

ArviZ: backend agnostic exploratory analysis of Bayesian models in Python

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Probabilistic programming is an emerging field of growing importance. In recent years, many libraries have been built to write probabilistic models as executable code. ArviZ proposes the use of a common data structure called InferenceData to ease the analysis of the results. To this end, ArviZ converts results from several libraries to InferenceData. It also provides functions to plot the results —using matplotlib or bokeh—, calculate relevant diagnostics or perform model checking. We therefore hope ArviZ will become a key tool in Bayesian analysis by providing users with computational tools to analyze and explore their results and to compare between different probabilistic programming libraries.

1 INTRODUCTION

The growth of both probabilistic programming languages and algorithms for the analysis of Bayesian inference results led to the introduction of the Python library ArviZ [Kumar et al. 2019]. Outside inference itself and sampling, ArviZ covers all the other aspects of Bayesian analysis. These tasks such as diagnoses of the quality of the inference, model criticism or preparation of the results for a particular audience are also key to the modelling process and require both numerical and visual tools. ArviZ aims to ease the use of a robust Bayesian workflow so users can concentrate on domain specific knowledge.

Following the structure of ArviZ’s source code itself, this paper divides all these tasks into 3 categories, each of which has its own section. Section 2 is about data storage of Bayesian inference results. Our goal is to define a storage schema compatible with netCDF [Unidata 2011]. This data structure should contain all relevant information to perform diagnostics on the inference run or to reproduce it. Sections 3 and 4 outline the algorithms and plotting functions implemented in ArviZ respectively.

2 DATA STORAGE SCHEME

One of ArviZ key features is its data storage scheme using InferenceData objects. InferenceData (built on top of xarray [Hoyer and Hamman 2017]) contain several groups, each of which is a multidimensional labeled array with one or several data variables (Figure 1).

These groups contain a specific quantity such as *posterior*, *observed data* or *sampler stats* (sampler quantities like divergencies, tree depth, or log likelihood). Groups in InferenceData directly translate to groups defined in netCDF files, making the storage of InferenceData as netCDF files straightforward. The full schema specification can be found on ArviZ documentation¹.

InferenceData objects are central to ArviZ, most ArviZ functions take InferenceData as input. Therefore, we provide native functions to convert between the outputs of several inference libraries and InferenceData. Table 1 shows the state of converter functions in ArviZ beta release 0.6.1 (latest release to date). Natively supported libraries are PyStan, CmdStan and CmdStanPy [Stan Development Team 2018a,b,c,d], PyMC3 [Salvatier et al. 2016], Pyro and NumPyro [Bingham et al. 2018], emcee [Foreman-Mackey et al. 2019, 2013] and TensorFlow Probability [Dillon et al. 2017]. In addition, there is also a function to convert dictionaries to InferenceData.

¹<https://arviz-devs.github.io/arviz/schema/schema.html>

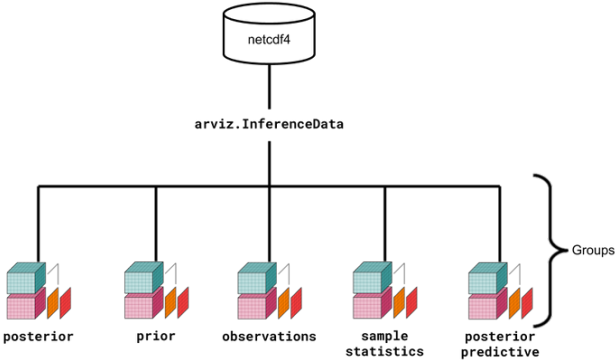


Fig. 1. Visual representation of the InferenceData structure.

Table 1. ArviZ converter functions summary

Inference Library	Sampler Stats	Posterior predictive	Observed data	Prior
PyStan, CmdStan, CmdStanPy	✓	✓	✓	✓
PyMC3	✓	✓	✓	✓
Pyro	✓ ²	✓	✓ ²	✓
NumPyro	✓	✓	✓	✓
emcee	Limited ³	Limited ³	✓	✗
tensorflow probability	Limited ⁴	✓	✓	✗

We are still working on the InferenceData scheme with two main goals in mind, support the storage of predictions, and storage of the arguments used when calling the sampler as well as the kind of sampler. This latter goal would allow to reproduce the sampling given the InferenceData object.

3 STATISTICS AND DIAGNOSTICS

ArviZ includes many statistics and diagnostics for Bayesian analysis such as the Gelman-Rubin statistic [Gelman and Rubin 1992] or the widely applicable Information Criterion [Watanabe 2010]. We strive to provide sensible defaults for all algorithms and to keep them up to date with the latest publications. Moreover, Numba [Lam et al. 2015] is used to speed up lengthy calculations.

3.1 Diagnostics

Many convergence assessment functions are available in ArviZ. az.rhat, az.ess and az.mcse implement the Gelman-Rubin statistic, effective sample size and Monte Carlo standard error respectively [Gelman et al. 2013; Gelman and Rubin 1992]. The improvements in Vehtari et al. [2019] have already been added to ArviZ and have been made the default for all 3 functions. Moreover, all 3 functions take as input a method to choose between the available versions of the algorithms. For example, the effective sample size can be calculated for the bulk or for quantiles

²For Pyro<1.0.0 there is only partial sampler stats support and no observed data available
³emcee’s blobs can be used to store sampler stats or even posterior predictive samples, however, blobs can store anything, so it is up to the user to customize them properly
⁴Only log likelihood data is retrieved

and with or without rank normalization. `az.bfmi` can be used to calculate Bayesian fraction of missing information [Betancourt 2016]. `az.geweke` implements the z-scores for convergence diagnostics [Geweke 1991].

An `az.summary` function is also provided for convenience to calculate several diagnostics together with statistics such as mean or variance. Its output can be directly printed in a readable manner.

3.2 Model comparison

ArviZ also provides functions for model comparison using the predictive accuracy as metric. Given that ArviZ is intended to analysis of Bayesian inference results and it aims to extend best practices, only the fully Bayesian algorithms have been implemented [Gelman et al. 2014]. `az.waic` computes the widely applicable information criterion [Watanabe 2010] and `az.loo` computes the leave one out cross validation using Pareto smoothed importance sampling [Vehtari et al. 2015, 2017].

`az.compare` can be used to compute the WAIC or LOO value for several models at the same time, effectively comparing them in a single line of code.

3.3 Model checking

One algorithm for model checking, `az.loo_pit`, has also been implemented recently, the leave one out cross validation probability integral transform (LOO-PIT) [Gabry et al. 2019]. This has been possible thanks to the versatility of `InferenceData`, which contains all the quantities needed for this calculation: observed data, posterior predictive samples and log likelihood data. It should be noted that the LOO-PIT result is generally analyzed visually in a qualitative way. This can also be done in ArviZ using native plotting functions.

In addition, the results from `az.loo` and `az.waic` can also be used for model checking to some extent.

4 DATA VISUALIZATION

Many of the algorithms described in Section 3 have complementary plots that extend them and ease their interpretability. Some examples are `az.plot_compare`, `az.plot_loo_pit` or `az.plot_ess` which complement the algorithms of the same name, but also `az.plot_khat` to complement `az.loo` or `az.plot_elpd` to complement either `az.waic` or `az.loo`.

ArviZ provides plotting functions suited for many different tasks: visualization of probability distributions, model checking, convergence diagnostics or model comparison. The documentation contains an [example gallery](#) showcasing all plots currently available in ArviZ. Figure 2 shows some of the recently added plots.

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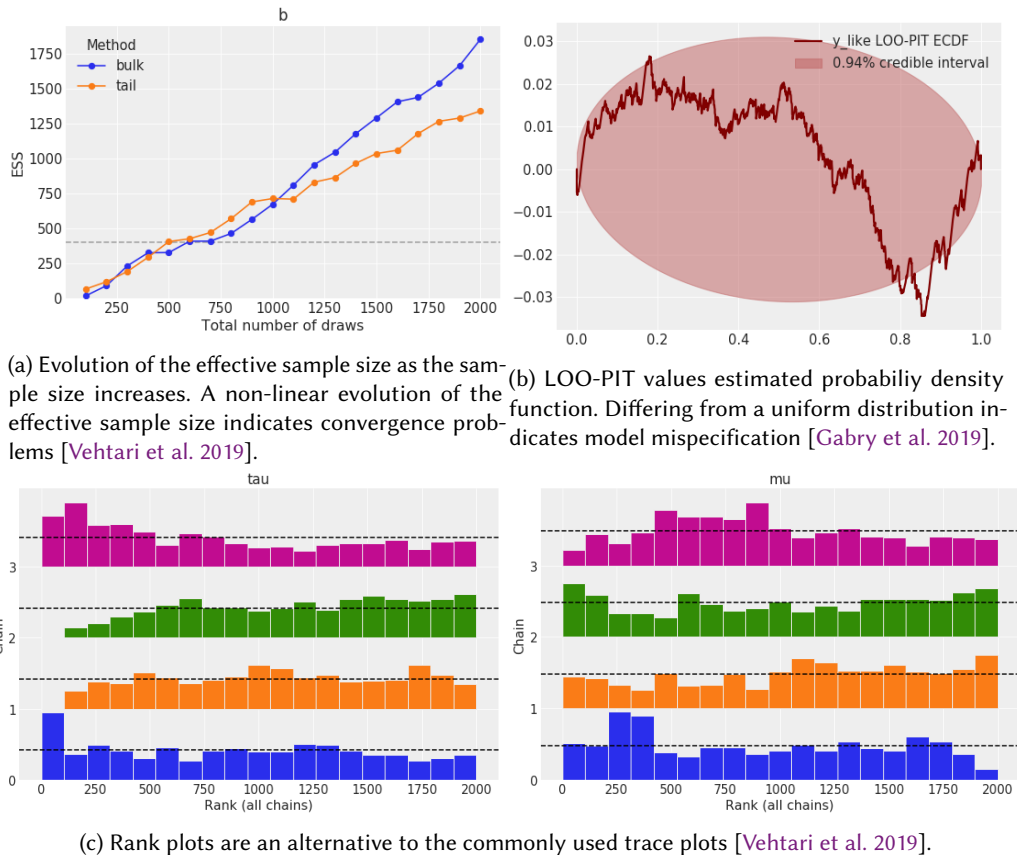


Fig. 2. Examples of plotting functions added to ArviZ during 2019.

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