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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 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.

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 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 (Hermans et al., 2020; Papamakarios et al., 2019; Papamakarios & Murray, 2016). Unlike classical methods from Approximate Bayesian Computation (ABC, Sisson et al. (2018)), 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 with 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 *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 any 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 (Tejero-Cantero et al., 2020), 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 (Boelts et al., 2022; Deistler, Goncalves, et al., 2022; Dirmeier et al., 2023; Dyer et al., 2022b; Glöckler et al., 2022; Gloeckler et al., 2023, 2024; Hermans et al., 2022; Linhart et al., 2024; Muratore et al., 2022; Spurio Mancini et al., 2023; Wiqvist et al., 2021) but has also fostered the application of SBI in various fields of research (Avecilla et al., 2022; Bernaerts et al., 2023; Boelts et al., 2023; Bondarenko et al., 2023; Confavreux et al., 2023; Deistler, Macke, et al., 2022; Dingeldein et al., 2023; Dyer et al., 2022a; Gao et al., 2024; Groschner et al., 2022; Hahn & Melchior, 2022; Hashemi et al., 2023; Jin et al., 2023; Lemos et al., 2024; Lowet et al., 2023; Mishra-Sharma & Cranmer, 2022; Myers-Joseph et al., 2024; Rößler et al., 2023; Wang et al., 2024).

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 (Figure 1).

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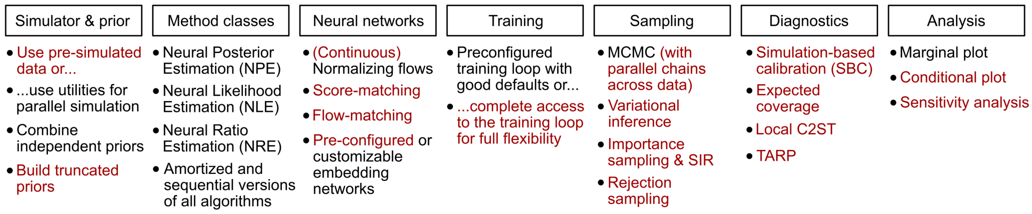

Figure 1: Features of the `sbi` package. Components that were added since the initial release described in Tejero-Cantero et al. (2020) are marked in red.

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, without needing 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` (Varoquaux, 2008). 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 simulation 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, running simulations with parameters likely to have resulted in the observation.

Neural networks and training: `sbi` implements a wide variety of state-of-the-art conditional density estimators for NPE and NLE, including normalizing flows (Greenberg et al., 2019; Papamakarios et al., 2021) (via `nflows` (Durkan et al., 2019) and `zuko` (Rozet, 2023)), diffusion models (Geffner et al., 2023; Simons et al., 2023; Song et al., 2021), mixture density networks (Bishop, 1994), and flow matching (Lipman et al., 2023; Wildberger et al., 2023) (via `zuko`), 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 multi-layer-perceptrons, convolutional networks, and permutation invariant networks). The neural networks can be trained with a pre-configured 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 (Abril-Pla et al., 2023; Bingham et al., 2019). `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) (Talts et al., 2018), expected coverage (Deistler, Goncalves, et al., 2022; Hermans et al., 2022), local C2ST (Linhart et al., 2024), and TARP (Lemos et al., 2023). Additionally, `sbi` offers visualization tools for the posterior, including marginal and conditional corner plots to visualize high-dimensional distributions, calibration plots, and wrappers for Arviz (Kumar et al., 2019) 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.

Related software

Since the original release of the sbi package, several other packages that implement neural network-based SBI algorithms have emerged. The Probabilists (2024) package offers neural posterior and neural ratio estimation, primarily targeting SBI researchers with a low-level API and full flexibility over the training loop (Lampe stopped being maintained in July 2024). The BayesFlow package (Stefan T. Radev et al., 2023) focuses on a set of amortized SBI algorithms based on posterior and likelihood estimation that have been developed in the respective research labs (Stefan T. Radev et al., 2020). The swyft package (undark-lab, 2023) specializes in algorithms based on neural ratio estimation. The sbijax package (Dirmeier et al., 2024) implements a set of inference methods in JAX.

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