

Simulation-Based Inference with Neural Posterior Estimation applied to X-ray spectral fitting Demonstration of working principles down to the Poisson regime

Didier Barret & Simon Dupourqué (IRAP, France)

Neural networks are being extensively used for modeling data, especially in the case where no likelihood can be formulated. Aims. Although in the case of X-ray spectral fitting, the likelihood is known, we aim to investigate the neural networks ability to recover the model parameters but also their associated uncertainties, and compare its performance with standard X-ray spectral fitting, whether following a frequentist or Bayesian approach.

We apply Simulation-Based Inference with Neural Posterior Estimation (SBI-NPE) to X-ray spectra. We train a network with simulated spectra generated from a multi-parameter source emission model folded through an instrument response, so that it learns the mapping between the simulated spectra and their parameters and returns the posterior distribution. The model parameters are sampled from a predefined prior distribution. To maximize the efficiency of the training of the neural network, yet limiting the size of the training sample to speed up the inference, we introduce a way to reduce the range of the priors, either through a classifier or a coarse and quick inference of one or multiple observations. For the sake of demonstrating working principles, we apply the technique to data generated from and recorded by the NICER X-ray instrument: a medium resolution X-ray spectrometer, covering the 0.2-12 keV band. We consider here simple X-ray emission models with up to 5 parameters.

SBI-NPE is demonstrated to work equally well as standard X-ray spectral fitting, both in the Gaussian and Poisson regimes, both on simulated and real data, yielding fully consistent results in terms of best fit parameters and posterior distributions. The inference time is comparable to or smaller than the one needed for Bayesian inference, when involving the computation of large Markov Chain Monte Carlo chains to derive the posterior distributions. On the other hand, once properly trained, an amortized SBI- NPE network generates the posterior distributions in no time (less than 1 second per spectrum on a 6-core laptop). We show that SBI-NPE is less sensitive to local minima trapping than standard fit statistic minimization techniques. With a simple model, we find that the neural network can be trained equally well on dimension-reduced spectra, via a Principal Component Decomposition, leading to a faster inference time with no significant degradation of the posteriors.

In this presentation, we will show that simulation-based inference with neural posterior estimation adds up as a complementary tool for X-ray spectral analysis, holding great potential for integration in pipelines developed for processing large data sets.