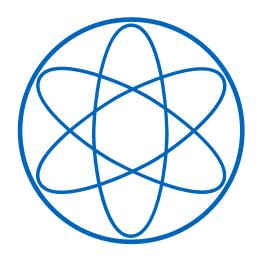


# Development and Benchmarking of a Bayesian Inference Pipeline for LHC Physics



Scientific Thesis for the procurance of the degree

BACHELOR OF SCIENCE

from the Physics Department at the Technical University of Munich.

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**Submitted on** September 22, 2022

Abstract

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Abbreviations

# Abbreviations

**BAT** Bayesian Analysis Toolkit.

**HMC** Hamiltonian Monte Carlo.

MCMC Markov chain Monte Carlo.

**NP** nuisance parameter.

**pdf** probability density function.

**POI** parameter of interest.

vi Abbreviations

# Introduction

# **Mathematical Preliminaries**

- 2.1 Frequentist versus Bayesian Inference
- 2.2 MCMC Sampling
- 2.2.1 Markov Chains
- 2.2.2 Metropolis Hastings
- 2.2.3 Hamiltonian Markov Chains

# HistFactory

- 3.1 Mathematical Description
- 3.2 Workspaces ...

# Bayesian Inference with HistFactory

#### 4.1 BAT

Bayesian Analysis Toolkit (BAT)

- 4.2 batty BAT to Python Interface
- 4.3 Priors from auxdata
- 4.4 Gradients for HamiltonianMC

#### 4.5 Python HistFactory Benchmarks

While running code on a PC, the execution time of a function varies due to other active processes. A typical run time statistic is illustrated in Figure 4.1.

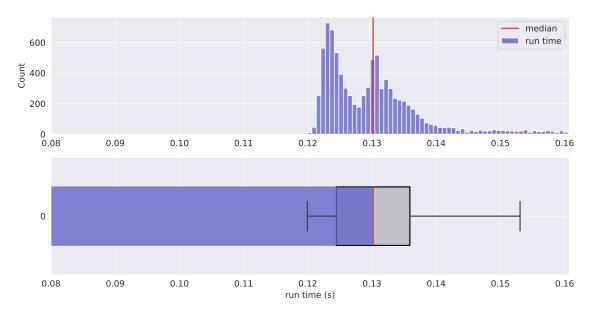
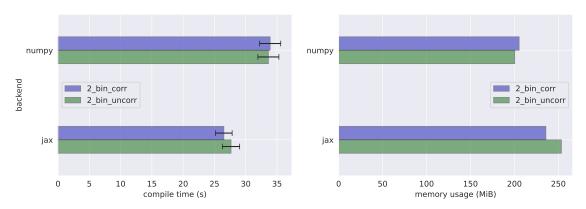


Figure 4.1: Run time statistics of (xx)

- use median instead mean
- use bar + box plot

#### 4.5.1 pyhf Backend

- jax vs numpy
- 2 simplemodels
- jax jitted log likelihood is 4 times faster with numpy backend



(a) Compile time and memory usage during compilation.

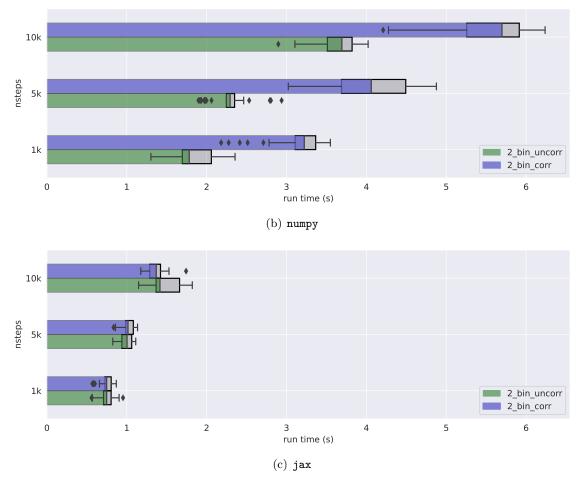


Figure 4.2: Compile benchmark and run time performance of bat\_sample() once using the numpy backend of pyhf and once with jax backend. The run time is evaluated for two different models XX.

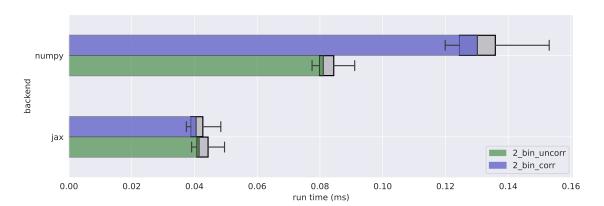


Figure 4.3: Run time of the log likelihood for two different HF models. XX

# Benchmarking the Python-Julia Pipeline against the Julia Implementation

#### 5.1 Overview

Calling Julia code from Python is accomplished by the PythonCall.jl module

#### 5.2 Benchmark Setup

•

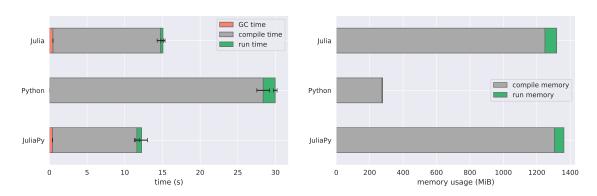


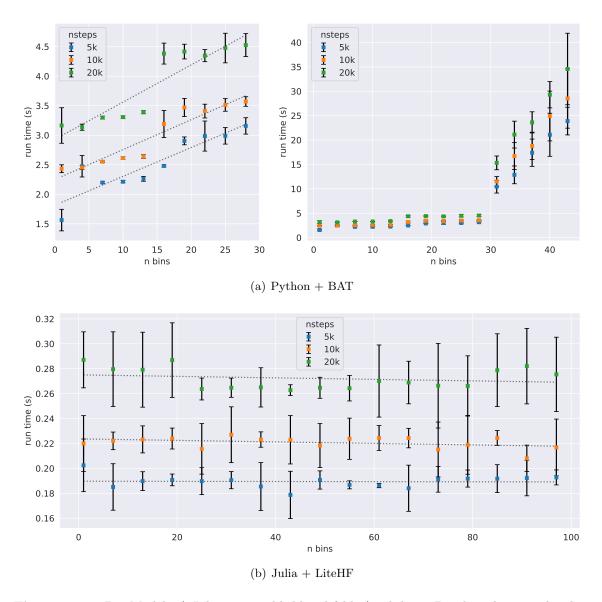
Figure 5.1: Total execution time for bat\_sample(). (10k steps) ...

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#### 5.3 Benchmarks

The pure-Julia implementation is about 10 times faster than the Python-Julia pipeline.

#### 5.3.1 n-Bin-Model



**Figure 5.2:** n-Bin Model. c) Julia + pyhf likelihood fehlt (noch keine Benchmarks gemacht, da LZ intensiv, in n $\tilde{A}$ zchster Version.)

- $\bullet$  simple model with uncorrelated background and n bins
- pure Julia "stable" runtime over 1 to 100 dimensional parameter vector (Ich check das nochmal ..)

 $\bullet\,$  Python jump at 30 dim parameter vector

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#### 5.3.2 Benchmarks for the "complex" Model

TODO: complex Model benchmarks

- In Progress..
- Ich hab mal Plots erzeugt, fur die simplemodels
  Hier hab ich nur gerade was durcheinandergebracht, ist in der naechsten Version drin (vmtl. mit dem complex model.)
- Ergebnis vorab:
  - pure-Julia ist wieder 10 x Schneller als Python + BAT
  - Python + BAT etwa vergleichbare Laufzeit wie Julia + pyhf likelihood

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# **Bibliography**

- [1] Lukas Heinrich, Matthew Feickert, and Giordon Stark. Python HistFactory pyhf. https://github.com/scikit-hep/pyhf, 2021.
- [2] Jeff Bezanson, Alan Edelman, Stefan Karpinski, and Viral B. Shah. Julia: A fresh approach to numerical computing. *SIAM Review*, 59(1):65–98, 9 2017.
- [3] Kyle Cranmer, Akira Shibata, Wouter Verkerke, Lorenzo Moneta, and George Lewis. Histfactory: A tool for creating statistical models for use with roofit and roostats. Technical report, 2012.
- [4] Kyle Cranmer. Practical statistics for the LHC. arXiv preprint arXiv:1503.07622, 2015.
- [5] Oliver Schulz, Frederik Beaujean, Allen Caldwell, Cornelius Grunwald, Vasyl Hafych, Kevin Kröninger, Salvatore La Cagnina, Lars Röhrig, and Lolian Shtembari. Bat.jl: A julia-based tool for bayesian inference. SN Computer Science, 2(3):210, Apr 2021.