# SBIAX: Density-estimation simulation-based inference in JAX.

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Summary

In a typical Bayesian inference problem, the data likelihood is not known. However, in recent years, machine learning methods for density estimation can allow for inference using an estimator of the data likelihood. This likelihood is created with neural networks that are trained on simulations - one of the many tools for simulation based inference (SBI, Cranmer et al. (2020)). In such analyses, density-estimation simulation-based inference methods can derive a posterior, which typically involves

- simulating a set of data and model parameters $\{(\xi, \pi)_0, ..., (\xi, \pi)_N\}$,
- obtaining a measurement $\hat{\xi}$,
- compressing the simulations and the measurements - usually with a neural network or linear compression - to a set of summaries $\{(x, \pi)_0, ..., (x, \pi)_N\}$ and $\hat{x}$,
- fitting an ensemble of normalising flow or similar density estimation algorithms (e.g. a Gaussian mixture model),
- the optional optimisation of the parameters for the architecture and fitting hyperparameters of the algorithms,
- sampling the ensemble posterior (using an MCMC sampler if the likelihood is fit directly) conditioned on the datavector to obtain parameter constraints on the parameters of a physical model, π.

sbiax is a code for implementing each of these steps. The code allows for Neural Likelihood Estimation (Alsing et al., 2019; Papamakarios, 2019) and Neural Posterior Estimation (Greenberg et al., 2019).

As shown in Homer 2024, SBI is shown to successfully obtain the correct posterior widths and coverages given enough simulations which agree with the analytic solution.

Statement of need

Simulation-based inference (SBI) covers a broad class of statistical techniques such as Approximate Bayesian Computation (ABC), Neural Ratio Estimation (NRE), Neural Likelihood Estimation (NLE) and Neural Posterior Estimation (NPE). These techniques can derive posterior distributions conditioned of noisy data vectors in a rigorous and efficient manner. In particular, density-estimation methods have emerged as a promising method, given their efficiency, using generative models to fit likelihoods or posteriors directly using simulations.

In the field of cosmology, SBI is of particular interest due to complexity and non-linearity of models for the expectations of non-standard summary statistics of the large-scale structure, as well as the non-Gaussian noise distributions for these statistics. The assumptions required for the complex analytic modelling of these statistics as well as the increasing dimensionality of

40 data returned by spectroscopic and photometric galaxy surveys limits the amount of information
41 that can be obtained on fundamental physical parameters. Therefore, the study and research
42 into current and future statistical methods for Bayesian inference is of paramount importance
43 for the field of cosmology.

44 The software we present, `sbiax`, is designed to be used by machine learning and physics
45 researchers for running Bayesian inferences using density-estimation SBI techniques. These
46 models can be fit easily with multi-accelerator training and inference within the code. This
47 code - written in `jax` (Bradbury et al., 2018) - allows for seemless integration of cutting edge
48 generative models to SBI, including continuous normalising flows (Grathwohl et al., 2018),
49 matched flows (Lipman et al., 2023), masked autoregressive flows (Papamakarios et al., 2018;
50 Ward, [release year of version]) and Gaussian mixture models - all of which are implemented in
51 the code. The code features integration with the `optuna` (Akiba et al., 2019) hyperparameter
52 optimisation framework which would be used to ensure consistent analyses, `blackjax` (Cabezas
53 et al., 2024) for fast MCMC sampling and `equinox` (Kidger & Garcia, 2021) for neural network
54 compression methods. The design of `sbiax` allows for new density estimation algorithms to be
55 trained and sampled from.

Density estimation with normalising flows

57 The use of density-estimation in SBI has been accelerated by the advent of normalising
58 flows. These models parameterise a change-of-variables $y = f_\phi(x; \pi)$ between a simple base
59 distribution (e.g. a multivariate unit Gaussian $\mathcal{G}[z|\mathbf{0}, \mathbf{I}]$) and an unknown distribution $q(x|\pi)$
60 (from which we have simulated samples x). Naturally, this is of particular importance in
61 inference problems in which the likelihood is not known. The change-of-variables is fit from data
62 by training neural networks to model the transformation in order to maximise the log-likelihood
63 of the simulated data x conditioned on the parameters π of a simulator model. The mapping
64 is expressed as

$$y = f_\phi(x; \pi),$$

65 where ϕ are the parameters of the neural network. The log-likelihood of the flow is expressed
66 as

$$\log p_\phi(x|\pi) = \log \mathcal{G}[f_\phi(x; \pi)|0, \mathbb{I}] + \log \left| \mathbf{J}_{f_\phi}(x; \pi) \right|,$$

67 This density estimate is fit to a set of N simulation-parameter pairs $\{(\xi, \pi)_0, ..., (\xi, \pi)_N\}$ by
68 minimising a Monte-Carlo estimate of the KL-divergence

$$
\begin{aligned}
\langle D_{KL}(q||p_\phi)\rangle_{\pi \sim p(\pi)} &= \int \mathrm{d}\pi \, p(\pi) \int \mathrm{d}x \, q(x|\pi) \log \frac{q(x|\pi)}{p_\phi(x|\pi)}, \\
&= \int \mathrm{d}\pi \int \mathrm{d}x \, p(\pi, x)[\log q(x|\pi) - \log p_\phi(x|\pi)], \\
&\geq - \int \mathrm{d}\pi \int \mathrm{d}x \, p(\pi, x) \log p_\phi(x|\pi), \\
&\approx -\frac{1}{N} \sum_{i=1}^{N} \log p_\phi(x_i|\pi_i),
\end{aligned}
\tag{1}
$$

69 where $q(x|\pi)$ is the unknown likelihood from which the simulations x are drawn. This applies
70 similarly for an estimator of the posterior (instead of the likelihood as shown here) and is the
71 basis of being able to estimate the likelihood or posterior directly when an analytic form is

72 not available. If the likelihood is fit from simulations, a prior is required and the posterior is
73 sampled via an MCMC given some measurement. This is implemented within the code.

74 An ensemble of density estimators (with parameters - e.g. the weights and biases of the
75 networks - denoted by $\{\phi_0, ..., \phi_J\}$) has a likelihood which is written as

$$p_{\text{ensemble}}(\xi|\pi) = \sum_{j=1}^{J} \alpha_i p_{\phi_i}(\hat{\xi}|\pi)$$

76 where

$$\alpha_i = \frac{\exp(p_{\phi_i}(\hat{\xi}|\pi))}{\sum_{j=1}^{J} \exp(p_{\phi_j}(\hat{\xi}|\pi))}$$

77 are the weights of each density estimator in the ensemble. This ensemble likelihood can be
78 easily sampled with an MCMC sampler. In Figure 1 we show an example posterior from
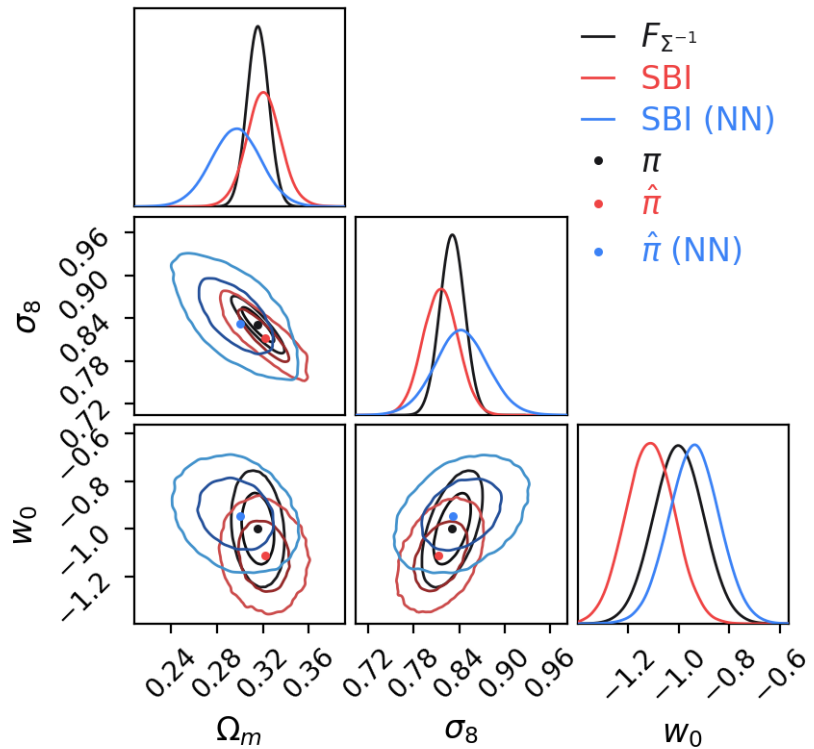79 applying SBI, with our code, using two compression methods separately.

Figure 1: An example of posteriors derived with `sbiax`. We fit a ensemble of two continuous normalising flows to a set of simulations of cosmic shear two-point functions. The expectation $\xi[\pi]$ is linearised with respect to π and a theoretical data covariance model Σ allows for easy sampling of many simulations - an ideal test arena for SBI methods. We derive two posteriors, from separate experiments, where a linear (red) or neural network compression (blue) is used. In black, the true analytic posterior is shown (note that for a finite set of simulations the posteriors will not overlap completely).

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