**pyhf**: pure-Python implementation of HistFactory with tensors and automatic differentiation

Matthew Feickert  
(University of Illinois at Urbana-Champaign)

matthew.feickert@cern.ch

CMS Analysis Tools Task Force Meeting

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pyhf team

Lukas Heinrich  
CERN

Matthew Feickert  
Illinois

Giordon Stark  
UCSC SCIPP

plus more than 20 contributors
Goals of physics analysis at the LHC

- Search for new physics
- Make precision measurements
- Provide constraints on models through setting best limits

- All require **building statistical models** and **fitting models** to data to perform statistical inference
- Model complexity can be huge for complicated searches
- **Problem:** Time to fit can be **many hours**
- **Goal:** Empower analysts with fast fits and expressive models
HistFactory Model

- A flexible probability density function (p.d.f.) template to build statistical models in high energy physics
- Developed in 2011 during work that lead to the Higgs discovery [CERN-OPEN-2012-016]
- Widely used by ATLAS for **measurements of known physics** (Standard Model) and **searches for new physics** (beyond the Standard Model)
HistFactory Template: at a glance

\[ f(\text{data}|\text{parameters}) = f(\vec{n}, \vec{a}|\vec{\eta}, \vec{\chi}) = \prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}(n_{cb}|\nu_{cb}(\vec{\eta}, \vec{\chi})) \prod_{\chi \in \vec{\chi}} c_\chi(a_\chi|\chi) \]

\( \vec{n} \): events, \( \vec{a} \): auxiliary data, \( \vec{\eta} \): unconstrained pars, \( \vec{\chi} \): constrained pars

\[ \nu_{cb}(\vec{\eta}, \vec{\chi}) = \sum_{s \in \text{samples}} \left( \sum_{\kappa \in \vec{\kappa}} \kappa_{scb}(\vec{\eta}, \vec{\chi}) \right) \left( \nu_{scb}^0(\vec{\eta}, \vec{\chi}) + \sum_{\Delta \in \vec{\Delta}} \Delta_{scb}(\vec{\eta}, \vec{\chi}) \right) \]

Use: Multiple disjoint channels (or regions) of binned distributions with multiple samples contributing to each with additional (possibly shared) systematics between sample estimates

Main pieces:

- **Main Poisson p.d.f. for simultaneous measurement of multiple channels**
- **Event rates** \( \nu_{cb}(\vec{\eta}, \vec{\chi}) \) (nominal rate \( \nu_{scb}^0 \) with rate modifiers)
  - encode systematic uncertainties (e.g. normalization, shape)
- **Constraint p.d.f. (+ data) for "auxiliary measurements"**
HistFactory Template: at a second glance

\[ f(\text{data}|\text{parameters}) = f(\vec{n}, \vec{a}|\vec{\eta}, \vec{\chi}) = \prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}(n_{cb}|\nu_{cb}(\vec{\eta}, \vec{\chi})) \prod_{\chi \in \vec{\chi}} c_\chi(a_\chi|\chi) \]

\( \vec{n} \): events, \( \vec{a} \): auxiliary data, \( \vec{\eta} \): unconstrained pars, \( \vec{\chi} \): constrained pars

\( \nu_{cb}(\vec{\eta}, \vec{\chi}) = \sum_{s \in \text{samples}} \left( \sum_{\kappa \in \vec{\kappa}} \kappa_{scb}(\vec{\eta}, \vec{\chi}) \right) \left( \nu_{0scb}(\vec{\eta}, \vec{\chi}) + \sum_{\Delta \in \vec{\Delta}} \Delta_{scb}(\vec{\eta}, \vec{\chi}) \right) \)

Use: Multiple disjoint channels (or regions) of binned distributions with multiple samples contributing to each with additional (possibly shared) systematics between sample estimates

Main pieces:

- **Main Poisson p.d.f. for simultaneous measurement of multiple channels**
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  - encode systematic uncertainties (e.g. normalization, shape)
- **Constraint p.d.f. (+ data) for "auxiliary measurements"**
In HEP common for systematic uncertainties to be specified with two template histograms: "up" and "down" variation for parameter $\theta \in \{\tilde{\eta}, \tilde{\chi}\}$

- "up" variation: model prediction for $\theta = +1$
- "down" variation: model prediction for $\theta = -1$
- Interpolation and extrapolation choices provide model predictions $\nu(\tilde{\theta})$ for any $\tilde{\theta}$

Constraint terms $c_j (a_j | \theta_j)$ used to model auxiliary measurements. Example for Normal (most common case):

- Mean of nuisance parameter $\theta_j$ with normalized width ($\sigma = 1$)
- Normal: auxiliary data $a_j = 0$ (aux data function of modifier type)
- Constraint term produces penalty in likelihood for pulling $\theta_j$ away from auxiliary measurement value
- As $\nu(\tilde{\theta})$ constraint terms inform rate modifiers (systematic uncertainties) during simultaneous fit

Image credit: Alex Held
HistFactory Template: grammar

\[ f(\text{data}|\text{parameters}) = f(\vec{n}, \vec{a} | \vec{\eta}, \vec{\chi}) = \prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}(n_{cb} | \nu_{cb}(\vec{\eta}, \vec{\chi})) \prod_{\chi \in \vec{\chi}} c_\chi(a_\chi | \chi) \]

Mathematical grammar for a simultaneous fit with:

- multiple "channels" (analysis regions, (stacks of) histograms) that can have multiple bins
- with systematic uncertainties that modify the event rate \( \nu_{cb}(\vec{\eta}, \vec{\chi}) \)
- coupled to a set of constraint terms

Example: Each bin is separate (1-bin) channel, each histogram (color) is a sample and share a normalization systematic uncertainty
HistFactory Template: implementation

\[ f(\text{data}|\text{parameters}) = \prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}(n_{cb}|\nu_{cb}(\eta, \chi)) \prod_{\chi \in \chi} c_{\chi}(a_{\chi}|\chi) \]

\( \vec{n} \): events, \( \vec{a} \): auxiliary data, \( \vec{\eta} \): unconstrained pars, \( \vec{\chi} \): constrained pars

This is a \textbf{mathematical representation}! Nowhere is any software spec defined

Until 2018 the only implementation of HistFactory has been in \textbf{ROOT}
**pyhf: HistFactory in pure Python**

- First non-ROOT implementation of the HistFactory p.d.f. template
  - DOI: 10.5281/zenodo.1169739
- pure-Python library as second implementation of HistFactory
  - `$ python -m pip install pyhf`
  - No dependence on ROOT!
- Open source tool for all of HEP
  - IRIS-HEP supported Scikit-HEP project
  - Used in ATLAS SUSY, Exotics, and Top groups in 18 published analyses
  - Used by Belle II (DOI: 10.1103/PhysRevLett.127.181802)
  - Used for reinterpretation in phenomenology paper (DOI: 10.1007/JHEP04(2019)144) and SModelS (DOI: 10.1016/j.cpc.2021.107909)
  - Keen to make a bridge to CMS!
Machine Learning Frameworks for Computation

- All numerical operations implemented in **tensor backends** through an API of \(n\)-dimensional array operations

- Using deep learning frameworks as computational backends allows for **exploitation of auto differentiation (autograd) and GPU acceleration**

- As huge buy in from industry we benefit for free as these frameworks are **continually improved** by professional software engineers (physicists are not)

- Show hardware acceleration giving **order of magnitude speedup** for some models!

- Improvements over traditional
  - 10 hrs to 30 min; 20 min to 10 sec
Automatic differentiation

With tensor library backends gain access to **exact (higher order) derivatives** — accuracy is only limited by floating point precision

\[
\frac{\partial L}{\partial \mu}, \frac{\partial L}{\partial \theta_i}
\]

Exploit **full gradient of the likelihood** with **modern optimizers** to help speedup fit!

Gain this through the frameworks creating **computational directed acyclic graphs** and then applying the chain rule (to the operations)
JSON spec fully describes the HistFactory model

- Human & machine readable **declarative** statistical models
- Industry standard
  - Will be with us forever
- Parsable by every language
  - Highly portable
  - Bidirectional translation with ROOT
- Versionable and easily preserved
  - JSON Schema describing HistFactory specification
  - Attractive for analysis preservation
  - Highly compressible

```json
{
  "channels": [  # List of regions
    { 
      "name": "singlechannel",
      "samples": [  # List of samples in region
        { 
          "name": "signal",
          "data": [20.0, 10.0],
          # list of rate factors and/or systematic uncertainties
          "modifiers": [ { "name": "mu", "type": "normfactor", "data": null} ]
        },
        { 
          "name": "background",
          "data": [50.0, 63.0],
          "modifiers": [ {"name": "uncorr_bkguncrt", "type": "shapesys", "data": [5.0, 12.0]} ]
        }
      ]
    }
  ],
  "observations": [  # Observed data
    { "name": "singlechannel", "data": [55.0, 62.0] }
  ],
  "measurements": [  # Parameter of interest
    { "name": "Measurement", "config": {"poi": "mu", "parameters": []} }
  ],
  "version": "1.0.0"  # Version of spec standard
}
```

JSON defining a single channel, two bin counting experiment with systematics
ATLAS validation and publication of likelihoods

New open release allows theorists to explore LHC data in a new way

The ATLAS collaboration releases full analysis likelihoods, a first for an LHC experiment

9 JANUARY, 2020 | By Katarina Anthony

((ATLAS, 2019) (CERN, 2020)
Large community adoption followed (2020 on)

**Charged lepton flavor violation at the EIC**

Vincenzo Cirigliano, Kaori Fuyuto, Christopher Lee, Emanuele Mereghetti and Bin Yan


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**EIC**

DOI: 10.1007/JHEP03 (2021)256

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**Sensitivity of future hadron colliders to leptoquark pair production in the di-muon di-jets channel**

B. [1]

value of \( \mu \) at which \( \text{CL}_{\text{S}} = 0.05 \). We compute the \( \text{CL}_{\text{S}} \) values using [pyhf](https://pyhf.readthedocs.io/en/stable/) [64], a Python implementation of [HistFactory](https://github.com/_histfactory/histfactory) [65]. By comparison with the theoretical

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**FCC**

DOI: 10.1140/epjc/s10052-020-7722-3

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**Search for \( B^{+} \to K^{+}\nu\bar{\nu} \) Decays Using an Inclusive Tagging Method at Belle II**

 statistical analysis to determine the signal yields is

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**Belle-II**

DOI: 10.1103/PhysRevLett.127.181802

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**How to discover QCD Instantons at the LHC**

Simone Amoroso, Deepak Kar, Matthias Schott

signal region selection are used to perform a counting experiment using the [pyhf](https://pyhf.readthedocs.io/en/stable/) package [56]. The systematic uncer-

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**LHC BSM**

DOI: 10.1140/epjc/s10052-020-8210-5

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**Lepton flavor violation and dilepton tails at the LHC**

Andrei Angelovska, Darius A. Faroughy, Olcvr Sumensari

sonian distributions. The 95% confidence level (CL) upper

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**LHC QCD**

DOI: 10.1140/epjc/s10052-021-09412-1

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**μ-Collider**

DOI: 10.1007/JHEP06(2021)133

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**ATLAS**

arXiv:2105.01676

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**Hunting wino and higgsino dark matter at the muon collider with disappearing tracks**

Rodolfo Capdevilla, Federico Meloni, Rosa Simoniello and Jose Zurita

The [pyhf](https://pyhf.readthedocs.io/en/stable/) software package [94, 95] was used to set limits on the expected discovery \( p \)-value and to set limits.
Extending and visualization: cabinetry

- **pyhf** focuses on the modeling (library not a framework)
- Leverage the design of the **Scikit-HEP ecosystem** and close communication between pyhf dev team and cabinetry lead dev Alexander Held
- **cabinetry** designs & steers template profile likelihood fits
- Uses pyhf as the inference engine
- Provides common visualization for inference validation

- Implementations for all **common inference tasks** exist
  - includes associated visualizations
  - results validated against **TRExFitter**

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Alex Held, ATLAS SUSY Workshop 2021
Run Example: Hypothesis test

```python
$ python -m pip install pyhf[jax,contrib]
$ pyhf contrib download https://doi.org/10.17182/hepdata.90607.v3/r3 1Lbb-pallet

import json
import pyhf

pyhf.set_backend("jax")  # Optional for speed
spec = json.load(open("1Lbb-pallet/BkgOnly.json"))
patchset = pyhf.PatchSet(json.load(open("1Lbb-pallet/patchset.json")))

workspace = pyhf.Workspace(spec)
model = workspace.model(patches=[patchset["C1N2_Wh_hbb_900_250"]])

test_poi = 1.0
data = workspace.data(model)
cls_obs, cls_exp_band = pyhf.infer.hypotest(
    test_poi, data, model, test_stat="qtilde", return_expected_set=True
)
print(f"Observed CLs: {cls_obs}")
# Observed CLs: 0.4573416902360917
print(f"Expected CLs band: {[exp.tolist() for exp in cls_exp_band]}")
# Expected CLs band: [0.014838293214187472, 0.05174259485911152, 0.16166970886709053, 0.4097850957724176, 0.7428200727035176]
```
import json
import matplotlib.pyplot as plt
import numpy as np
import pyhf
from pyhf.contrib.viz.brazil import plot_results

pyhf.set_backend("jax")  # Optional for speed

spec = json.load(open("1Lbb-pallet/BkgOnly.json"))
patchset = pyhf.PatchSet(json.load(open("1Lbb-pallet/patchset.json")))

workspace = pyhf.Workspace(spec)
model = workspace.model(patches=[patchset["C1N2_Wh_hbb_900_250"]])

test_pois = np.linspace(0, 5, 41)  # POI step of 0.125
data = workspace.data(model)
obs_limit, exp_limits, (test_pois, results) = pyhf.infer.intervals.upperlimit(data, model, test_pois, return_results=True)

print(f"Observed limit: {obs_limit}"
  # Observed limit: 2.547958147632675
print(f"Expected limits: {[limit.tolist() for limit in exp_limits]}
  # Expected limits: [0.7065311975182036, 1.0136453820160332, 1.5766626372587724, 2.558234487679955, 4.105381941514062]

fig, ax = plt.subplots()
artists = plot_results(test_pois, results, ax=ax)
fig.savefig("upper_limit.pdf")
import json
import cabinetry
import pyhf
from cabinetry.model_utils import prediction
from pyhf.contrib.utils import download

# download the ATLAS bottom-squarks analysis probability models from HEPData
download("https://www.hepdata.net/record/resource/1935437?view=true", "bottom-squarks")

# construct a workspace from a background-only model and a signal hypothesis
bkg_only_workspace = pyhf.Workspace(json.load(open("bottom-squarks/RegionC/BkgOnly.json")))
patchset = pyhf.PatchSet(json.load(open("bottom-squarks/RegionC/patchset.json")))
workspace = patchset.apply(bkg_only_workspace, "sbottom_600_280_150")

# construct the probability model and observations
model, data = cabinetry.model_utils.model_and_data(workspace)

# produce visualizations of the pre-fit model and observed data
prefit_model = prediction(model)
cabinetry.visualize.data_mc(prefit_model, data)

# fit the model to the observed data
fit_results = cabinetry.fit.fit(model, data)

# produce visualizations of the post-fit model and observed data
postfit_model = prediction(model, fit_results=fit_results)
cabinetry.visualize.data_mc(postfit_model, data)
Core part of IRIS-HEP Analysis Systems pipeline

- Analysis Systems pipeline: deployable stack of experiment agnostic infrastructure
  - c.f. demonstration at IRIS-HEP Analysis Grand Challenge Tools Workshop 2021
- Accelerating fitting (reducing time to insight (statistical inference)!) \( (\text{pyhf} + \text{cabinetry}) \)
- An enabling technology for reinterpretation \( (\text{pyhf} + \text{RECAST}) \)
Call to action: pyhf and Combine interoperability

- Long standing (2018) question: Is it possible for Combine users to use pyhf?
- How to translate between Combine and HistFactory models?
- ...or, what is needed in a HistFactory v2 spec to be an acceptable alternative for Combine?
- The pyhf dev team wants to work to make this happen!

Fun fact! It was Lindsey Gray who first asked about this possibility when Matthew was presenting at the US LUA 2018 meeting. Thanks Lindesy!
Call to action: Thoughts from Combine dev team

- At November 2021 publication of statistical models workshop Andrew Gilbert (CMS Combine team dev) gave suggestions for starting places
- Recommends that instead of starting from scratch start from Combine Python parser and then work on datacard translator
- Alex Held has taken some preliminary first steps in the past with a datacard-to-pyhf project on GitHub

Serialising combine models

- Could pyhf be used?
  - The combine and HistFactory/pyhf feature sets are roughly similar
  - Close enough that a basic converter from datacards to pyhf JSON format should not be too difficult
  - Harder to make the pyhf likelihood exactly equivalent to the combine one (and if not identical, the likelihood is not preserved)
  - Some things (MC stat uncertainties) are definitely handled differently... other things (e.g. shape morphing) may appear to be the same, but subtle details may differ
  - Unclear if other commonly used features available (e.g. writing bin contents for some processes as generic formulae (RooFormulaVars))

Andrew Gilbert,
Publication of statistical models workshop 2021
Call to action: Funding for work

- Tools useful for the whole particle physics community is core to IRIS-HEP's mission
  - As an IRIS-HEP supported project pyhf wants to support CMS users
- IRIS-HEP offers paid (up to 3 FTE-months) Fellow positions
  - https://iris-hep.org/fellows.html
- IRIS-HEP Analysis Systems team has a Fellow project for pyhf + Combine open now
  - Matthew would be a project mentor
Summary

- **Accelerated** fitting library
  - reducing time to insight/inference!
  - Hardware acceleration on GPUs and vectorized operations
  - Backend agnostic Python API and CLI

- **Flexible** declarative schema
  - JSON: ubiquitous, universal support, versionable

- Enabling technology for **reinterpretation**
  - JSON Patch files for efficient computation of new signal models
  - Unifying tool for theoretical and experimental physicists

- Project in growing **Pythonic HEP ecosystem**
  - Openly developed on GitHub and welcome contributions
  - Comprehensive open tutorials
  - Ask us about Scikit-HEP and IRIS-HEP!
Thanks for listening!

Come talk with us!

www.scikit-hep.org/pyhf
Backup
Why is the likelihood important?

- High information-density summary of analysis
- Almost everything we do in the analysis ultimately affects the likelihood and is encapsulated in it
  - Trigger
  - Detector
  - Combined Performance / Physics Object Groups
  - Systematic Uncertainties
  - Event Selection
- Unique representation of the analysis to reuse and preserve
Full likelihood serialization...

...making good on 19 year old agreement to publish likelihoods

Massimo Corradi

It seems to me that there is a general consensus that what is really meaningful for an experiment is likelihood, and almost everybody would agree on the prescription that experiments should give their likelihood function for these kinds of results. Does everybody agree on this statement, to publish likelihoods?

Louis Lyons

Any disagreement? Carried unanimously. That's actually quite an achievement for this Workshop.

(1st Workshop on Confidence Limits, CERN, 2000)

This hadn't been done in HEP until 2019

- In an "open world" of statistics this is a difficult problem to solve
- What to preserve and how? All of ROOT?
- Idea: Focus on a single more tractable binned model first
JSON Patch for signal model (reinterpretation)

JSON Patch gives ability to **easily mutate model**
Think: test a **new theory** with a **new patch**!
(c.f. Lukas Heinrich's RECAST talk from Snowmass 2021 Computational Frontier Workshop)

Combined with RECAST gives powerful tool for **reinterpretation studies**

```bash
# Using CLI
$ pyhf cls example.json | jq '.CLs_obs 0.053994246621274014
$ cat new_signal.json
{   "op": "replace",   "path": "/channels/0/samples/0/data",   "value": [10.0, 6.0] }
$ pyhf cls example.json --patch new_signal.json | jq '.CLs_obs 0.3536906623262466
```
Likelihoods preserved on HEPData

- **pyhf pallet:**
  - Background-only model JSON stored
  - Hundreds of signal model JSON Patches stored together as a `pyhf "patch set"` file
  - Fully preserve and publish the full statistical model and observations to give likelihood with own DOI!

![Image of HEPData interface](image.png)

```bash
$ tree pyhf-pallet
pyhf-pallet
|-- BkgOnly.json
|-- patchset.json
|-- README.md
0 directories, 3 files
```
...can be used from HEPData

- **pyhf pallet**:  
  - Background-only model JSON stored  
  - Hundreds of signal model JSON Patches stored together as a `pyhf "patch set" file`

- Fully preserve and publish the full statistical model and observations to give likelihood

```bash
# pyhf pallet for the SUSY EWK 1Lbb analysis
$ pyhf contrib download https://doi.org/10.17182/hepdata.90607.v3/r3 1Lbb-pallet && cd 1Lbb-pallet

# verify patchset is valid
$ pyhf patchset verify BkgOnly.json patchset.json
All good.

# signal model: m1 = 900, m2 = 300 (chain CLI API output)
$ cat BkgOnly.json |
  | pyhf cls --patch <(pyhf patchset extract --name C1N2_Wh_hbb_900_300 patchset.json) | 
  | jq .Cls_obs
0.5004165245329418

# new signal model: m1 = 900, m2 = 400 (use serialized CLI API output)
$ pyhf patchset extract --name C1N2_Wh_hbb_900_400 --output-file C1N2_Wh_hbb_900_400_patch.json patchset.json
$ pyhf cls --patch C1N2_Wh_hbb_900_400_patch.json BkgOnly.json | jq .Cls_obs
0.573500726833779
```
Rapid adoption in ATLAS...

- 18 ATLAS SUSY, Exotics, Top analyses with full probability models published to HEPData
- ATLAS SUSY will be continuing to publish full Run 2 likelihoods
- 3L eRJR, doi:10.17182/hepdata.90607 (2020)
- ss3L search, doi:10.17182/hepdata.91214 (2020)

SUSY EWK 3L RPV analysis (ATLAS-CONF-2020-009): Exclusion curves as a function of mass and branching fraction to $Z$ bosons
• pyhf likelihoods discussed in
  o Higgs boson potential at colliders: status and perspectives
• SModelS team has implemented a SModelS/pyhf interface [arXiv:2009.01809]
  o tool for interpreting simplified-model results from the LHC
  o designed to be used by theorists
  o SModelS authors giving tutorial later today!

  o Compare simplified likelihood (bestSR) to full likelihood (pyhf) using SModelS
References


6. ATLAS collaboration, *Search for bottom-squark pair production with the ATLAS detector in final states containing Higgs bosons, b-jets and missing transverse momentum*, 2019

7. ATLAS collaboration, *Reproducing searches for new physics with the ATLAS experiment through publication of full statistical likelihoods*, 2019

8. ATLAS collaboration, *Search for bottom-squark pair production with the ATLAS detector in final states containing Higgs bosons, b-jets and missing transverse momentum: HEPData entry*, 2019
The end.