ArviZ: backend agnostic exploratory analysis of Bayesian models in Python

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In recent years, many libraries have been built to specify probabilistic models as executable code. ArviZ proposes the use of a common data structure called `InferenceData` to ease and unify common types of analysese of these models. To this end, ArviZ converts results from several libraries to `InferenceData`. It also provides functions to flexibly plot the results using different libraries, 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 across different probabilistic programming libraries (PPL). By unifying the common pre and post modeling toolset the workflow is simpler for both PPL designers and Bayesian practitioners. For practitioners it simplifies the steps after inference. For PPL designers it allows them to focus on building their modeling langauge and inference, and deferring pre and post inference tasks to ArviZ

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 questions.

Following the structure of ArviZ's source code itself, this paper divides these tasks into 3 categories, each of which has its own section. Section 2 is about data storage of Bayesian inference results. Section 3 outlines the statistical and diagnostic algorithms provided by ArviZ, while Section 4 provides an overview of plotting functions implemented in ArviZ.

2 DATA STORAGE SCHEMA

One of ArviZ's key features is its data storage schema. Our goal is to define a storage schema compatible with netCDF [Unidata 2011]. This data structure, called `InferenceData`, should contain all relevant information to perform diagnostics on the inference run or to reproduce it. `InferenceData` (built on top of xarray [Hoyer and Hamman 2017]) contains several groups, each of which is a multidimensional labeled array with one or several data variables (Figure 1).

These groups contain data related to a specific collection such as *posterior*, *observed data*, or *sampler stats* (sampler quantities like divergences, tree depth, or log likelihood). Groups in `InferenceData` directly translate to groups defined in netCDF files, making their storage as netCDF files straightforward. The full schema specification can be found in ArviZ documentation[1].

[1] https://arviz-devs.github.io/arviz/schema/schema.html

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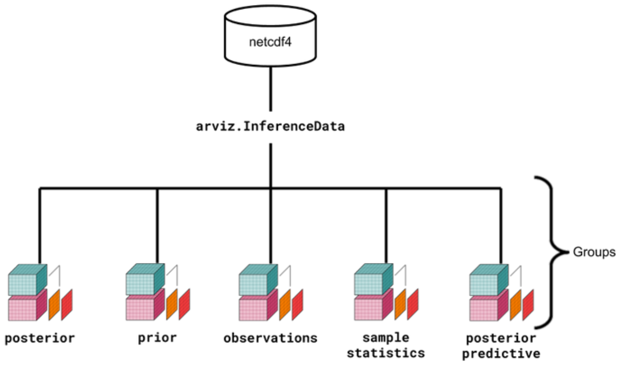


Fig. 1. Visual representation of the `InferenceData` structure.

`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 of NumPy arrays to `InferenceData`.

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]	✓	✓	✗

Future design goals of `InferenceData` include two main goals: support the storage of out-of-sample posterior predictive samples, and storage of the arguments used when calling the sampler as well as the kind of sampler. The latter goal would allow reproducible sampling given the `InferenceData` object.

3 STATISTICS AND DIAGNOSTICS

ArviZ includes many statistics and diagnostics for Bayesian analysis such as the $\hat{R}$ statistic [Gelman and Rubin 1992; Vehtari et al. 2019] 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

[2] For Pyro<1.0.0 there is only partial sampler stats support and no observed data available

[3] emcee'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

[4] Only log likelihood data is retrieved

publications. Moreover, when installed, Numba [Lam et al. 2015] is optionally used to speed up expensive calculations.

3.1 Diagnostics

Many convergence assessment functions are available in ArviZ. `rhat`, `ess` and `mcse` implement the $\hat{R}$ 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 three functions. Moreover, all three 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 and with or without rank normalization. The `bfmi` function can be used to calculate Bayesian fraction of missing information [Betancourt 2016], and the `geweke` function implements z-scores for convergence diagnostics [Geweke 1991].

A `summary` function is also provided for convenience to calculate several diagnostics together with some statistics such as mean, standard deviation or highest posterior density intervals. 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]. The `waic` function computes the widely applicable information criterion [Watanabe 2010], and the `loo` function computes the leave one out cross validation using Pareto smoothed importance sampling [Vehtari et al. 2015, 2017].

For iterative model building, the `compare` function 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, the `loo_pit` function, 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 `loo` and `waic` functions can also be used for model checking to some extent.

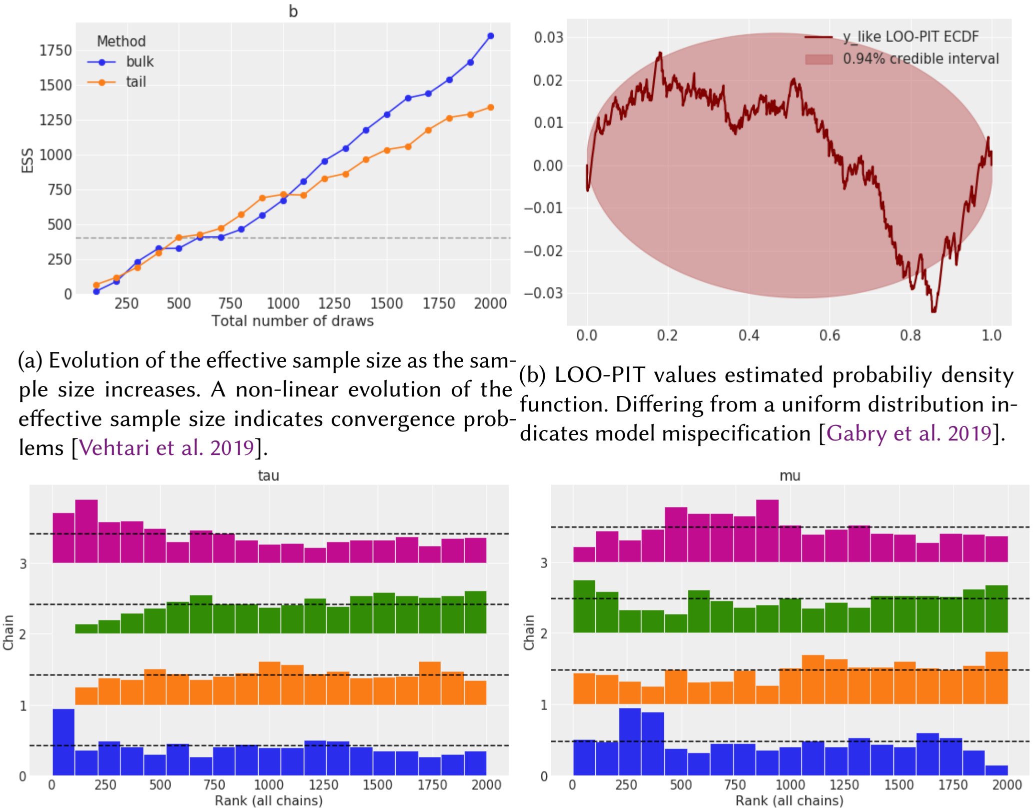
4 DATA VISUALIZATION

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

ArviZ provides plotting functions suited to many different tasks: visualization of probabiliy distributions, model checking, convergence diagnostics, or model comparison. The documentation contains an example gallery[5] showcasing all plots currently available in ArviZ. Figure 2 shows some of the recently added plots.

[5] https://arviz-devs.github.io/arviz/examples/index.html

Additionally, the plots may use either Matplotlib [Hunter 2007], which is versatile and well tested, especially for preparing static plots, or Bokeh [Bokeh Development Team 2019], which allows for interactivity and web-based graphics.



(a) Evolution of the effective sample size as the sample size increases. A non-linear evolution of the effective sample size indicates convergence problems [Vehtari et al. 2019].

(b) LOO-PIT values estimated probabiliy density function. Differing from a uniform distribution indicates model mispecification [Gabry et al. 2019].

(c) Rank plots are an alternative to the commonly used trace plots [Vehtari et al. 2019].

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

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