: 10.48550/arXiv.1912.11554.
- [56] Hong Ge, Kai Xu, and Zoubin Ghahramani. Turing: a language for flexible probabilistic inference. In *International Conference on Artificial Intelligence and Statistics, AISTATS 2018, 9-11 April 2018, Playa Blanca, Lanzarote, Canary Islands, Spain*, pages 1682–1690, 2018. URL <http://proceedings.mlr.press/v84/ge18b.html>.
- [57] Arnaud Quera-Bofarull, Joel Dyer, Anisoara Calinescu, J. Doyne Farmer, and Michael Wooldridge. Blackbirds: Black-box inference for differentiable simulators. *Journal of Open Source Software*, 8(89):5776, 2023. doi: 10.21105/joss.05776. URL <https://doi.org/10.21105/joss.05776>.
- [58] François Rozet, Arnaud Delaunoy, Benjamin Miller, et al. Lampe: Likelihood-free amortized posterior estimation. *Statistical Software*, 2021.
- [59] Stefan T. Radev, Marvin Schmitt, Lukas Schumacher, Lasse Elsemüller, Valentin Pratz, Yannik Schälte, Ullrich Köthe, and Paul-Christian Bürkner. BayesFlow: Amortized Bayesian workflows with neural networks. *Journal of Open Source Software*, 8(89):5702, 2023. doi: 10.21105/joss.05702.
- [60] undark lab. Swyft: A system for scientific simulation-based inference at scale. <https://github.com/undark-lab/swyft>, 2023. Version 0.4.5.
- [61] Simon Dirmeier, Simone Ulzega, Antonietta Mira, and Carlo Albert. Simulation-based inference with the python package sbijax, 2024.