pyhf Documentation

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CONTENTS

Measurements in High Energy Physics (HEP) rely on determining the compatibility of observed collision events with theoretical predictions. The relationship between them is often formalised in a statistical *model* $f(x|)$ describing the probability of data x given model parameters . Given observed data, the *likelihood* $\mathcal{L}()$ then serves as the basis to test hypotheses on the parameters . For measurements based on binned data (*histograms*), the family of statistical models has been widely used in both Standard Model measurements [intro-4] as well as searches for new physics [intro-5]. In this package, a declarative, plain-text format for describing -based likelihoods is presented that is targeted for reinterpretation and long-term preservation in analysis data repositories such as HEPData [intro-3].

CHAPTER

ONE

HISTFACTORY

Statistical models described using [intro-2] center around the simultaneous measurement of disjoint binned distributions (*channels*) observed as event counts . For each channel, the overall expected event rate[1] is the sum over a number of physics processes (*samples*). The sample rates may be subject to parametrised variations, both to express the effect of *free parameters* [2] and to account for systematic uncertainties as a function of *constrained parameters* . The degree to which the latter can cause a deviation of the expected event rates from the nominal rates is limited by *constraint terms*. In a frequentist framework these constraint terms can be viewed as *auxiliary measurements* with additional global observable data , which paired with the channel data completes the observation $x = (,)$. In addition to the partition of the full parameter set into free and constrained parameters $= (,)$, a separate partition $= (,)$ will be useful in the context of hypothesis testing, where a subset of the parameters are declared *parameters of interest* and the remaining ones as *nuisance parameters* .

$$f(x|) = f(x|\overbrace{,}^{\text{free}}\underbrace{)}_{\text{constrained}} = f(x|\overbrace{,}^{\text{parameters of interest}}\underbrace{)}_{\text{nuisance parameters}} \tag{1.1}$$

Thus, the overall structure of a probability model is a product of the analysis-specific model term describing the measurements of the channels and the analysis-independent set of constraint terms:

$$f(,|,) = \underbrace{\prod_{c\in\text{ channels}}\prod_{b\in\text{ bins}_c}\text{Pois}\left(n_{cb}\,|\,\nu_{cb}\,(,)\right)}_{\substack{\text{Simultaneous measurement}\\ \text{of multiple channels}}}\quad\underbrace{\prod_{\in} c(a|\,)}_{\substack{\text{constraint terms}\\ \text{for } x201C\text{auxiliary measurements} x201D}}\quad, \tag{1.2}$$

where within a certain integrated luminosity we observe n_{cb} events given the expected rate of events $\nu_{cb}(,)$ as a function of unconstrained parameters and constrained parameters . The latter has corresponding one-dimensional constraint terms $c_(a|\,)$ with auxiliary data a constraining the parameter . The event rates ν_{cb} are defined as

$$\nu_{cb}\,() = \sum_{s\in\text{ samples}}\nu_{scb}\,(,) = \sum_{s\in\text{ samples}}\underbrace{\left(\prod_{\kappa\in\,\kappa}\kappa_{scb}\,(,)\right)}_{\text{multiplicative modifiers}}\underbrace{\left(\nu^0_{scb}\,(,) + \sum_{\Delta\in\Delta}\Delta_{scb}\,(,)\right)}_{\text{additive modifiers}}. \tag{1.3}$$

The total rates are the sum over sample rates ν_{csb}, each determined from a *nominal rate* ν^0_{scb} and a set of multiplicative and additive denoted *rate modifiers* $\kappa()$ and $\Delta()$. These modifiers are functions of (usually a single) model parameters. Starting from constant nominal rates, one can derive the per-bin event rate modification by iterating over all sample rate modifications as shown in (1.3).

As summarised in *Modifiers and Constraints*, rate modifications are defined in for bin b, sample s, channel c. Each modifier is represented by a parameter $\phi \in \{\gamma, \alpha, \lambda, \mu\}$. By convention bin-wise parameters are denoted with γ and

[1] Here rate refers to the number of events expected to be observed within a given data-taking interval defined through its integrated luminosity. It often appears as the input parameter to the Poisson distribution, hence the name "rate".

[2] These *free parameters* frequently include the of a given process, i.e. its cross-section normalised to a particular reference cross-section such as that expected from the Standard Model or a given BSM scenario.

interpolation parameters with α. The luminosity λ and scale factors μ affect all bins equally. For constrained modifiers, the implied constraint term is given as well as the necessary input data required to construct it. σ_b corresponds to the relative uncertainty of the event rate, whereas δ_b is the event rate uncertainty of the sample relative to the total event rate $\nu_b = \sum_s \nu_{sb}^0$.

Modifiers implementing uncertainties are paired with a corresponding default constraint term on the parameter limiting the rate modification. The available modifiers may affect only the total number of expected events of a sample within a given channel, i.e. only change its normalisation, while holding the distribution of events across the bins of a channel, i.e. its "shape", invariant. Alternatively, modifiers may change the sample shapes. Here supports correlated an uncorrelated bin-by-bin shape modifications. In the former, a single nuisance parameter affects the expected sample rates within the bins of a given channel, while the latter introduces one nuisance parameter for each bin, each with their own constraint term. For the correlated shape and normalisation uncertainties, makes use of interpolating functions, f_p and g_p, constructed from a small number of evaluations of the expected rate at fixed values of the parameter α[3]. For the remaining modifiers, the parameter directly affects the rate.

Table 1: Modifiers and Constraints

Description	Modification	Constraint Term c	Input
Uncorrelated Shape	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \mathrm{Pois}\left(r_b = \sigma_b^{-2} \middle\vert \rho_b = \sigma_b^{-2}\gamma_b\right)$	σ_b
Correlated Shape	$\Delta_{scb}(\alpha) = f_p\left(\alpha \middle\vert \Delta_{scb,\alpha=-1}, \Delta_{scb,\alpha=1}\right)$	$\mathrm{Gaus}\left(a = 0 \middle\vert \alpha, \sigma = 1\right)$	$\Delta_{scb,\alpha=\pm1}$
Normalisation Unc.	$\kappa_{scb}(\alpha) = g_p\left(\alpha \middle\vert \kappa_{scb,\alpha=-1}, \kappa_{scb,\alpha=1}\right)$	$\mathrm{Gaus}\left(a = 0 \middle\vert \alpha, \sigma = 1\right)$	$\kappa_{scb,\alpha=\pm1}$
MC Stat. Uncertainty	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \mathrm{Gaus}\left(a_{\gamma_b} = 1 \middle\vert \gamma_b, \delta_b\right)$	$\delta_b^2 = \sum_s \delta_{sb}^2$
Luminosity	$\kappa_{scb}(\lambda) = \lambda$	$\mathrm{Gaus}\left(l = \lambda_0 \middle\vert \lambda, \sigma_\lambda\right)$	$\lambda_0, \sigma_\lambda$
Normalisation	$\kappa_{scb}(\mu_b) = \mu_b$		
Data-driven Shape	$\kappa_{scb}(\gamma_b) = \gamma_b$		

Given the likelihood $\mathcal{L}()$, constructed from observed data in all channels and the implied auxiliary data, *measurements* in the form of point and interval estimates can be defined. The majority of the parameters are *nuisance parameters* — parameters that are not the main target of the measurement but are necessary to correctly model the data. A small subset of the unconstrained parameters may be declared as *parameters of interest* for which measurements hypothesis tests are performed, e.g. profile likelihood methods [intro-1]. The *Symbol Notation* table provides a summary of all the notation introduced in this documentation.

[3] This is usually constructed from the nominal rate and measurements of the event rate at $\alpha = \pm 1$, where the value of the modifier at $\alpha = \pm 1$ must be provided and the value at $\alpha = 0$ corresponds to the corresponding identity operation of the modifier, i.e. $f_p(\alpha = 0) = 0$ and $g_p(\alpha = 0) = 1$ for additive and multiplicative modifiers respectively. See Section 4.1 in [intro-2].

Table 2: Symbol Notation

Symbol	Name
$f(x\|)$	model
$\mathcal{L}()$	likelihood
$x = \{,\}$	full dataset (including auxiliary data)
	channel data (or event counts)
	auxiliary data
$\nu()$	calculated event rates
$= \{,\} = \{,\}$	all parameters
	free parameters
	constrained parameters
	parameters of interest
	nuisance parameters
$\kappa()$	multiplicative rate modifier
$\Delta()$	additive rate modifier
$c_(a_\|)$	constraint term for constrained parameter
σ	relative uncertainty in the constrained parameter

CHAPTER

TWO

DECLARATIVE FORMATS

While flexible enough to describe a wide range of LHC measurements, the design of the specification is sufficiently simple to admit a *declarative format* that fully encodes the statistical model of the analysis. This format defines the channels, all associated samples, their parameterised rate modifiers and implied constraint terms as well as the measurements. Additionally, the format represents the mathematical model, leaving the implementation of the likelihood minimisation to be analysis-dependent and/or language-dependent. Originally XML was chosen as a specification language to define the structure of the model while introducing a dependence on to encode the nominal rates and required input data of the constraint terms [intro-2]. Using this specification, a model can be constructed and evaluated within the framework.

This package introduces an updated form of the specification based on the ubiquitous plain-text JSON format and its schema-language *JSON Schema*. Described in more detail in *Likelihood Specification*, this schema fully specifies both structure and necessary constrained data in a single document and thus is implementation independent.

CHAPTER

THREE

ADDITIONAL MATERIAL

3.1 Footnotes

3.2 Bibliography

CHAPTER

FOUR

LIKELIHOOD SPECIFICATION

The structure of the JSON specification of models follows closely the original XML-based specification [likelihood-2].

4.1 Workspace

```
{
    "$schema": "http://json-schema.org/draft-06/schema#",
    "$id": "https://scikit-hep.org/pyhf/schemas/1.0.0/workspace.json",
    "$ref": "defs.json#/definitions/workspace"
}
```

The overall document in the above code snippet describes a *workspace*, which includes

- **channels**: The channels in the model, which include a description of the samples within each channel and their possible parametrised modifiers.
- **measurements**: A set of measurements, which define among others the parameters of interest for a given statistical analysis objective.
- **observations**: The observed data, with which a likelihood can be constructed from the model.

A workspace consists of the channels, one set of observed data, but can include multiple measurements. If provided a JSON file, one can quickly check that it conforms to the provided workspace specification as follows:

```
import json, requests, jsonschema

workspace = json.load(open("/path/to/analysis_workspace.json"))
# if no exception is raised, it found and parsed the schema
schema = requests.get("https://scikit-hep.org/pyhf/schemas/1.0.0/workspace.json").json()
# If no exception is raised by validate(), the instance is valid.
jsonschema.validate(instance=workspace, schema=schema)
```

4.2 Channel

A channel is defined by a channel name and a list of samples [likelihood-1].

```
{
    "channel": {
        "type": "object",
        "properties": {
            "name": { "type": "string" },
            "samples": { "type": "array", "items": {"$ref": "#/definitions/sample"},
↪"minItems": 1 }
        },
        "required": ["name", "samples"],
        "additionalProperties": false
    },
}
```

The Channel specification consists of a list of channel descriptions. Each channel, an analysis region encompassing one or more measurement bins, consists of a `name` field and a `samples` field (see *Channel*), which holds a list of sample definitions (see *Sample*). Each sample definition in turn has a `name` field, a `data` field for the nominal event rates for all bins in the channel, and a `modifiers` field of the list of modifiers for the sample.

4.3 Sample

A sample is defined by a sample name, the sample event rate, and a list of modifiers [likelihood-1].

```
{
    "sample": {
        "type": "object",
        "properties": {
            "name": { "type": "string" },
            "data": { "type": "array", "items": {"type": "number"}, "minItems": 1 },
            "modifiers": {
                "type": "array",
                "items": {
                    "anyOf": [
                        { "$ref": "#/definitions/modifier/histosys" },
                        { "$ref": "#/definitions/modifier/lumi" },
                        { "$ref": "#/definitions/modifier/normfactor" },
                        { "$ref": "#/definitions/modifier/normsys" },
                        { "$ref": "#/definitions/modifier/shapefactor" },
                        { "$ref": "#/definitions/modifier/shapesys" },
                        { "$ref": "#/definitions/modifier/staterror" }
                    ]
                }
            }
        },
        "required": ["name", "data", "modifiers"],
        "additionalProperties": false
    },
}
```

4.4 Modifiers

The modifiers that are applicable for a given sample are encoded as a list of JSON objects with three fields. A name field, a type field denoting the class of the modifier, and a data field which provides the necessary input data as denoted in *Modifiers and Constraints*.

Based on the declared modifiers, the set of parameters and their constraint terms are derived implicitly as each type of modifier unambiguously defines the constraint terms it requires. Correlated shape modifiers and normalisation uncertainties have compatible constraint terms and thus modifiers can be declared that *share* parameters by re-using a name[1] for multiple modifiers. That is, a variation of a single parameter causes a shift within sample rates due to both shape and normalisation variations.

We review the structure of each modifier type below.

4.4.1 Uncorrelated Shape (shapesys)

To construct the constraint term, the relative uncertainties σ_b are necessary for each bin. Therefore, we record the absolute uncertainty as an array of floats, which combined with the nominal sample data yield the desired σ_b. An example is shown below:

```
{ "name": "mod_name", "type": "shapesys", "data": [1.0, 1.5, 2.0] }
```

An example of an uncorrelated shape modifier with three absolute uncertainty terms for a 3-bin channel.

Warning: Nuisance parameters will not be allocated for any bins where either

- the samples nominal expected rate is zero, or
- the absolute uncertainty is zero.

These values are, in the context of uncorrelated shape uncertainties, unphysical. If this situation occurs, one needs to go back and understand the inputs as this is undefined behavior in HistFactory.

The previous example will allocate three nuisance parameters for `mod_name`. The following example will allocate only two nuisance parameters for a 3-bin channel:

```
{ "name": "mod_name", "type": "shapesys", "data": [1.0, 0.0, 2.0] }
```

4.4.2 Correlated Shape (histosys)

This modifier represents the same source of uncertainty which has a different effect on the various sample shapes, hence a correlated shape. To implement an interpolation between sample distribution shapes, the distributions with a "downward variation" ("lo") associated with $\alpha = -1$ and an "upward variation" ("hi") associated with $\alpha = +1$ are provided as arrays of floats. An example is shown below:

```
{ "name": "mod_name", "type": "histosys", "data": {"hi_data": [20,15], "lo_data": [10,␣
↪10]} }
```

An example of a correlated shape modifier with absolute shape variations for a 2-bin channel.

[1] The name of a modifier specifies the parameter set it is controlled by. Modifiers with the same name share parameter sets.

4.4.3 Normalisation Uncertainty (normsys)

The normalisation uncertainty modifies the sample rate by a overall factor $\kappa(\alpha)$ constructed as the interpolation between downward ("lo") and upward ("hi") as well as the nominal setting, i.e. $\kappa(-1) = \kappa_{\alpha=-1}$, $\kappa(0) = 1$ and $\kappa(+1) = \kappa_{\alpha=+1}$. In the modifier definition we record $\kappa_{\alpha=+1}$ and $\kappa_{\alpha=-1}$ as floats. An example is shown below:

```
{ "name": "mod_name", "type": "normsys", "data": {"hi": 1.1, "lo": 0.9} }
```

An example of a normalisation uncertainty modifier with scale factors recorded for the up/down variations of an n-bin channel.

4.4.4 MC Statistical Uncertainty (staterror)

As the sample counts are often derived from Monte Carlo (MC) datasets, they necessarily carry an uncertainty due to the finite sample size of the datasets. As explained in detail in [likelihood-2], adding uncertainties for each sample would yield a very large number of nuisance parameters with limited utility. Therefore a set of bin-wise scale factors γ_b is introduced to model the overall uncertainty in the bin due to MC statistics. The constrained term is constructed as a set of Gaussian constraints with a central value equal to unity for each bin in the channel. The scales σ_b of the constraint are computed from the individual uncertainties of samples defined within the channel relative to the total event rate of all samples: $\delta_{csb} = \sigma_{csb} / \sum_s \nu^0_{scb}$. As not all samples are within a channel are estimated from MC simulations, only the samples with a declared statistical uncertainty modifier enter the sum. An example is shown below:

```
{ "name": "mod_name", "type": "staterror", "data": [0.1] }
```

An example of a statistical uncertainty modifier.

4.4.5 Luminosity (lumi)

Sample rates derived from theory calculations, as opposed to data-driven estimates, are scaled to the integrated luminosity corresponding to the observed data. As the luminosity measurement is itself subject to an uncertainty, it must be reflected in the rate estimates of such samples. As this modifier is of global nature, no additional per-sample information is required and thus the data field is nulled. This uncertainty is relevant, in particular, when the parameter of interest is a signal cross-section. The luminosity uncertainty σ_λ is provided as part of the parameter configuration included in the measurement specification discussed in *Measurements*. An example is shown below:

```
{ "name": "mod_name", "type": "lumi", "data": null }
```

An example of a luminosity modifier.

4.4.6 Unconstrained Normalisation (normfactor)

The unconstrained normalisation modifier scales the event rates of a sample by a free parameter μ. Common use cases are the signal rate of a possible BSM signal or simultaneous in-situ measurements of background samples. Such parameters are frequently the parameters of interest of a given measurement. No additional per-sample data is required. An example is shown below:

```
{ "name": "mod_name", "type": "normfactor", "data": null }
```

An example of a normalisation modifier.

4.4.7 Data-driven Shape (shapefactor)

In order to support data-driven estimation of sample rates (e.g. for multijet backgrounds), the data-driven shape modifier adds free, bin-wise multiplicative parameters. Similarly to the normalisation factors, no additional data is required as no constraint is defined. An example is shown below:

```
{ "name": "mod_name", "type": "shapefactor", "data": null }
```

An example of an uncorrelated shape modifier.

4.5 Data

The data provided by the analysis are the observed data for each channel (or region). This data is provided as a mapping from channel name to an array of floats, which provide the observed rates in each bin of the channel. The auxiliary data is not included as it is an input to the likelihood that does not need to be archived and can be determined automatically from the specification. An example is shown below:

```
{ "chan_name_one": [10, 20], "chan_name_two": [4, 0]}
```

An example of channel data.

4.6 Measurements

Given the data and the model definitions, a measurement can be defined. In the current schema, the measurements defines the name of the parameter of interest as well as parameter set configurations.[2] Here, the remaining information not covered through the channel definition is provided, e.g. for the luminosity parameter. For all modifiers, the default settings can be overridden where possible:

- **inits**: Initial value of the parameter.
- **bounds**: Interval bounds of the parameter.
- **auxdata**: Auxiliary data for the associated constraint term.
- **sigmas**: Associated uncertainty of the parameter.

An example is shown below:

```
{
    "name": "MyMeasurement",
    "config": {
        "poi": "SignalCrossSection", "parameters": [
            { "name":"lumi", "auxdata":[1.0],"sigmas":[0.017], "bounds":[[0.915,1.085]],
↪"inits":[1.0] },
            { "name":"mu_ttbar", "bounds":[[0, 5]] },
            { "name":"rw_1CR", "fixed":true }
        ]
    }
}
```

[2] In this context a parameter set corresponds to a named lower-dimensional subspace of the full parameters . In many cases these are one-dimensional subspaces, e.g. a specific interpolation parameter α or the luminosity parameter λ. For multi-bin channels, however, e.g. all bin-wise nuisance parameters of the uncorrelated shape modifiers are grouped under a single name. Therefore in general a parameter set definition provides arrays of initial values, bounds, etc.

An example of a measurement. This measurement, which scans over the parameter of interest `SignalCrossSection`, is setting configurations for the luminosity modifier, changing the default bounds for the normfactor modifier named `mu_ttbar`, and specifying that the modifier `rw_1CR` is held constant (`fixed`).

4.7 Observations

This is what we evaluate the hypothesis testing against, to determine the compatibility of signal+background hypothesis to the background-only hypothesis. This is specified as a list of objects, with each object structured as

- **name**: the channel for which the observations are recorded
- **data**: the bin-by-bin observations for the named channel

An example is shown below:

```
{
    "name": "channel1",
    "data": [110.0, 120.0]
}
```

An example of an observation. This observation recorded for a 2-bin channel `channel1`, has values `110.0` and `120.0`.

4.8 Toy Example

```
{
    "channels": [
        { "name": "singlechannel",
          "samples": [
            { "name": "signal",
              "data": [5.0, 10.0],
              "modifiers": [ { "name": "mu", "type": "normfactor", "data": null} ]
            },
            { "name": "background",
              "data": [50.0, 60.0],
              "modifiers": [ {"name": "uncorr_bkguncrt", "type": "shapesys", "data": [5.
↪0, 12.0]} ]
            }
          ]
        }
    ],
    "observations": [
        { "name": "singlechannel", "data": [50.0, 60.0] }
    ],
    "measurements": [
        { "name": "Measurement", "config": {"poi": "mu", "parameters": []} }
    ],
    "version": "1.0.0"
}
```

In the above example, we demonstrate a simple measurement of a single two-bin channel with two samples: a signal sample and a background sample. The signal sample has an unconstrained normalisation factor μ, while the background

sample carries an uncorrelated shape systematic controlled by parameters γ_1 and γ_2. The background uncertainty for the bins is 10% and 20% respectively.

4.9 Additional Material

4.9.1 Footnotes

4.9.2 Bibliography

CHAPTER

FIVE

FUNDAMENTALS

Notebooks:

[1]:
```
%pylab inline
from ipywidgets import interact
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
```

```
Populating the interactive namespace from numpy and matplotlib
```

5.1 Piecewise Linear Interpolation

References: https://cds.cern.ch/record/1456844/files/CERN-OPEN-2012-016.pdf

We wish to understand interpolation using the piecewise linear function. This is `interpcode=0` in the above reference. This function is defined as (nb: vector denotes bold)

$$\eta_s(\vec{\alpha}) = \sigma^0_{sb}(\vec{\alpha}) + \underbrace{\sum_{p\in \text{Syst}} I_{\text{lin.}}(\alpha_p; \sigma^0_{sb}, \sigma^+_{psb}, \sigma^-_{psb})}_{\text{deltas to calculate}}$$

with

$$I_{\text{lin.}}(\alpha; I^0, I^+, I^-) = \begin{cases} \alpha(I^+ - I^0) & \alpha \geq 0 \\ \alpha(I^0 - I^-) & \alpha < 0 \end{cases}$$

In this notebook, we'll demonstrate the technical implementation of these interplations starting from simple dimensionality and increasing the dimensions as we go along. In all situations, we'll consider a single systematic that we wish to interpolate, such as Jet Energy Scale (JES).

Let's define the interpolate function. This function will produce the deltas we would like to calculate and sum with the nominal measurement to determine the interpolated measurements value.

[2]:
```
def interpolate_deltas(down, nom, up, alpha):
    delta_up = up - nom
    delta_down = nom - down
    if alpha > 0:
        return delta_up * alpha
    else:
        return delta_down * alpha
```

Why are we calculating deltas? This is some additional foresight that you, the reader, may not have yet. Multiple interpolation schemes exist but they all rely on calculating the change with respect to the nominal measurement (the delta).

5.1.1 Case 1: The Single-binned Histogram

Let's first start with considering evaluating the total number of events after applying JES corrections. This is the single-bin case. Code that runs through event selection will vary the JES parameter and provide three histograms, each with a single bin. These three histograms represent the nominal-, up-, and down- variations of the JES nuisance parameter.

When processing, we find that there are 10 events nominally, and when we vary the JES parameter downwards, we only measure 8 events. When varying upwards, we measure 15 events.

[3]:
```
down_1 = np.array([8])
nom_1 = np.array([10])
up_1 = np.array([15])
```

We would like to generate a function $f(\alpha_{\text{JES}})$ that linearly interpolates the number of events for us so we can scan the phase-space for calculating PDFs. The `interpolate_deltas()` function defined above does this for us.

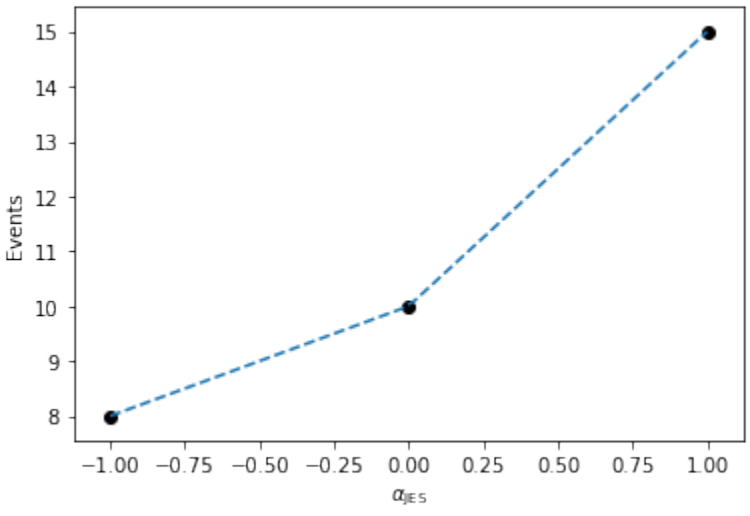
[4]:
```
alphas = np.linspace(-1.0, 1.0)
deltas = [interpolate_deltas(down_1, nom_1, up_1, alpha) for alpha in alphas]
deltas[:5]
```

[4]:
```
[array([-2.]),
 array([-1.91836735]),
 array([-1.83673469]),
 array([-1.75510204]),
 array([-1.67346939])]
```

So now that we've generated the deltas from the nominal measurement, we can plot this to see how the linear interpolation works in the single-bin case, where we plot the measured values in black, and the interpolation in dashed, blue.

[5]:
```
plt.plot(alphas, [nom_1 + delta for delta in deltas], linestyle='--')
plt.scatter((-1, 0, 1), (down_1, nom_1, up_1), color='k')
plt.xlabel(r'$\alpha_\mathrm{JES}$')
plt.ylabel(r'Events')
```

[5]:
```
Text(0,0.5,'Events')
```



Here, we can imagine building a 1-dimensional tensor (column-vector) of measurements as a function of α_{JES} with each row in the column vector corresponding to a given α_{JES} value.

5.1.2 Case 2: The Multi-binned Histogram

Now, let's increase the computational difficulty a little by increasing the dimensionality. Assume instead of a single-bin measurement, we have more measurements! We are good physicists after all. Imagine continuing on the previous example, where we add more bins, perhaps because we got more data. Imagine that this was binned by collection year, where we observed 10 events in the first year, 10.5 the next year, and so on...

[6]:
```
down_hist = np.linspace(8, 10, 11)
nom_hist = np.linspace(10, 13, 11)
up_hist = np.linspace(15, 20, 11)
```

Now, we still need to interpolate. Just like before, we have varied JES upwards and downwards to determine the corresponding histograms of variations. In order to interpolate, we need to interpolate by bin for each bin in the three histograms we have here (or three measurements if you prefer).

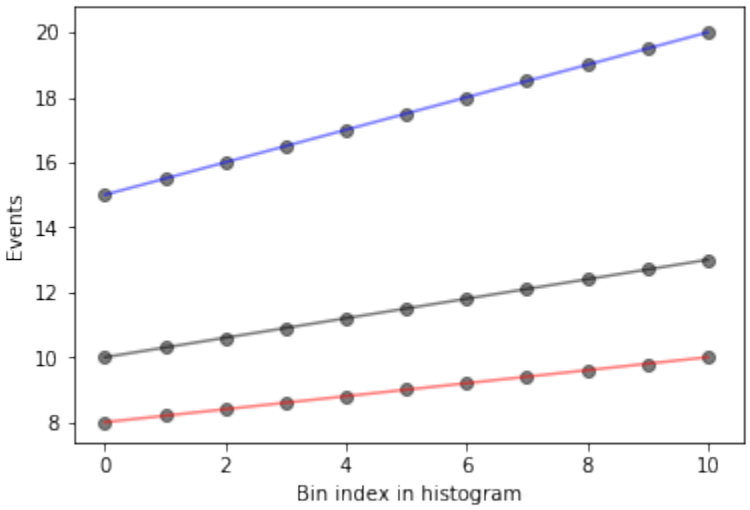
Let's go ahead and plot these histograms as a function of the bin index with black as the nominal measurements, red and blue as the down and up variations respectively. The black points are the measurements we have, and for each bin, we would like to interpolate to get an interpolated histogram that represents the measurement as a function of α_{JES}.

[7]:
```
def plot_measurements(down_hist, nom_hist, up_hist):
    bincenters = np.arange(len(nom_hist))
    for i, h in enumerate(zip(up_hist, nom_hist, down_hist)):
        plt.scatter([i] * len(h), h, color='k', alpha=0.5)

    for c, h in zip(['r', 'k', 'b'], [down_hist, nom_hist, up_hist]):
        plt.plot(bincenters, h, color=c, linestyle='-', alpha=0.5)

    plt.xlabel('Bin index in histogram')
    plt.ylabel('Events')


plot_measurements(down_hist, nom_hist, up_hist)
```

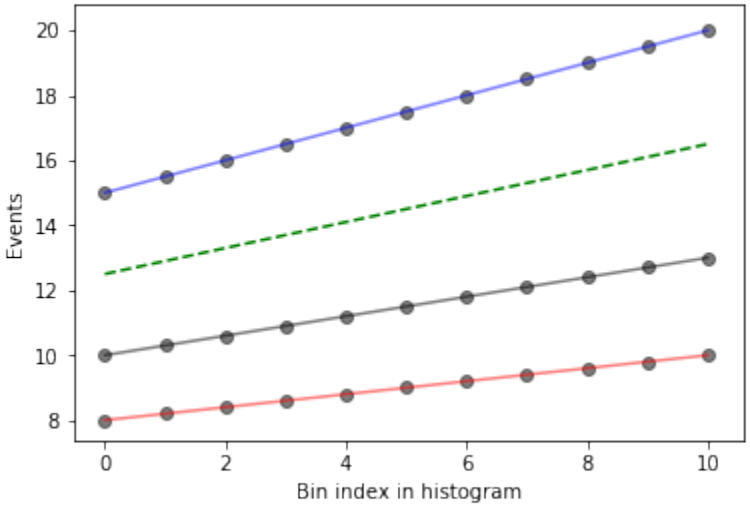


What does this look like if we evaluate at a single $\alpha_{\text{JES}} = 0.5$? We'll write a function that interpolates and then plots the interpolated values as a function of bin index, in green, dashed.

[8]:
```
def plot_interpolated_histogram(alpha, down_hist, nom_hist, up_hist):
    bincenters = np.arange(len(nom_hist))
    interpolated_vals = [
        nominal + interpolate_deltas(down, nominal, up, alpha)
        for down, nominal, up in zip(down_hist, nom_hist, up_hist)
    ]

    plot_measurements(down_hist, nom_hist, up_hist)
    plt.plot(bincenters, interpolated_vals, color='g', linestyle='--')


plot_interpolated_histogram(0.5, down_hist, nom_hist, up_hist)
```



We can go one step further in visualization and see what it looks like for different α_{JES} using iPyWidget's interactivity. Change the slider to get an idea of how the interpolation works.

[9]:
```
x = interact(
    lambda alpha: plot_interpolated_histogram(alpha, down_hist, nom_hist, up_hist),
    alpha=(-1, 1, 0.1),
)
```

```
aW50ZXJhY3RpdmUoY2hpbGRyZW49KEZsb2F0U2xpZGVyKHZhbHVlPTAuMCwgZGVzY3JpcHRpb249dSdhbHBoYScsIG1heD0xLjAsIG1p
```

The magic in `plot_interpolated_histogram()` happens to be that for a given α_{JES}, we iterate over all measurements bin-by-bin to calculate the interpolated value

```
[nominal + interpolate_deltas(down, nominal, up, alpha) for down, nominal, up in zip(...
↪hists...)]
```

So you can imagine that we're building up a 2-dimensional tensor with each row corresponding to a different α_{JES} and each column corresponding to the bin index of the histograms (or measurements). Let's go ahead and build a 3-dimensional representation of our understanding so far!

[10]:
```
def interpolate_alpha_range(alphas, down_hist, nom_hist, up_hist):
    at_alphas = []
    for alpha in alphas:
```

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```
        interpolated_hist_at_alpha = [
            nominal + interpolate_deltas(down, nominal, up, alpha)
            for down, nominal, up in zip(down_hist, nom_hist, up_hist)
        ]
        at_alphas.append(interpolated_hist_at_alpha)
    return np.array(at_alphas)
```

And then with this, we are interpolating over all histograms bin-by-bin and producing a 2-dimensional tensor with each row corresponding to a specific value of α_{JES}.

[11]:
```
alphas = np.linspace(-1, 1, 11)

interpolated_vals_at_alphas = interpolate_alpha_range(
    alphas, down_hist, nom_hist, up_hist
)

print(interpolated_vals_at_alphas[alphas == -1])
print(interpolated_vals_at_alphas[alphas == 0])
print(interpolated_vals_at_alphas[alphas == 1])
```

```
[[ 8.   8.2  8.4  8.6  8.8  9.   9.2  9.4  9.6  9.8 10. ]]
[[10.  10.3 10.6 10.9 11.2 11.5 11.8 12.1 12.4 12.7 13. ]]
[[15.  15.5 16.  16.5 17.  17.5 18.  18.5 19.  19.5 20. ]]
```

We have a way to generate the 2-dimensional tensor. Let's go ahead and add in all dimensions. Additionally, we'll add in some extra code to show the projection of the 2-d plots that we made earlier to help understand the 3-d plot a bit better. Like before, let's plot specifically colored lines for $\alpha_{\text{JES}} = 0.5$ as well as provide an interactive session.

[13]:
```
def plot_wire(alpha):
    alphas = np.linspace(-1, 1, 51)
    at_alphas = interpolate_alpha_range(alphas, down_hist, nom_hist, up_hist)
    bincenters = np.arange(len(nom_hist))
    x, y = np.meshgrid(bincenters, alphas)
    z = np.asarray(at_alphas)
    bottom = np.zeros_like(x)
    fig = plt.figure(figsize=(10, 10))
    ax1 = fig.add_subplot(111, projection='3d')
    ax1.plot_wireframe(x, y, z, alpha=0.3)

    x, y = np.meshgrid(bincenters, [alpha])
    z = interpolate_alpha_range([alpha], down_hist, nom_hist, up_hist)

    ax1.plot_wireframe(x, y, z, edgecolor='g', linestyle='--')
    ax1.set_xlim(0, 10)
    ax1.set_ylim(-1.0, 1.5)
    ax1.set_zlim(0, 25)
    ax1.view_init(azim=-125)
    ax1.set_xlabel('Bin Index')
    ax1.set_ylabel(r'$\alpha_\mathrm{JES}$')
    ax1.set_zlabel('Events')

    # add in 2D plot goodness
```

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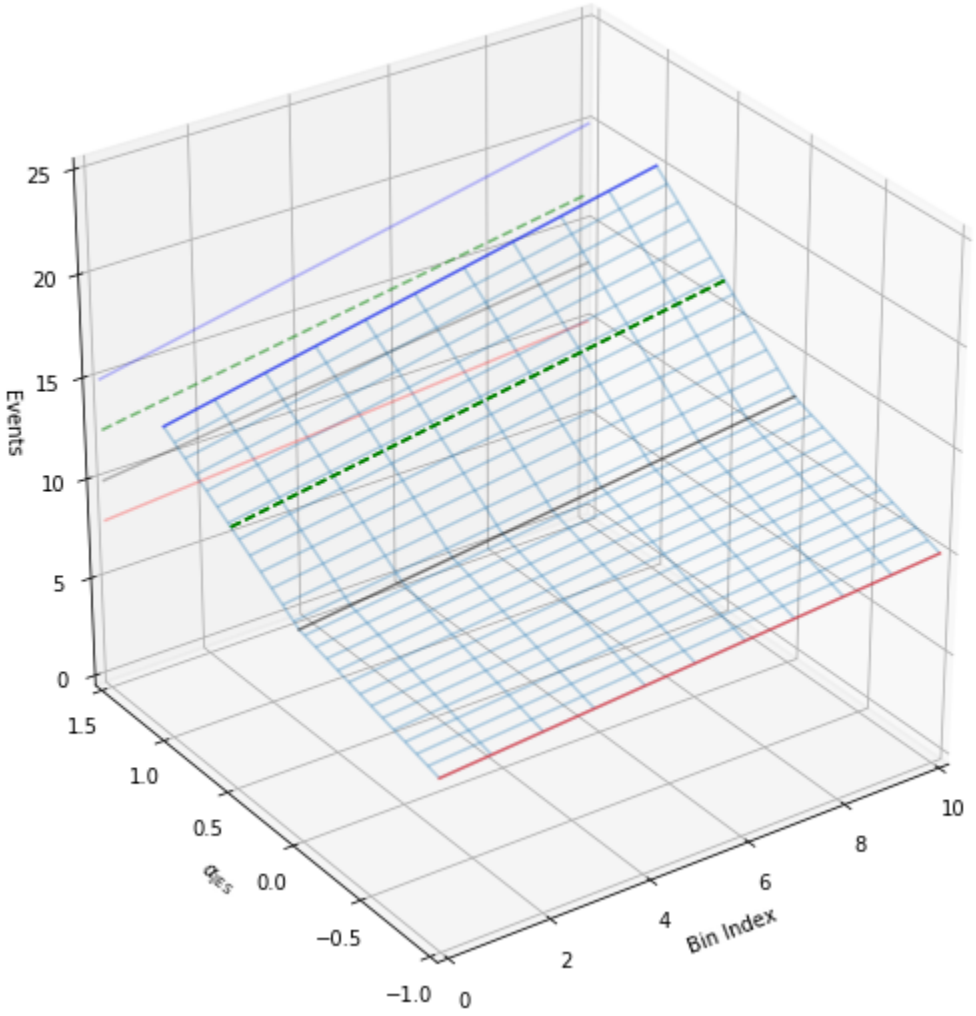
```
    for c, h, zs in zip(
        ['r', 'k', 'b'], [down_hist, nom_hist, up_hist], [-1.0, 0.0, 1.0]
    ):
        ax1.plot(bincenters, h, color=c, linestyle='-', alpha=0.5, zdir='y', zs=zs)
        ax1.plot(bincenters, h, color=c, linestyle='-', alpha=0.25, zdir='y', zs=1.5)

    ax1.plot(bincenters, z.T, color='g', linestyle='--', zdir='y', zs=alpha)
    ax1.plot(bincenters, z.T, color='g', linestyle='--', alpha=0.5, zdir='y', zs=1.5)

    plt.show()


plot_wire(0.5)

interact(plot_wire, alpha=(-1, 1, 0.1))
```



```
aW50ZXJhY3RpdmUoY2hpbGRyZW49KEZsb2F0U2xpZGVyKHZhbHVlPTAuMCwgZGVzY3JpcHRpb249dSdhbHBoYScsIG1heD0xLjAsIG1p
```

[13]:
```
<function __main__.plot_wire>
```

5.2 Tensorizing Interpolators

This notebook will introduce some tensor algebra concepts about being able to convert from calculations inside for-loops into a single calculation over the entire tensor. It is assumed that you have some familiarity with what interpolation functions are used for in `pyhf`.

To get started, we'll load up some functions we wrote whose job is to generate sets of histograms and alphas that we will compute interpolations for. This allows us to generate random, structured input data that we can use to test the tensorized form of the interpolation function against the original one we wrote. For now, we will consider only the `numpy` backend for simplicity, but can replace `np` to `pyhf.tensorlib` to achieve identical functionality.

The function `random_histosets_alphasets_pair` will produce a pair `(histogramsets, alphasets)` of histograms and alphas for those histograms that represents the type of input we wish to interpolate on.

[1]:
```
import numpy as np


def random_histosets_alphasets_pair(
    nsysts=150, nhistos_per_syst_upto=300, nalphas=1, nbins_upto=1
):
    def generate_shapes(histogramssets, alphasets):
        h_shape = [len(histogramssets), 0, 0, 0]
        a_shape = (len(alphasets), max(map(len, alphasets)))
        for hs in histogramssets:
            h_shape[1] = max(h_shape[1], len(hs))
            for h in hs:
                h_shape[2] = max(h_shape[2], len(h))
                for sh in h:
                    h_shape[3] = max(h_shape[3], len(sh))
        return tuple(h_shape), a_shape

    def filled_shapes(histogramssets, alphasets):
        # pad our shapes with NaNs
        histos, alphas = generate_shapes(histogramssets, alphasets)
        histos, alphas = np.ones(histos) * np.nan, np.ones(alphas) * np.nan
        for i, syst in enumerate(histogramssets):
            for j, sample in enumerate(syst):
                for k, variation in enumerate(sample):
                    histos[i, j, k, : len(variation)] = variation
        for i, alphaset in enumerate(alphasets):
            alphas[i, : len(alphaset)] = alphaset
        return histos, alphas

    nsyst_histos = np.random.randint(1, 1 + nhistos_per_syst_upto, size=nsysts)
    nhistograms = [np.random.randint(1, nbins_upto + 1, size=n) for n in nsyst_histos]
    random_alphas = [np.random.uniform(-1, 1, size=nalphas) for n in nsyst_histos]
```

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```
    random_histogramssets = [
        [  # all histos affected by systematic $nh
            [  # sample $i, systematic $nh
                np.random.uniform(10 * i + j, 10 * i + j + 1, size=nbin).tolist()
                for j in range(3)
            ]
            for i, nbin in enumerate(nh)
        ]
        for nh in nhistograms
    ]
    h, a = filled_shapes(random_histogramssets, random_alphas)
    return h, a
```

5.2.1 The (slow) interpolations

In all cases, the way we do interpolations is as follows:

1. Loop over both the `histogramssets` and `alphasets` simultaneously (e.g. using python's `zip()`)
2. Loop over all histograms set in the set of histograms sets that correspond to the histograms affected by a given systematic
3. Loop over all of the alphas in the set of alphas
4. Loop over all the bins in the histogram sets simultaneously (e.g. using python's `zip()`)
5. Apply the interpolation across the same bin index

This is already exhausting to think about, so let's put this in code form. Depending on the kind of interpolation being done, we'll pass in `func` as an argument to the top-level interpolation loop to switch between linear (`interpcode=0`) and non-linear (`interpcode=1`).

[2]:
```
def interpolation_looper(histogramssets, alphasets, func):
    all_results = []
    for histoset, alphaset in zip(histogramssets, alphasets):
        all_results.append([])
        set_result = all_results[-1]
        for histo in histoset:
            set_result.append([])
            histo_result = set_result[-1]
            for alpha in alphaset:
                alpha_result = []
                for down, nom, up in zip(histo[0], histo[1], histo[2]):
                    v = func(down, nom, up, alpha)
                    alpha_result.append(v)
                histo_result.append(alpha_result)
    return all_results
```

And we can also define our linear and non-linear interpolations we'll consider in this notebook that we wish to tensorize.

[3]:
```
def interpolation_linear(histogramssets, alphasets):
    def summand(down, nom, up, alpha):
        delta_up = up - nom
        delta_down = nom - down
```

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```
        if alpha > 0:
            delta = delta_up * alpha
        else:
            delta = delta_down * alpha
        return nom + delta

    return interpolation_looper(histogramssets, alphasets, summand)


def interpolation_nonlinear(histogramssets, alphasets):
    def product(down, nom, up, alpha):
        delta_up = up / nom
        delta_down = down / nom
        if alpha > 0:
            delta = delta_up ** alpha
        else:
            delta = delta_down ** (-alpha)
        return nom * delta

    return interpolation_looper(histogramssets, alphasets, product)
```

We will also define a helper function that allows us to pass in two functions we wish to compare the outputs for:

[4]:
```
def compare_fns(func1, func2):
    h, a = random_histosets_alphasets_pair()

    def _func_runner(func, histssets, alphasets):
        return np.asarray(func(histssets, alphasets))

    old = _func_runner(func1, h, a)
    new = _func_runner(func2, h, a)

    return (np.all(old[~np.isnan(old)] == new[~np.isnan(new)]), (h, a))
```

For the rest of the notebook, we will detail in explicit form how the linear interpolator gets tensorized, step-by-step. The same sequence of steps will be shown for the non-linear interpolator – but it is left up to the reader to understand the steps.

5.2.2 Tensorizing the Linear Interpolator

Step 0

Step 0 requires converting the innermost conditional check on `alpha > 0` into something tensorizable. This also means the calculation itself is going to become tensorized. So we will convert from

```
if alpha > 0:
    delta =  delta_up*alpha
else:
    delta =  delta_down*alpha
```

to

```
delta = np.where(alpha > 0, delta_up*alpha, delta_down*alpha)
```

Let's make that change now, and let's check to make sure we still do the calculation correctly.

[5]:
```
# get the internal calculation to use tensorlib backend
def new_interpolation_linear_step0(histogramssets, alphasets):
    all_results = []
    for histoset, alphaset in zip(histogramssets, alphasets):
        all_results.append([])
        set_result = all_results[-1]
        for histo in histoset:
            set_result.append([])
            histo_result = set_result[-1]
            for alpha in alphaset:
                alpha_result = []
                for down, nom, up in zip(histo[0], histo[1], histo[2]):
                    delta_up = up - nom
                    delta_down = nom - down
                    delta = np.where(alpha > 0, delta_up * alpha, delta_down * alpha)
                    v = nom + delta
                    alpha_result.append(v)
                histo_result.append(alpha_result)
    return all_results
```

And does the calculation still match?

[6]:
```
result, (h, a) = compare_fns(interpolation_linear, new_interpolation_linear_step0)
print(result)
```

```
True
```

[7]:
```
%%timeit
interpolation_linear(h, a)
```

```
189 ms ± 6.14 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[8]:
```
%%timeit
new_interpolation_linear_step0(h, a)
```

```
255 ms ± 11.7 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Great! We're a little bit slower right now, but that's expected. We're just getting started.

Step 1

In this step, we would like to remove the innermost `zip()` call over the histogram bins by calculating the interpolation between the histograms in one fell swoop. This means, instead of writing something like

```
for down,nom,up in zip(histo[0],histo[1],histo[2]):
    delta_up = up - nom
    ...
```

one can instead write

```
delta_up = histo[2] - histo[1]
...
```

taking advantage of the automatic broadcasting of operations on input tensors. This sort of feature of the tensor backends allows us to speed up code, such as interpolation.

[9]:
```
# update the delta variations to remove the zip() call and remove most-nested loop
def new_interpolation_linear_step1(histogramssets, alphasets):
    all_results = []
    for histoset, alphaset in zip(histogramssets, alphasets):
        all_results.append([])
        set_result = all_results[-1]
        for histo in histoset:
            set_result.append([])
            histo_result = set_result[-1]
            for alpha in alphaset:
                alpha_result = []
                deltas_up = histo[2] - histo[1]
                deltas_dn = histo[1] - histo[0]
                calc_deltas = np.where(alpha > 0, deltas_up * alpha, deltas_dn * alpha)
                v = histo[1] + calc_deltas
                alpha_result.append(v)
                histo_result.append(alpha_result)
    return all_results
```

And does the calculation still match?

[10]:
```
result, (h, a) = compare_fns(interpolation_linear, new_interpolation_linear_step1)
print(result)
```

```
True
```

[11]:
```
%%timeit
interpolation_linear(h, a)
```

```
188 ms ± 7.14 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[12]:
```
%%timeit
new_interpolation_linear_step1(h, a)
```

```
492 ms ± 42.8 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Great!

Step 2

In this step, we would like to move the giant array of the deltas calculated to the beginning – outside of all loops – and then only take a subset of it for the calculation itself. This allows us to figure out the entire structure of the input for the rest of the calculations as we slowly move towards including `einsum()` calls (einstein summation). This means we would like to go from

```
for histo in histoset:
    delta_up = histo[2] - histo[1]
...
```

to

```
all_deltas = ...
for nh, histo in enumerate(histoset):
    deltas = all_deltas[nh]
    ...
```

Again, we are taking advantage of the automatic broadcasting of operations on input tensors to calculate all the deltas in a single action.

[13]:
```
# figure out the giant array of all deltas at the beginning and only take subsets of it␣
↪for the calculation
def new_interpolation_linear_step2(histogramssets, alphasets):
    all_results = []

    allset_all_histo_deltas_up = histogramssets[:, :, 2] - histogramssets[:, :, 1]
    allset_all_histo_deltas_dn = histogramssets[:, :, 1] - histogramssets[:, :, 0]

    for nset, (histoset, alphaset) in enumerate(zip(histogramssets, alphasets)):
        set_result = []

        all_histo_deltas_up = allset_all_histo_deltas_up[nset]
        all_histo_deltas_dn = allset_all_histo_deltas_dn[nset]

        for nh, histo in enumerate(histoset):
            alpha_deltas = []
            for alpha in alphaset:
                alpha_result = []
                deltas_up = all_histo_deltas_up[nh]
                deltas_dn = all_histo_deltas_dn[nh]
                calc_deltas = np.where(alpha > 0, deltas_up * alpha, deltas_dn * alpha)
                alpha_deltas.append(calc_deltas)
            set_result.append([histo[1] + d for d in alpha_deltas])
        all_results.append(set_result)
    return all_results
```

And does the calculation still match?

[14]:
```
result, (h, a) = compare_fns(interpolation_linear, new_interpolation_linear_step2)
print(result)
```

```
True
```

[15]:
```
%%timeit
interpolation_linear(h, a)
```

```
179 ms ± 12.4 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[16]:
```
%%timeit
new_interpolation_linear_step2(h, a)
```

```
409 ms ± 20.8 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Great!

Step 3

In this step, we get to introduce einstein summation to generalize the calculations we perform across many dimensions in a more concise, straightforward way. See this blog post for some more details on einstein summation notation. In short, it allows us to write

$$c_j = \sum_i \sum_k = A_{ik} B_{kj} \qquad \rightarrow \qquad \texttt{einsum("ij,jk->i", A, B)}$$

in a much more elegant way to express many kinds of common tensor operations such as dot products, transposes, outer products, and so on. This step is generally the hardest as one needs to figure out the corresponding `einsum` that keeps the calculation preserved (and matching). To some extent it requires a lot of trial and error until you get a feel for how einstein summation notation works.

As a concrete example of a conversion, we wish to go from something like

```
for nh,histo in enumerate(histoset):
    for alpha in alphaset:
        deltas_up    = all_histo_deltas_up[nh]
        deltas_dn    = all_histo_deltas_dn[nh]
        calc_deltas  = np.where(alpha > 0, deltas_up*alpha, deltas_dn*alpha)
        ...
```

to get rid of the loop over `alpha`

```
for nh,histo in enumerate(histoset):
    alphas_times_deltas_up = np.einsum('i,j->ij',alphaset,all_histo_deltas_up[nh])
    alphas_times_deltas_dn = np.einsum('i,j->ij',alphaset,all_histo_deltas_dn[nh])
    masks = np.einsum('i,j->ij',alphaset > 0,np.ones_like(all_histo_deltas_dn[nh]))

    alpha_deltas  = np.where(masks,alphas_times_deltas_up, alphas_times_deltas_dn)
    ...
```

In this particular case, we need an outer product that multiplies across the `alphaset` to the corresponding `histoset` for the up/down variations. Then we just need to select from either the up variation calculation or the down variation calculation based on the sign of alpha. Try to convince yourself that the einstein summation does what the for-loop does, but a little bit more concisely, and perhaps more clearly! How does the function look now?

[17]:
```
# remove the loop over alphas, starts using einsum to help generalize to more dimensions
def new_interpolation_linear_step3(histogramssets, alphasets):
    all_results = []

    allset_all_histo_deltas_up = histogramssets[:, :, 2] - histogramssets[:, :, 1]
    allset_all_histo_deltas_dn = histogramssets[:, :, 1] - histogramssets[:, :, 0]

    for nset, (histoset, alphaset) in enumerate(zip(histogramssets, alphasets)):
        set_result = []

        all_histo_deltas_up = allset_all_histo_deltas_up[nset]
        all_histo_deltas_dn = allset_all_histo_deltas_dn[nset]

        for nh, histo in enumerate(histoset):
            alphas_times_deltas_up = np.einsum(
                'i,j->ij', alphaset, all_histo_deltas_up[nh]
            )
```

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```
            alphas_times_deltas_dn = np.einsum(
                'i,j->ij', alphaset, all_histo_deltas_dn[nh]
            )
            masks = np.einsum(
                'i,j->ij', alphaset > 0, np.ones_like(all_histo_deltas_dn[nh])
            )

            alpha_deltas = np.where(
                masks, alphas_times_deltas_up, alphas_times_deltas_dn
            )
            set_result.append([histo[1] + d for d in alpha_deltas])

        all_results.append(set_result)
    return all_results
```

And does the calculation still match?

[18]:
```
result, (h, a) = compare_fns(interpolation_linear, new_interpolation_linear_step3)
print(result)
```

```
True
```

[19]:
```
%%timeit
interpolation_linear(h, a)
```

```
166 ms ± 11.6 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[20]:
```
%%timeit
new_interpolation_linear_step3(h, a)
```

```
921 ms ± 133 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Great! Note that we've been getting a little bit slower during these steps. It will all pay off in the end when we're fully tensorized! A lot of the internal steps are overkill with the heavy einstein summation and broadcasting at the moment, especially for how many loops in we are.

Step 4

Now in this step, we will move the einstein summations to the outer loop, so that we're calculating it once! This is the big step, but a little bit easier because all we're doing is adding extra dimensions into the calculation. The underlying calculation won't have changed. At this point, we'll also rename from `i` and `j` to `a` and `b` for `alpha` and `bin` (as in the bin in the histogram). To continue the notation as well, here's a summary of the dimensions involved:

- `s` will be for the set under consideration (e.g. the modifier)
- `a` will be for the alpha variation
- `h` will be for the histogram affected by the modifier
- `b` will be for the bin of the histogram

So we wish to move the `einsum` code from

```
for nset,(histoset, alphaset) in enumerate(zip(histogramssets,alphasets)):
    ...
```

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```
    for nh,histo in enumerate(histoset):
        alphas_times_deltas_up = np.einsum('i,j->ij',alphaset,all_histo_deltas_up[nh])
            ...
```

to

```
all_alphas_times_deltas_up = np.einsum('...',alphaset,all_histo_deltas_up)
for nset,(histoset, alphaset) in enumerate(zip(histogramssets,alphasets)):
    ...

    for nh,histo in enumerate(histoset):
        ...
```

So how does this new function look?

[21]:
```
# move the einsums to outer loops to get ready to get rid of all loops
def new_interpolation_linear_step4(histogramssets, alphasets):
    allset_all_histo_deltas_up = histogramssets[:, :, 2] - histogramssets[:, :, 1]
    allset_all_histo_deltas_dn = histogramssets[:, :, 1] - histogramssets[:, :, 0]
    allset_all_histo_nom = histogramssets[:, :, 1]

    allsets_all_histos_alphas_times_deltas_up = np.einsum(
        'sa,shb->shab', alphasets, allset_all_histo_deltas_up
    )
    allsets_all_histos_alphas_times_deltas_dn = np.einsum(
        'sa,shb->shab', alphasets, allset_all_histo_deltas_dn
    )
    allsets_all_histos_masks = np.einsum(
        'sa,s...u->s...au', alphasets > 0, np.ones_like(allset_all_histo_deltas_dn)
    )

    allsets_all_histos_deltas = np.where(
        allsets_all_histos_masks,
        allsets_all_histos_alphas_times_deltas_up,
        allsets_all_histos_alphas_times_deltas_dn,
    )

    all_results = []
    for nset, histoset in enumerate(histogramssets):
        all_histos_deltas = allsets_all_histos_deltas[nset]
        set_result = []
        for nh, histo in enumerate(histoset):
            set_result.append([d + histoset[nh, 1] for d in all_histos_deltas[nh]])
        all_results.append(set_result)
    return all_results
```

And does the calculation still match?

[22]:
```
result, (h, a) = compare_fns(interpolation_linear, new_interpolation_linear_step4)
print(result)
```

```
True
```

[23]:
```
%%timeit
interpolation_linear(h, a)
```

```
160 ms ± 5 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[24]:
```
%%timeit
new_interpolation_linear_step4(h, a)
```

```
119 ms ± 3.19 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

Great! And look at that huge speed up in time already, just from moving the multiple, heavy einstein summation calculations up through the loops. We still have some more optimizing to do as we still have explicit loops in our code. Let's keep at it, we're almost there!

Step 5

The hard part is mostly over. We have to now think about the nominal variations. Recall that we were trying to add the nominals to the deltas in order to compute the new value. In practice, we'll return the delta variation only, but we'll show you how to get rid of this last loop. In this case, we want to figure out how to change code like

```
all_results    = []
for nset,histoset in enumerate(histogramssets):
    all_histos_deltas = allsets_all_histos_deltas[nset]
    set_result = []
    for nh,histo in enumerate(histoset):
        set_result.append([d + histoset[nh,1] for d in all_histos_deltas[nh]])
    all_results.append(set_result)
```

to get rid of that most-nested loop

```
all_results    = []
for nset,histoset in enumerate(histogramssets):
    # look ma, no more loops inside!
```

So how does this look?

[25]:
```
# slowly getting rid of our loops to build the right output tensor -- gotta think about␣
↪nominals
def new_interpolation_linear_step5(histogramssets, alphasets):
    allset_all_histo_deltas_up = histogramssets[:, :, 2] - histogramssets[:, :, 1]
    allset_all_histo_deltas_dn = histogramssets[:, :, 1] - histogramssets[:, :, 0]
    allset_all_histo_nom = histogramssets[:, :, 1]

    allsets_all_histos_alphas_times_deltas_up = np.einsum(
        'sa,shb->shab', alphasets, allset_all_histo_deltas_up
    )
    allsets_all_histos_alphas_times_deltas_dn = np.einsum(
        'sa,shb->shab', alphasets, allset_all_histo_deltas_dn
    )
    allsets_all_histos_masks = np.einsum(
        'sa,s...u->s...au', alphasets > 0, np.ones_like(allset_all_histo_deltas_dn)
    )
```

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```
    allsets_all_histos_deltas = np.where(
        allsets_all_histos_masks,
        allsets_all_histos_alphas_times_deltas_up,
        allsets_all_histos_alphas_times_deltas_dn,
    )

    all_results = []

    for nset, (_, alphaset) in enumerate(zip(histogramssets, alphasets)):
        all_histos_deltas = allsets_all_histos_deltas[nset]
        noms = histogramssets[nset, :, 1]

        all_histos_noms_repeated = np.einsum('a,hn->han', np.ones_like(alphaset), noms)

        set_result = all_histos_deltas + all_histos_noms_repeated
        all_results.append(set_result)
    return all_results
```

And does the calculation still match?

[26]:
```
result, (h, a) = compare_fns(interpolation_linear, new_interpolation_linear_step5)
print(result)
```

```
True
```

[27]:
```
%%timeit
interpolation_linear(h, a)
```

```
160 ms ± 8.28 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[28]:
```
%%timeit
new_interpolation_linear_step5(h, a)
```

```
1.57 ms ± 75.2 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

Fantastic! And look at the speed up. We're already faster than the for-loop and we're not even done yet.

Step 6

The final frontier. Also probably the best Star Wars episode. In any case, we have one more for-loop that needs to die in a slab of carbonite. This should be much easier now that you're more comfortable with tensor broadcasting and einstein summations.

What does the function look like now?

[29]:
```
def new_interpolation_linear_step6(histogramssets, alphasets):
    allset_allhisto_deltas_up = histogramssets[:, :, 2] - histogramssets[:, :, 1]
    allset_allhisto_deltas_dn = histogramssets[:, :, 1] - histogramssets[:, :, 0]
    allset_allhisto_nom = histogramssets[:, :, 1]

    # x is dummy index

    allsets_allhistos_alphas_times_deltas_up = np.einsum(
```

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```
        'sa,shb->shab', alphasets, allset_allhisto_deltas_up
    )
    allsets_allhistos_alphas_times_deltas_dn = np.einsum(
        'sa,shb->shab', alphasets, allset_allhisto_deltas_dn
    )
    allsets_allhistos_masks = np.einsum(
        'sa,sxu->sxau',
        np.where(alphasets > 0, np.ones(alphasets.shape), np.zeros(alphasets.shape)),
        np.ones(allset_allhisto_deltas_dn.shape),
    )

    allsets_allhistos_deltas = np.where(
        allsets_allhistos_masks,
        allsets_allhistos_alphas_times_deltas_up,
        allsets_allhistos_alphas_times_deltas_dn,
    )
    allsets_allhistos_noms_repeated = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_allhisto_nom
    )
    set_results = allsets_allhistos_deltas + allsets_allhistos_noms_repeated
    return set_results
```

And does the calculation still match?

[30]:
```
result, (h, a) = compare_fns(interpolation_linear, new_interpolation_linear_step6)
print(result)
```

```
True
```

[31]:
```
%%timeit
interpolation_linear(h, a)
```

```
156 ms ± 6.29 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[32]:
```
%%timeit
new_interpolation_linear_step6(h, a)
```

```
468 µs ± 37.1 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

And we're done tensorizing it. There are some more improvements that could be made to make this interpolation calculation even more robust – but for now we're done.

5.2.3 Tensorizing the Non-Linear Interpolator

This is very, very similar to what we've done for the case of the linear interpolator. As such, we will provide the resulting functions for each step, and you can see how things perform all the way at the bottom. Enjoy and learn at your own pace!

[33]:
```
def interpolation_nonlinear(histogramssets, alphasets):
    all_results = []
    for histoset, alphaset in zip(histogramssets, alphasets):
        all_results.append([])
```

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```
        set_result = all_results[-1]
        for histo in histoset:
            set_result.append([])
            histo_result = set_result[-1]
            for alpha in alphaset:
                alpha_result = []
                for down, nom, up in zip(histo[0], histo[1], histo[2]):
                    delta_up = up / nom
                    delta_down = down / nom
                    if alpha > 0:
                        delta = delta_up ** alpha
                    else:
                        delta = delta_down ** (-alpha)
                    v = nom * delta
                    alpha_result.append(v)
                histo_result.append(alpha_result)
    return all_results


def new_interpolation_nonlinear_step0(histogramssets, alphasets):
    all_results = []
    for histoset, alphaset in zip(histogramssets, alphasets):
        all_results.append([])
        set_result = all_results[-1]
        for histo in histoset:
            set_result.append([])
            histo_result = set_result[-1]
            for alpha in alphaset:
                alpha_result = []
                for down, nom, up in zip(histo[0], histo[1], histo[2]):
                    delta_up = up / nom
                    delta_down = down / nom
                    delta = np.where(
                        alpha > 0,
                        np.power(delta_up, alpha),
                        np.power(delta_down, np.abs(alpha)),
                    )
                    v = nom * delta
                    alpha_result.append(v)
                histo_result.append(alpha_result)
    return all_results


def new_interpolation_nonlinear_step1(histogramssets, alphasets):
    all_results = []
    for histoset, alphaset in zip(histogramssets, alphasets):
        all_results.append([])
        set_result = all_results[-1]
        for histo in histoset:
            set_result.append([])
            histo_result = set_result[-1]
            for alpha in alphaset:
```

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```
                alpha_result = []
                deltas_up = np.divide(histo[2], histo[1])
                deltas_down = np.divide(histo[0], histo[1])
                bases = np.where(alpha > 0, deltas_up, deltas_down)
                exponents = np.abs(alpha)
                calc_deltas = np.power(bases, exponents)
                v = histo[1] * calc_deltas
                alpha_result.append(v)
                histo_result.append(alpha_result)
    return all_results


def new_interpolation_nonlinear_step2(histogramssets, alphasets):
    all_results = []

    allset_all_histo_deltas_up = np.divide(
        histogramssets[:, :, 2], histogramssets[:, :, 1]
    )
    allset_all_histo_deltas_dn = np.divide(
        histogramssets[:, :, 0], histogramssets[:, :, 1]
    )

    for nset, (histoset, alphaset) in enumerate(zip(histogramssets, alphasets)):
        set_result = []

        all_histo_deltas_up = allset_all_histo_deltas_up[nset]
        all_histo_deltas_dn = allset_all_histo_deltas_dn[nset]

        for nh, histo in enumerate(histoset):
            alpha_deltas = []
            for alpha in alphaset:
                alpha_result = []
                deltas_up = all_histo_deltas_up[nh]
                deltas_down = all_histo_deltas_dn[nh]
                bases = np.where(alpha > 0, deltas_up, deltas_down)
                exponents = np.abs(alpha)
                calc_deltas = np.power(bases, exponents)
                alpha_deltas.append(calc_deltas)
            set_result.append([histo[1] * d for d in alpha_deltas])
        all_results.append(set_result)
    return all_results


def new_interpolation_nonlinear_step3(histogramssets, alphasets):
    all_results = []

    allset_all_histo_deltas_up = np.divide(
        histogramssets[:, :, 2], histogramssets[:, :, 1]
    )
    allset_all_histo_deltas_dn = np.divide(
        histogramssets[:, :, 0], histogramssets[:, :, 1]
    )
```

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```
    for nset, (histoset, alphaset) in enumerate(zip(histogramssets, alphasets)):
        set_result = []

        all_histo_deltas_up = allset_all_histo_deltas_up[nset]
        all_histo_deltas_dn = allset_all_histo_deltas_dn[nset]

        for nh, histo in enumerate(histoset):
            # bases and exponents need to have an outer product, to essentially tile or␣
↪repeat over rows/cols
            bases_up = np.einsum(
                'a,b->ab', np.ones(alphaset.shape), all_histo_deltas_up[nh]
            )
            bases_dn = np.einsum(
                'a,b->ab', np.ones(alphaset.shape), all_histo_deltas_dn[nh]
            )
            exponents = np.einsum(
                'a,b->ab', np.abs(alphaset), np.ones(all_histo_deltas_up[nh].shape)
            )

            masks = np.einsum(
                'a,b->ab', alphaset > 0, np.ones(all_histo_deltas_dn[nh].shape)
            )
            bases = np.where(masks, bases_up, bases_dn)
            alpha_deltas = np.power(bases, exponents)
            set_result.append([histo[1] * d for d in alpha_deltas])

        all_results.append(set_result)
    return all_results


def new_interpolation_nonlinear_step4(histogramssets, alphasets):
    all_results = []

    allset_all_histo_nom = histogramssets[:, :, 1]
    allset_all_histo_deltas_up = np.divide(
        histogramssets[:, :, 2], allset_all_histo_nom
    )
    allset_all_histo_deltas_dn = np.divide(
        histogramssets[:, :, 0], allset_all_histo_nom
    )

    bases_up = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_all_histo_deltas_up
    )
    bases_dn = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_all_histo_deltas_dn
    )
    exponents = np.einsum(
        'sa,shb->shab', np.abs(alphasets), np.ones(allset_all_histo_deltas_up.shape)
    )
```

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```
    masks = np.einsum(
        'sa,shb->shab', alphasets > 0, np.ones(allset_all_histo_deltas_up.shape)
    )
    bases = np.where(masks, bases_up, bases_dn)

    allsets_all_histos_deltas = np.power(bases, exponents)

    all_results = []
    for nset, histoset in enumerate(histogramssets):
        all_histos_deltas = allsets_all_histos_deltas[nset]
        set_result = []
        for nh, histo in enumerate(histoset):
            set_result.append([histoset[nh, 1] * d for d in all_histos_deltas[nh]])
        all_results.append(set_result)
    return all_results


def new_interpolation_nonlinear_step5(histogramssets, alphasets):
    all_results = []

    allset_all_histo_nom = histogramssets[:, :, 1]
    allset_all_histo_deltas_up = np.divide(
        histogramssets[:, :, 2], allset_all_histo_nom
    )
    allset_all_histo_deltas_dn = np.divide(
        histogramssets[:, :, 0], allset_all_histo_nom
    )

    bases_up = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_all_histo_deltas_up
    )
    bases_dn = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_all_histo_deltas_dn
    )
    exponents = np.einsum(
        'sa,shb->shab', np.abs(alphasets), np.ones(allset_all_histo_deltas_up.shape)
    )

    masks = np.einsum(
        'sa,shb->shab', alphasets > 0, np.ones(allset_all_histo_deltas_up.shape)
    )
    bases = np.where(masks, bases_up, bases_dn)

    allsets_all_histos_deltas = np.power(bases, exponents)

    all_results = []
    for nset, (_, alphaset) in enumerate(zip(histogramssets, alphasets)):
        all_histos_deltas = allsets_all_histos_deltas[nset]
        noms = allset_all_histo_nom[nset]
        all_histos_noms_repeated = np.einsum('a,hn->han', np.ones_like(alphaset), noms)
        set_result = all_histos_deltas * all_histos_noms_repeated
        all_results.append(set_result)
```

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```
    return all_results


def new_interpolation_nonlinear_step6(histogramssets, alphasets):
    all_results = []

    allset_all_histo_nom = histogramssets[:, :, 1]
    allset_all_histo_deltas_up = np.divide(
        histogramssets[:, :, 2], allset_all_histo_nom
    )
    allset_all_histo_deltas_dn = np.divide(
        histogramssets[:, :, 0], allset_all_histo_nom
    )

    bases_up = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_all_histo_deltas_up
    )
    bases_dn = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_all_histo_deltas_dn
    )
    exponents = np.einsum(
        'sa,shb->shab', np.abs(alphasets), np.ones(allset_all_histo_deltas_up.shape)
    )

    masks = np.einsum(
        'sa,shb->shab', alphasets > 0, np.ones(allset_all_histo_deltas_up.shape)
    )
    bases = np.where(masks, bases_up, bases_dn)

    allsets_all_histos_deltas = np.power(bases, exponents)
    allsets_allhistos_noms_repeated = np.einsum(
        'sa,shb->shab', np.ones(alphasets.shape), allset_all_histo_nom
    )
    set_results = allsets_all_histos_deltas * allsets_allhistos_noms_repeated
    return set_results
```

[34]:
```
result, (h, a) = compare_fns(interpolation_nonlinear, new_interpolation_nonlinear_step0)
print(result)
```

```
True
```

[35]:
```
%%timeit
interpolation_nonlinear(h, a)
```

```
149 ms ± 9.45 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[36]:
```
%%timeit
new_interpolation_nonlinear_step0(h, a)
```

```
527 ms ± 29.2 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[37]:
```
result, (h, a) = compare_fns(interpolation_nonlinear, new_interpolation_nonlinear_step1)
print(result)
```

```
True
```

[38]:
```
%%timeit
interpolation_nonlinear(h, a)
```

```
150 ms ± 5.21 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[39]:
```
%%timeit
new_interpolation_nonlinear_step1(h, a)
```

```
456 ms ± 17.9 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[40]:
```
result, (h, a) = compare_fns(interpolation_nonlinear, new_interpolation_nonlinear_step2)
print(result)
```

```
True
```

[41]:
```
%%timeit
interpolation_nonlinear(h, a)
```

```
154 ms ± 4.49 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[42]:
```
%%timeit
new_interpolation_nonlinear_step2(h, a)
```

```
412 ms ± 31 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[43]:
```
result, (h, a) = compare_fns(interpolation_nonlinear, new_interpolation_nonlinear_step3)
print(result)
```

```
True
```

[44]:
```
%%timeit
interpolation_nonlinear(h, a)
```

```
145 ms ± 5.15 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[45]:
```
%%timeit
new_interpolation_nonlinear_step3(h, a)
```

```
1.28 s ± 74.4 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[46]:
```
result, (h, a) = compare_fns(interpolation_nonlinear, new_interpolation_nonlinear_step4)
print(result)
```

```
True
```

[47]:
```
%%timeit
interpolation_nonlinear(h, a)
```

```
147 ms ± 8.4 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[48]:
```
%%timeit
new_interpolation_nonlinear_step4(h, a)
```

```
120 ms ± 3.06 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[49]:
```
result, (h, a) = compare_fns(interpolation_nonlinear, new_interpolation_nonlinear_step5)
print(result)
```

```
True
```

[50]:
```
%%timeit
interpolation_nonlinear(h, a)
```

```
151 ms ± 5.29 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[51]:
```
%%timeit
new_interpolation_nonlinear_step5(h, a)
```

```
2.65 ms ± 57.6 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

[52]:
```
result, (h, a) = compare_fns(interpolation_nonlinear, new_interpolation_nonlinear_step6)
print(result)
```

```
True
```

[53]:
```
%%timeit
interpolation_nonlinear(h, a)
```

```
156 ms ± 3.35 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[54]:
```
%%timeit
new_interpolation_nonlinear_step6(h, a)
```

```
1.49 ms ± 16 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

5.3 Empirical Test Statistics

In this notebook we will compute test statistics empirically from pseudo-experiment and establish that they behave as assumed in the asymptotic approximation.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
import pyhf

np.random.seed(0)
plt.rcParams.update({"font.size": 14})
```

First, we define the statistical model we will study.

- the signal expected event rate is 10 events
- the background expected event rate is 100 events
- a 10% uncertainty is assigned to the background

The expected event rates are chosen to lie comfortably in the asymptotic regime.

[2]:
```
model = pyhf.simplemodels.uncorrelated_background(
    signal=[10.0], bkg=[100.0], bkg_uncertainty=[10.0]
)
```

The test statistics based on the profile likelihood described in arXiv:1007.1727 cover scanarios for both

- POI allowed to float to negative values (unbounded; $\mu \in [-10, 10]$)
- POI constrained to non-negative values (bounded; $\mu \in [0, 10]$)

For consistency, test statistics (t_μ, q_μ) associated with bounded POIs are usually denoted with a tilde $(\tilde{t}_\mu, \tilde{q}_\mu)$.

We set up the bounds for the fit as follows

[3]:
```
unbounded_bounds = model.config.suggested_bounds()
unbounded_bounds[model.config.poi_index] = (-10, 10)

bounded_bounds = model.config.suggested_bounds()
```

Next we draw some synthetic datasets (also referrerd to as "toys" or pseudo-experiments). We will "throw" 300 toys:

[4]:
```
true_poi = 1.0
n_toys = 300
toys = model.make_pdf(pyhf.tensorlib.astensor([true_poi, 1.0])).sample((n_toys,))
```

In the asymptotic treatment the test statistics are described as a function of the data's best-fit POI value $\hat{\mu}$.

So let's run some fits so we can plots the empirical test statistics against $\hat{\mu}$ to observed the emergence of the asymptotic behavior.

[5]:
```
pars = np.asarray(
    [pyhf.infer.mle.fit(toy, model, par_bounds=unbounded_bounds) for toy in toys]
)
fixed_params = model.config.suggested_fixed()
```

We can now calculate all four test statistics described in `arXiv:1007.1727`

[6]:
```
test_poi = 1.0
tmu = np.asarray(
    [
        pyhf.infer.test_statistics.tmu(
            test_poi,
            toy,
            model,
            init_pars=model.config.suggested_init(),
            par_bounds=unbounded_bounds,
            fixed_params=fixed_params,
        )
        for toy in toys
    ]
)
```

[7]:
```
tmu_tilde = np.asarray(
    [
        pyhf.infer.test_statistics.tmu_tilde(
            test_poi,
```

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```
            toy,
            model,
            init_pars=model.config.suggested_init(),
            par_bounds=bounded_bounds,
            fixed_params=fixed_params,
        )
        for toy in toys
    ]
)
```

[8]:
```
qmu = np.asarray(
    [
        pyhf.infer.test_statistics.qmu(
            test_poi,
            toy,
            model,
            init_pars=model.config.suggested_init(),
            par_bounds=unbounded_bounds,
            fixed_params=fixed_params,
        )
        for toy in toys
    ]
)
```

[9]:
```
qmu_tilde = np.asarray(
    [
        pyhf.infer.test_statistics.qmu_tilde(
            test_poi,
            toy,
            model,
            init_pars=model.config.suggested_init(),
            par_bounds=bounded_bounds,
            fixed_params=fixed_params,
        )
        for toy in toys
    ]
)
```

Let's plot all the test statistics we have computed

[10]:
```
muhat = pars[:, model.config.poi_index]
muhat_sigma = np.std(muhat)
```

We can check the asymptotic assumption that $\hat{\mu}$ is distributed normally around it's true value $\mu' = 1$

[11]:
```
fig, ax = plt.subplots()
fig.set_size_inches(7, 5)

ax.set_xlabel(r"$\hat{\mu}$")
ax.set_ylabel("Density")
ax.set_ylim(top=0.5)
```

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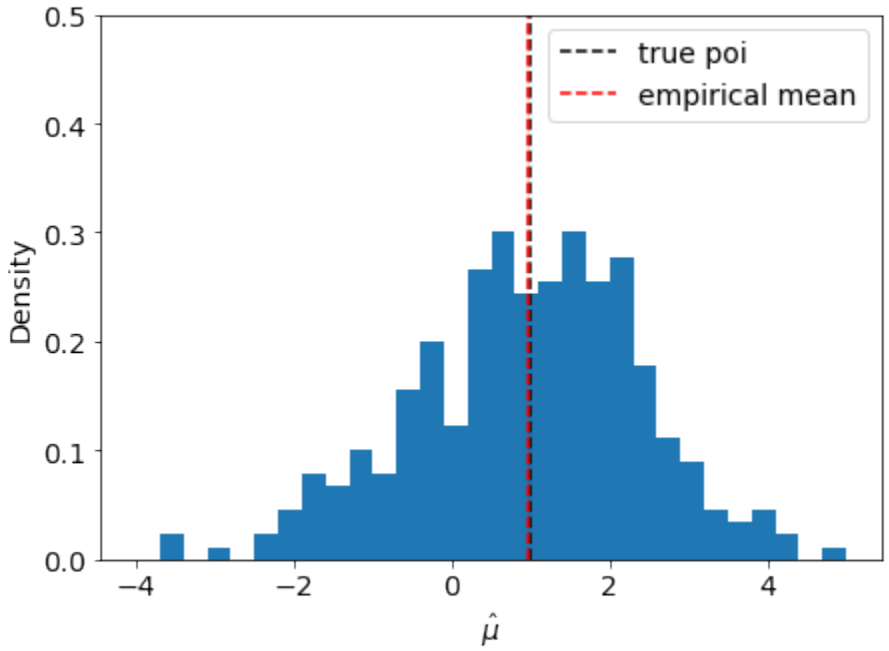
```
ax.hist(muhat, bins=np.linspace(-4, 5, 31), density=True)
ax.axvline(true_poi, label="true poi", color="black", linestyle="dashed")
ax.axvline(np.mean(muhat), label="empirical mean", color="red", linestyle="dashed")
ax.legend();
```



Here we define the asymptotic profile likelihood test statistics:

$$t_\mu = \frac{(\mu - \hat{\mu})^2}{\sigma^2}$$

$$\tilde{t}_\mu = \begin{cases} t_\mu, & \hat{\mu} > 0 \\ t_\mu - t_0, & \text{else} \end{cases}$$

$$q_\mu = \begin{cases} t_\mu, & \hat{\mu} < \mu \\ 0, & \text{else} \end{cases}$$

$$\tilde{q}_\mu = \begin{cases} \tilde{t}_\mu, & \hat{\mu} < \mu \\ 0, & \text{else} \end{cases}$$

[12]:
```
def tmu_asymp(mutest, muhat, sigma):
    return (mutest - muhat) ** 2 / sigma ** 2


def tmu_tilde_asymp(mutest, muhat, sigma):
    a = tmu_asymp(mutest, muhat, sigma)
    b = tmu_asymp(mutest, muhat, sigma) - tmu_asymp(0.0, muhat, sigma)
    return np.where(muhat > 0, a, b)


def qmu_asymp(mutest, muhat, sigma):
```

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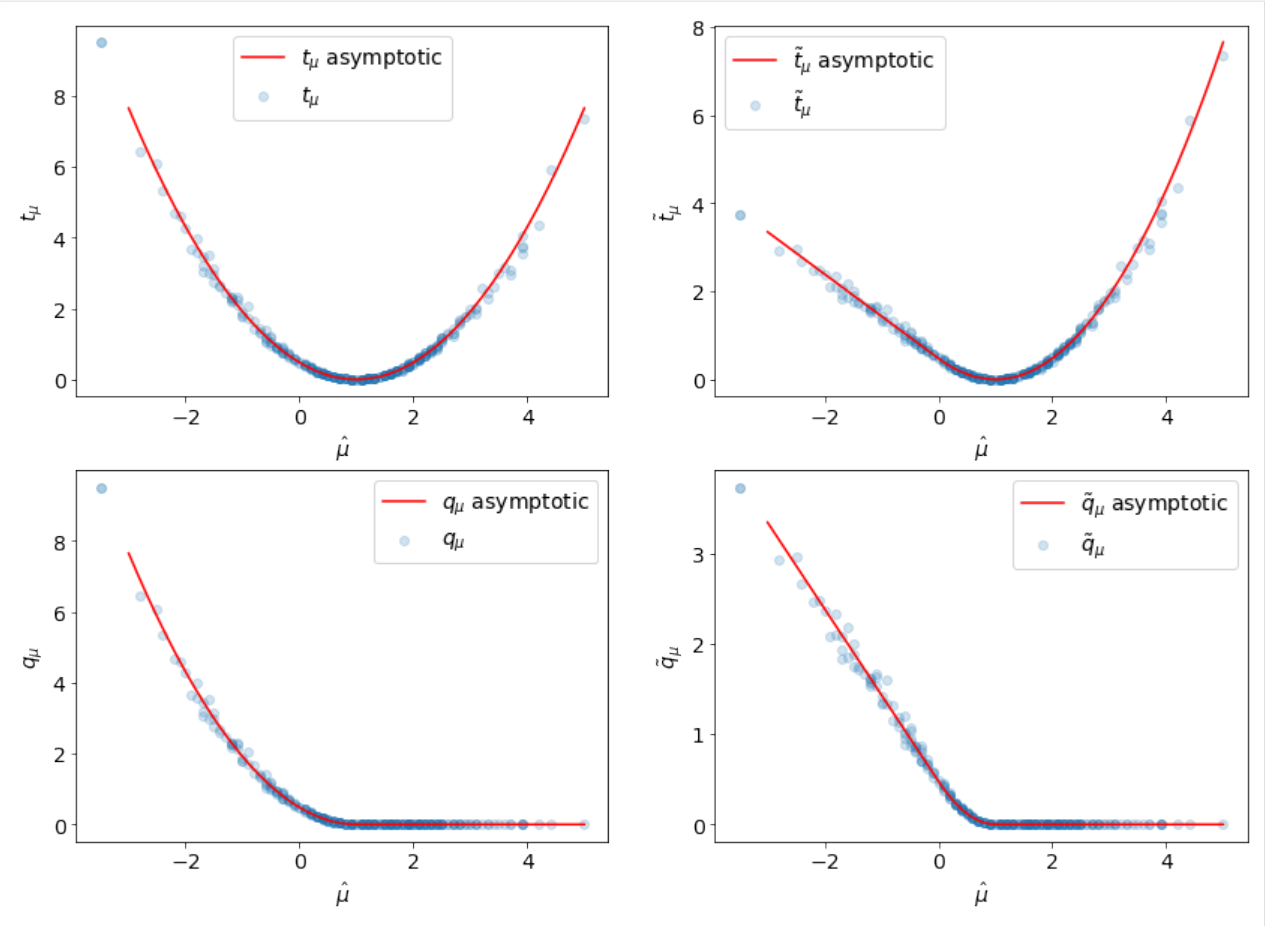
```
    return np.where(
        muhat < mutest, tmu_asymp(mutest, muhat, sigma), np.zeros_like(muhat)
    )


def qmu_tilde_asymp(mutest, muhat, sigma):
    return np.where(
        muhat < mutest, tmu_tilde_asymp(mutest, muhat, sigma), np.zeros_like(muhat)
    )
```

And now we can compare them to the empirical values:

[13]:
```
muhat_asymp = np.linspace(-3, 5)
fig, axarr = plt.subplots(2, 2)
fig.set_size_inches(14, 10)

labels = [r"$t_{\mu}$", "$\\tilde{t}_{\\mu}$", r"$q_{\mu}$", "$\\tilde{q}_{\\mu}$"]
data = [
    (tmu, tmu_asymp),
    (tmu_tilde, tmu_tilde_asymp),
    (qmu, qmu_asymp),
    (qmu_tilde, qmu_tilde_asymp),
]

for ax, (label, d) in zip(axarr.ravel(), zip(labels, data)):
    empirical, asymp_func = d
    ax.scatter(muhat, empirical, alpha=0.2, label=label)
    ax.plot(
        muhat_asymp,
        asymp_func(1.0, muhat_asymp, muhat_sigma),
        label=f"{label} asymptotic",
        c="r",
    )
    ax.set_xlabel(r"$\hat{\mu}$")
    ax.set_ylabel(f"{label}")
    ax.legend(loc="best")
```



5.4 Using Calculators

One low-level functionality of `pyhf` when it comes to statistical fits is the idea of a calculator to evaluate with `asymptotics` or `toybased` hypothesis testing.

This notebook will introduce very quickly what these calculators are meant to do and how they are used internally in the code. We'll set up a simple model for demonstration and then show how the calculators come into play.

[1]:
```
import numpy as np
import pyhf

np.random.seed(0)
```

[2]:
```
model = pyhf.simplemodels.uncorrelated_background([6], [9], [3])
data = [9] + model.config.auxdata
```

5.4.1 The high-level API

If the only thing you are interested in is the hypothesis test result you can just run the high-level API to get it:

[3]:
```
CLs_obs, CLs_exp = pyhf.infer.hypotest(1.0, data, model, return_expected_set=True)
print(f'CLs_obs = {CLs_obs}')
print(f'CLs_exp = {CLs_exp}')
```

```
CLs_obs = 0.1677886052335611
CLs_exp = [array(0.0159689), array(0.05465771), array(0.16778861), array(0.41863467),␣
↪array(0.74964133)]
```

5.4.2 The low-level API

Under the hood, the hypothesis test computes *test statistics* (such as $q_\mu, \tilde{q}_\mu$) and uses *calculators* in order to assess how likely the computed test statistic value is under various hypotheses. The goal is to provide a consistent API that understands how you wish to perform your hypothesis test.

Let's look at the `asymptotics` calculator and then do the same thing for the `toybased`.

Asymptotics

First, let's create the calculator for asymptotics using the $\tilde{q}_\mu$ test statistic.

[4]:
```
asymp_calc = pyhf.infer.calculators.AsymptoticCalculator(
    data, model, test_stat='qtilde'
)
```

Now from this, we want to perform the fit and compute the value of the test statistic from which we can get our p-values:

[5]:
```
teststat = asymp_calc.teststatistic(poi_test=1.0)
print(f'qtilde = {teststat}')
```

```
qtilde = 0.0
```

In addition to this, we can ask the calculator for the distributions of the test statistic for the background-only and signal+background hypotheses:

[6]:
```
sb_dist, b_dist = asymp_calc.distributions(poi_test=1.0)
```

From these distributions, we can ask for the p-value of the test statistic and use this to calculate the CL_s — a "modified" p-value.

[7]:
```
p_sb = sb_dist.pvalue(teststat)
p_b = b_dist.pvalue(teststat)
p_s = p_sb / p_b

print(f'CL_sb = {p_sb}')
print(f'CL_b = {p_b}')
print(f'CL_s = CL_sb / CL_b = {p_s}')
```

```
CL_sb = 0.08389430261678055
CL_b = 0.5
CL_s = CL_sb / CL_b = 0.1677886052335611
```

In a similar procedure, we can do the same thing for the expected CL_s values as well. We need to get the expected value of the test statistic at each $\pm\sigma$ and then ask for the expected p-value associated with each value of the test statistic.

[8]:
```
teststat_expected = [b_dist.expected_value(i) for i in [2, 1, 0, -1, -2]]
p_expected = [sb_dist.pvalue(t) / b_dist.pvalue(t) for t in teststat_expected]
p_expected
```

[8]:
```
[0.01596890401598493,
 0.05465770873260968,
 0.1677886052335611,
 0.4186346709326618,
 0.7496413276864433]
```

However, these sorts of steps are somewhat time-consuming and lengthy, and depending on the calculator chosen, may differ a little bit. The calculator API also serves to harmonize the extraction of the observed p-values:

[9]:
```
p_sb, p_b, p_s = asymp_calc.pvalues(teststat, sb_dist, b_dist)

print(f'CL_sb = {p_sb}')
print(f'CL_b = {p_b}')
print(f'CL_s = CL_sb / CL_b = {p_s}')
```

```
CL_sb = 0.08389430261678055
CL_b = 0.5
CL_s = CL_sb / CL_b = 0.1677886052335611
```

and the expected p-values:

[10]:
```
p_exp_sb, p_exp_b, p_exp_s = asymp_calc.expected_pvalues(sb_dist, b_dist)

print(f'exp. CL_sb = {p_exp_sb}')
print(f'exp. CL_b = {p_exp_b}')
print(f'exp. CL_s = CL_sb / CL_b = {p_exp_s}')
```

```
exp. CL_sb = [array(0.00036329), array(0.00867173), array(0.0838943), array(0.35221608),␣
↪array(0.73258689)]
exp. CL_b = [array(0.02275013), array(0.15865525), array(0.5), array(0.84134475),␣
↪array(0.97724987)]
exp. CL_s = CL_sb / CL_b = [array(0.0159689), array(0.05465771), array(0.16778861),␣
↪array(0.41863467), array(0.74964133)]
```

Toy-Based

The calculator API abstracts away a lot of the differences between various strategies, such that it returns what you want, regardless of whether you choose to perform asymptotics or toy-based testing. It hopefully delivers a simple but powerful API for you!

Let's create a toy-based calculator and "throw" 500 toys.

[11]:
```
toy_calc = pyhf.infer.calculators.ToyCalculator(
    data, model, test_stat='qtilde', ntoys=500
)
```

Like before, we'll ask for the test statistic. Unlike the asymptotics case, where we compute the Asimov dataset and perform a series of fits, here we are just evaluating the test statistic for the observed data.

[12]:
```
teststat = toy_calc.teststatistic(poi_test=1.0)
print(f'qtilde = {teststat}')
```

```
qtilde = 1.902590865638981
```

[13]:
```
inits = model.config.suggested_init()
bounds = model.config.suggested_bounds()
fixeds = model.config.suggested_fixed()
pyhf.infer.test_statistics.qmu_tilde(1.0, data, model, inits, bounds, fixeds)
```

[13]:
```
array(1.90259087)
```

So now the next thing to do is get our distributions. This is where, in the case of toys, we fit each and every single toy that we've randomly sampled from our model.

Note, again, that the API for the calculator is the same as in the asymptotics case.

[14]:
```
sb_dist, b_dist = toy_calc.distributions(poi_test=1.0)
```

From these distributions, we can ask for the p-value of the test statistic and use this to calculate the $\mathrm{CL_s}$.

[15]:
```
p_sb, p_b, p_s = toy_calc.pvalues(teststat, sb_dist, b_dist)

print(f'CL_sb = {p_sb}')
print(f'CL_b = {p_b}')
print(f'CL_s = CL_sb / CL_b = {p_s}')
```

```
CL_sb = 0.084
CL_b = 0.52
CL_s = CL_sb / CL_b = 0.16153846153846155
```

In a similar procedure, we can do the same thing for the expected $\mathrm{CL_s}$ values as well. We need to get the expected value of the test statistic at each $\pm\sigma$ and then ask for the expected p-value associated with each value of the test statistic.

[16]:
```
p_exp_sb, p_exp_b, p_exp_s = toy_calc.expected_pvalues(sb_dist, b_dist)

print(f'exp. CL_sb = {p_exp_sb}')
print(f'exp. CL_b = {p_exp_b}')
print(f'exp. CL_s = CL_sb / CL_b = {p_exp_s}')
```

```
exp. CL_sb = [array(0.), array(0.008), array(0.084), array(0.318), array(1.)]
exp. CL_b = [array(0.02540926), array(0.17), array(0.52), array(0.846), array(1.)]
exp. CL_s = CL_sb / CL_b = [array(0.), array(0.04594333), array(0.16153846), array(0.
↪37939698), array(1.)]
```

CHAPTER

SIX

EXAMPLES

Try out in Binder!

Notebooks:

6.1 ShapeFactor

[1]:
```
import logging
import json
import numpy as np
import matplotlib.pyplot as plt

import pyhf
from pyhf.contrib.viz import brazil

logging.basicConfig(level=logging.INFO)
```

[2]:
```
def prep_data(sourcedata):
    spec = {
        'channels': [
            {
                'name': 'signal',
                'samples': [
                    {
                        'name': 'signal',
                        'data': sourcedata['signal']['bindata']['sig'],
                        'modifiers': [
                            {'name': 'mu', 'type': 'normfactor', 'data': None}
                        ],
                    },
                    {
                        'name': 'bkg1',
                        'data': sourcedata['signal']['bindata']['bkg1'],
                        'modifiers': [
                            {
                                'name': 'coupled_shapefactor',
                                'type': 'shapefactor',
                                'data': None,
                            }
                        ],
```

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```
                    },
                ],
            },
            {
                'name': 'control',
                'samples': [
                    {
                        'name': 'background',
                        'data': sourcedata['control']['bindata']['bkg1'],
                        'modifiers': [
                            {
                                'name': 'coupled_shapefactor',
                                'type': 'shapefactor',
                                'data': None,
                            }
                        ],
                    }
                ],
            },
        ]
    }
    pdf = pyhf.Model(spec)
    data = []
    for channel in pdf.config.channels:
        data += sourcedata[channel]['bindata']['data']
    data = data + pdf.config.auxdata
    return data, pdf
```

[3]:
```
source = {
    "channels": {
        "signal": {
            "binning": [2, -0.5, 1.5],
            "bindata": {
                "data": [220.0, 230.0],
                "bkg1": [100.0, 70.0],
                "sig": [20.0, 20.0],
            },
        },
        "control": {
            "binning": [2, -0.5, 1.5],
            "bindata": {"data": [200.0, 300.0], "bkg1": [100.0, 100.0]},
        },
    }
}

data, pdf = prep_data(source['channels'])
print(f'data: {data}')

init_pars = pdf.config.suggested_init()
print(f'expected data: {pdf.expected_data(init_pars)}')

par_bounds = pdf.config.suggested_bounds()
```

```
INFO:pyhf.pdf:Validating spec against schema: model.json
INFO:pyhf.pdf:adding modifier mu (1 new nuisance parameters)
INFO:pyhf.pdf:adding modifier coupled_shapefactor (2 new nuisance parameters)
```

```
data: [200.0, 300.0, 220.0, 230.0]
expected data: [100. 100. 120.  90.]
```

[4]:
```
print(f'initialization parameters: {pdf.config.suggested_init()}')

unconpars = pyhf.infer.mle.fit(data, pdf)
print(f'parameters post unconstrained fit: {unconpars}')
```

```
initialization parameters: [1.0, 1.0, 1.0]
parameters post unconstrained fit: [1.00004623 1.99998941 3.00000438]
```

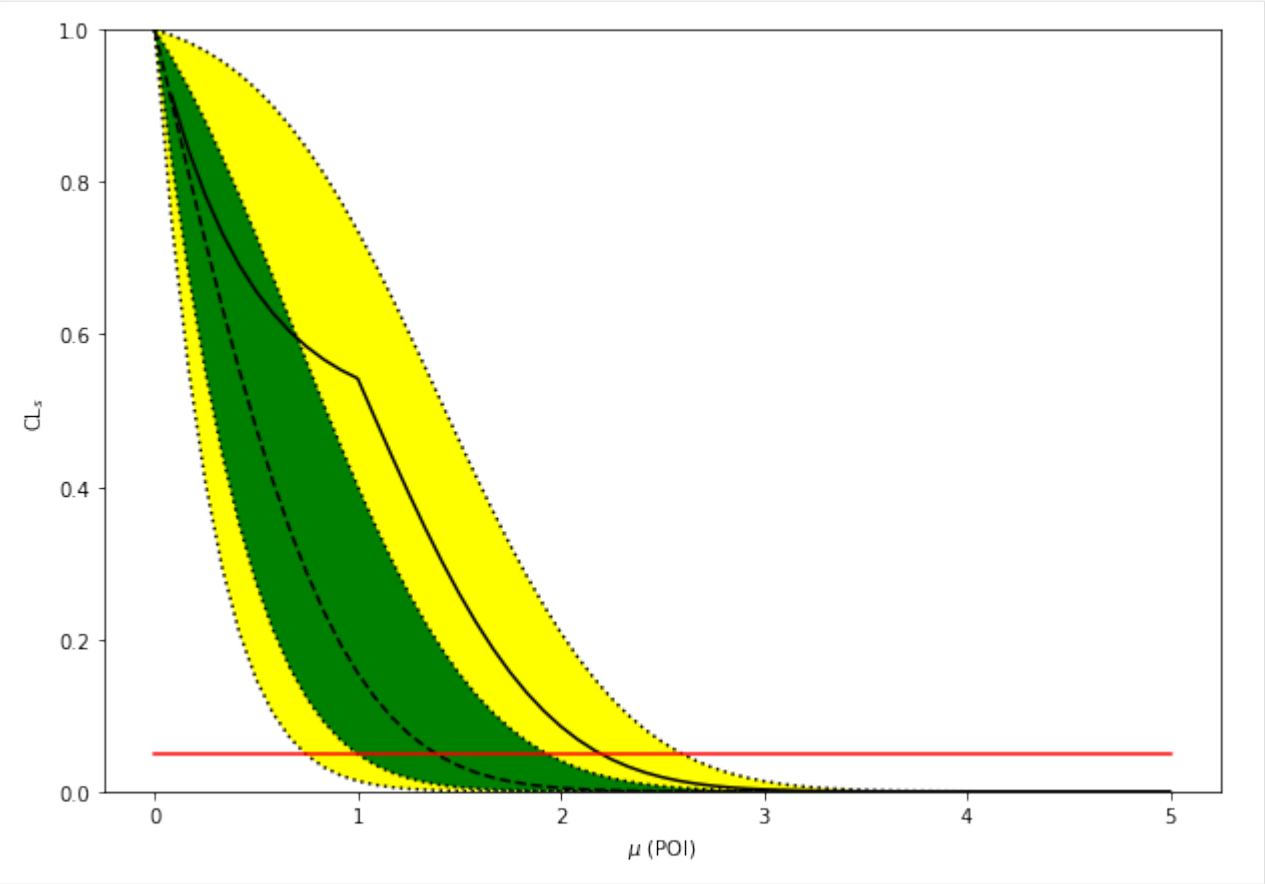
```
/srv/conda/envs/notebook/lib/python3.7/site-packages/pyhf/tensor/numpy_backend.py:334:␣
↪RuntimeWarning: divide by zero encountered in log
  return n * np.log(lam) - lam - gammaln(n + 1.0)
```

[5]:
```
obs_limit, exp_limits, (poi_tests, tests) = pyhf.infer.intervals.upperlimit(
    data, pdf, np.linspace(0, 5, 61), level=0.05, return_results=True
)
```

```
/srv/conda/envs/notebook/lib/python3.7/site-packages/pyhf/infer/calculators.py:352:␣
↪RuntimeWarning: invalid value encountered in double_scalars
  teststat = (qmu - qmu_A) / (2 * self.sqrtqmuA_v)
```

[6]:
```
fig, ax = plt.subplots(figsize=(10, 7))
artists = brazil.plot_results(poi_tests, tests, test_size=0.05, ax=ax)
print(f'expected upper limits: {exp_limits}')
print(f'observed upper limit : {obs_limit}')
```

```
expected upper limits: [array(0.74138115), array(0.994935), array(1.38451391), array(1.
↪92899382), array(2.59407668)]
observed upper limit : 2.1945969322493744
```



6.2 XML Import/Export

[1]:
```
# NB: python -m pip install pyhf[xmlio]
import pyhf
```

[2]:
```
!ls -lavh ../../../validation/xmlimport_input
```

```
total 1752
drwxr-xr-x   7 kratsg  staff   238B Oct 16 22:20 .
drwxr-xr-x  21 kratsg  staff   714B Apr  4 14:26 ..
drwxr-xr-x   6 kratsg  staff   204B Feb 27 17:13 config
drwxr-xr-x   7 kratsg  staff   238B Feb 27 23:41 data
-rw-r--r--   1 kratsg  staff   850K Oct 16 22:20 log
drwxr-xr-x  17 kratsg  staff   578B Nov 15 12:24 results
-rw-r--r--   1 kratsg  staff    21K Oct 16 22:20 scan.pdf
```

6.2.1 Importing

In order to convert HistFactory XML+ROOT to the pyhf JSON spec for likelihoods, you need to point the command-line interface `pyhf xml2json` at the top-level XML file. Additionally, as the HistFactory XML specification often uses relative paths, you might need to specify the base directory `--basedir` from which all other files are located, as specified in the top-level XML. The command will be of the format

```
pyhf xml2json {top-level XML} --basedir {base directory}
```

This will print the JSON representation of the XML+ROOT specified. If you wish to store this as a JSON file, you simply need to redirect it

```
pyhf xml2json {top-level XML} --basedir {base directory} > spec.json
```

[3]:
```
!pyhf xml2json --hide-progress ../../../validation/xmlimport_input/config/example.xml --
↪basedir ../../../validation/xmlimport_input | tee xml_importexport.json
```


```
{
    "channels": [
        {
            "name": "channel1",
            "samples": [
                {
                    "data": [
                        20.0,
                        10.0
                    ],
                    "modifiers": [
                        {
                            "data": {
                                "hi": 1.05,
                                "lo": 0.95
                            },
                            "name": "syst1",
                            "type": "normsys"
                        },
                        {
                            "data": null,
                            "name": "SigXsecOverSM",
                            "type": "normfactor"
                        }
                    ],
                    "name": "signal"
                },
                {
                    "data": [
                        100.0,
                        0.0
                    ],
                    "modifiers": [
                        {
                            "data": null,
                            "name": "lumi",
                            "type": "lumi"
```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```
                    },
                    {
                        "data": [
                            5.000000074505806,
                            0.0
                        ],
                        "name": "staterror_channel1",
                        "type": "staterror"
                    },
                    {
                        "data": {
                            "hi": 1.05,
                            "lo": 0.95
                        },
                        "name": "syst2",
                        "type": "normsys"
                    }
                ],
                "name": "background1"
            },
            {
                "data": [
                    0.0,
                    100.0
                ],
                "modifiers": [
                    {
                        "data": null,
                        "name": "lumi",
                        "type": "lumi"
                    },
                    {
                        "data": [
                            0.0,
                            10.0
                        ],
                        "name": "staterror_channel1",
                        "type": "staterror"
                    },
                    {
                        "data": {
                            "hi": 1.05,
                            "lo": 0.95
                        },
                        "name": "syst3",
                        "type": "normsys"
                    }
                ],
                "name": "background2"
            }
        ]
    }
```


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```
    ],
    "data": {
        "channel1": [
            122.0,
            112.0
        ]
    },
    "toplvl": {
        "measurements": [
            {
                "config": {
                    "parameters": [
                        {
                            "auxdata": [
                                1.0
                            ],
                            "bounds": [
                                [
                                    0.5,
                                    1.5
                                ]
                            ],
                            "fixed": true,
                            "inits": [
                                1.0
                            ],
                            "name": "lumi",
                            "sigmas": [
                                0.1
                            ]
                        },
                        {
                            "fixed": true,
                            "name": "alpha_syst1"
                        }
                    ],
                    "poi": "SigXsecOverSM"
                },
                "name": "GaussExample"
            },
            {
                "config": {
                    "parameters": [
                        {
                            "auxdata": [
                                1.0
                            ],
                            "bounds": [
                                [
                                    0.5,
                                    1.5
                                ]
```


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```
                        ],
                        "fixed": true,
                        "inits": [
                            1.0
                        ],
                        "name": "lumi",
                        "sigmas": [
                            0.1
                        ]
                    },
                    {
                        "fixed": true,
                        "name": "alpha_syst1"
                    }
                ],
                "poi": "SigXsecOverSM"
            },
            "name": "GammaExample"
        },
        {
            "config": {
                "parameters": [
                    {
                        "auxdata": [
                            1.0
                        ],
                        "bounds": [
                            [
                                0.5,
                                1.5
                            ]
                        ],
                        "fixed": true,
                        "inits": [
                            1.0
                        ],
                        "name": "lumi",
                        "sigmas": [
                            0.1
                        ]
                    },
                    {
                        "fixed": true,
                        "name": "alpha_syst1"
                    }
                ],
                "poi": "SigXsecOverSM"
            },
            "name": "LogNormExample"
        },
        {
            "config": {
```


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```
                    "parameters": [
                        {
                            "auxdata": [
                                1.0
                            ],
                            "bounds": [
                                [
                                    0.5,
                                    1.5
                                ]
                            ],
                            "fixed": true,
                            "inits": [
                                1.0
                            ],
                            "name": "lumi",
                            "sigmas": [
                                0.1
                            ]
                        },
                        {
                            "fixed": true,
                            "name": "alpha_syst1"
                        }
                    ],
                    "poi": "SigXsecOverSM"
                },
                "name": "ConstExample"
            }
        ],
        "resultprefix": "./results/example"
    }
}
```

6.2.2 Exporting

In order to convert the pyhf JSON to the HistFactory XML+ROOT spec for likelihoods, you need to point the command-line interface `pyhf json2xml` at the JSON file you want to convert. As everything is specified in a single file, there is no need to deal with base directories or looking up additional files. This will produce output XML+ROOT in the `--output-dir=./` directory (your current working directory), storing XML configs under `--specroot=config` and the data file under `--dataroot=data`. The XML configs are prefixed with `--resultprefix=FitConfig` by default, so that the top-level XML file will be located at `{output dir}/{prefix}.xml`. The command will be of the format

```
pyhf json2xml {JSON spec}
```

Note that the output directory must already exist.

[4]:
```
!mkdir -p output
!pyhf json2xml xml_importexport.json --output-dir output
!ls -lavh output/*
```

```
/Users/jovyan/pyhf/src/pyhf/writexml.py:120: RuntimeWarning: invalid value encountered␣
↪in true_divide
  attrs['HistoName'], np.divide(modifierspec['data'], sampledata).tolist()
-rw-r--r--  1 kratsg  staff   822B Apr  9 09:36 output/FitConfig.xml

output/config:
total 8
drwxr-xr-x  3 kratsg  staff   102B Apr  9 09:36 .
drwxr-xr-x  5 kratsg  staff   170B Apr  9 09:36 ..
-rw-r--r--  1 kratsg  staff   1.0K Apr  9 09:36 FitConfig_channel1.xml

output/data:
total 96
drwxr-xr-x  3 kratsg  staff   102B Apr  9 09:36 .
drwxr-xr-x  5 kratsg  staff   170B Apr  9 09:36 ..
-rw-r--r--  1 kratsg  staff    46K Apr  9 09:36 data.root
```

[5]:
```
!rm xml_importexport.json
!rm -rf output/
```

[1]:
```
import pyhf
import pandas
import numpy as np
import altair as alt
```

6.3 Visualization with Altair

Altair is a python API for generating Vega visuazliation specifications. We demonstracte how to use this to build an interactive chart of pyhf results.

6.3.1 Preparing the data

Altair reads the data as a pandas dataframe, so we create one.

[2]:
```
model = pyhf.simplemodels.uncorrelated_background([7], [20], [5])
data = [25] + model.config.auxdata
```

[3]:
```
muscan = np.linspace(0, 5, 31)
results = [
    pyhf.infer.hypotest(mu, data, model, return_expected_set=True) for mu in muscan
]
```

[4]:
```
data = np.concatenate(
    [
        muscan.reshape(-1, 1),
        np.asarray([r[0] for r in results]).reshape(-1, 1),
        np.asarray([r[1] for r in results]).reshape(-1, 5),
    ],
    axis=1,
```

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```
)
df = pandas.DataFrame(data, columns=["mu", "obs"] + [f"exp_{i}" for i in range(5)])
df.head()
```

[4]:

	mu	obs	exp_0	exp_1	exp_2	exp_3	exp_4
0	0.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1	0.166667	0.885208	0.670809	0.771258	0.870322	0.949235	0.989385
2	0.333333	0.795986	0.438838	0.581516	0.743696	0.890881	0.975022
3	0.500000	0.726450	0.279981	0.428500	0.623443	0.825621	0.956105
4	0.666667	0.672216	0.174235	0.308524	0.512383	0.754629	0.931866

6.3.2 Defining the Chart

We need to filled areas for the 1,2 sigma bands and two lines for the expected and observed CLs value. For interactivity we add a hovering label of the observed result

[5]:
```
band1 = (
    alt.Chart(df)
    .mark_area(opacity=0.5, color="green")
    .encode(x="mu", y="exp_1", y2="exp_3")
)

band2 = (
    alt.Chart(df)
    .mark_area(opacity=0.5, color="yellow")
    .encode(x="mu", y="exp_0", y2="exp_4")
)

line1 = alt.Chart(df).mark_line(color="black").encode(x="mu", y="obs")

line2 = (
    alt.Chart(df).mark_line(color="black", strokeDash=[5, 5]).encode(x="mu", y="exp_2")
)

nearest = alt.selection_single(
    nearest=True, on="mouseover", fields=["mu"], empty="none"
)


point = (
    alt.Chart(df)
    .mark_point(color="black")
    .encode(x="mu", y="obs", opacity=alt.condition(nearest, alt.value(1), alt.value(0)))
    .add_selection(nearest)
)

text = line1.mark_text(align="left", dx=5, dy=-5).encode(
    text=alt.condition(nearest, "obs", alt.value(" "))
)


band2 + band1 + line1 + line2 + point + text
```

[5]:
```
alt.LayerChart(...)
```

6.4 Hello World, pyhf style

Two bin counting experiment with a background uncertainty

[1]:
```
import pyhf
```

Returning the observed and expected CL_s

[2]:
```
model = pyhf.simplemodels.uncorrelated_background(
    signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
)
data = [51, 48] + model.config.auxdata
test_mu = 1.0
CLs_obs, CLs_exp = pyhf.infer.hypotest(
    test_mu, data, model, test_stat="qtilde", return_expected=True
)
print(f"Observed: {CLs_obs}, Expected: {CLs_exp}")
```

```
Observed: 0.052515541856109765, Expected: 0.06445521290832805
```

Returning the observed CL_s, CL_{s+b}, and CL_b

[3]:
```
CLs_obs, p_values = pyhf.infer.hypotest(
    test_mu, data, model, test_stat="qtilde", return_tail_probs=True
)
print(f"Observed CL_s: {CLs_obs}, CL_sb: {p_values[0]}, CL_b: {p_values[1]}")
```

```
Observed CL_s: 0.052515541856109765, CL_sb: 0.023324961200974572, CL_b: 0.
↪44415349012077077
```

A reminder that

$$\mathrm{CL}_s = \frac{\mathrm{CL}_{s+b}}{\mathrm{CL}_b} = \frac{p_{s+b}}{1-p_b}$$

[4]:
```
assert CLs_obs == p_values[0] / p_values[1]
```

Returning the expected CL_s band values

[5]:
```
import numpy as np
```

[6]:
```
CLs_obs, CLs_exp_band = pyhf.infer.hypotest(
    test_mu, data, model, test_stat="qtilde", return_expected_set=True
)
print(f"Observed CL_s: {CLs_obs}\n")
for p_value, n_sigma in enumerate(np.arange(-2, 3)):
    print(
        "Expected CL_s{}: {}".format(
            "      " if n_sigma == 0 else f"({n_sigma} )",
```

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```
            CLs_exp_band[p_value],
        )
    )
```

```
Observed CL_s: 0.052515541856109765

Expected CL_s(-2 ): 0.0026064088679947964
Expected CL_s(-1 ): 0.013820657528619273
Expected CL_s      : 0.06445521290832805
Expected CL_s(1 ): 0.23526103626937836
Expected CL_s(2 ): 0.5730418174887743
```

6.5 Multi-bin Poisson

[1]:
```
import logging
import json
import math
import numpy as np
import matplotlib.pyplot as plt

import pyhf
from pyhf import Model, optimizer
from pyhf.simplemodels import uncorrelated_background
from pyhf.contrib.viz import brazil

from scipy.interpolate import griddata
import scrapbook as sb
```

[2]:
```
def plot_histo(ax, binning, data):
    bin_width = (binning[2] - binning[1]) / binning[0]
    bin_leftedges = np.linspace(binning[1], binning[2], binning[0] + 1)[:-1]
    bin_centers = [le + bin_width / 2.0 for le in bin_leftedges]
    ax.bar(bin_centers, data, 1, alpha=0.5)


def plot_data(ax, binning, data):
    errors = [math.sqrt(d) for d in data]
    bin_width = (binning[2] - binning[1]) / binning[0]
    bin_leftedges = np.linspace(binning[1], binning[2], binning[0] + 1)[:-1]
    bin_centers = [le + bin_width / 2.0 for le in bin_leftedges]
    ax.bar(
        bin_centers,
        data,
        0,
        yerr=errors,
        linewidth=0,
        error_kw=dict(ecolor='k', elinewidth=1),
    )
    ax.scatter(bin_centers, data, c='k')
```

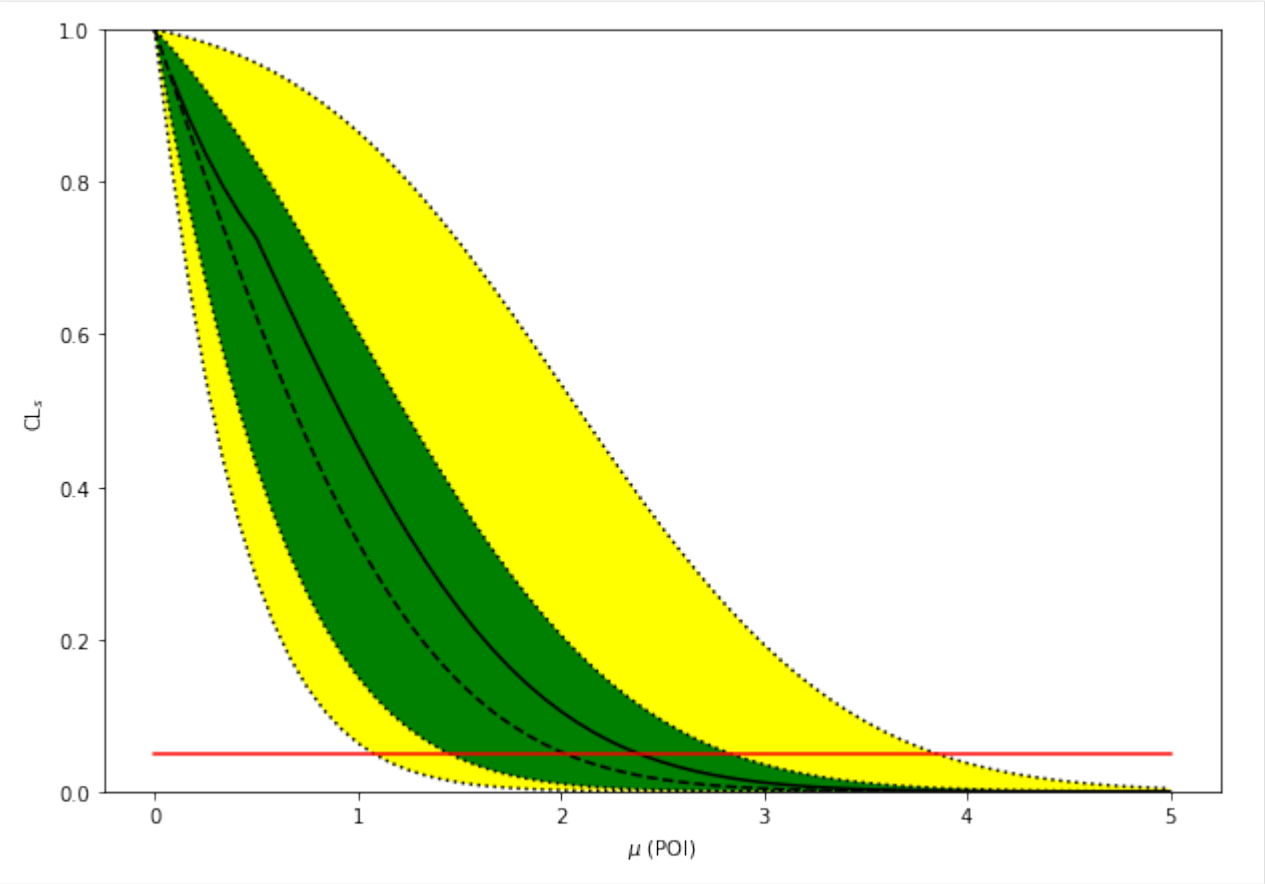
[3]:
```
validation_datadir = '../../validation/data'
```

[4]:
```
source = json.load(open(validation_datadir + '/1bin_example1.json'))
model = uncorrelated_background(
    source['bindata']['sig'], source['bindata']['bkg'], source['bindata']['bkgerr']
)
data = source['bindata']['data'] + model.config.auxdata

init_pars = model.config.suggested_init()
par_bounds = model.config.suggested_bounds()

obs_limit, exp_limits, (poi_tests, tests) = pyhf.infer.intervals.upperlimit(
    data, model, np.linspace(0, 5, 61), level=0.05, return_results=True
)
```

```
/srv/conda/envs/notebook/lib/python3.7/site-packages/pyhf/infer/calculators.py:352:␣
↪RuntimeWarning: invalid value encountered in double_scalars
  teststat = (qmu - qmu_A) / (2 * self.sqrtqmuA_v)
```

[5]:
```
fig, ax = plt.subplots(figsize=(10, 7))
artists = brazil.plot_results(poi_tests, tests, test_size=0.05, ax=ax)
print(f'expected upper limits: {exp_limits}')
print(f'observed upper limit : {obs_limit}')
```

```
expected upper limits: [array(1.07644221), array(1.44922838), array(2.01932904), array(2.
↪83213651), array(3.84750318)]
observed upper limit : 2.381026330918668
```



[6]:
```
source = {
    "binning": [2, -0.5, 1.5],
    "bindata": {
        "data": [120.0, 145.0],
        "bkg": [100.0, 150.0],
        "bkgerr": [15.0, 20.0],
        "sig": [30.0, 45.0],
    },
}


my_observed_counts = source['bindata']['data']

model = uncorrelated_background(
    source['bindata']['sig'], source['bindata']['bkg'], source['bindata']['bkgerr']
)
data = my_observed_counts + model.config.auxdata


binning = source['binning']

nompars = model.config.suggested_init()
```

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```
bonly_pars = [x for x in nompars]
bonly_pars[model.config.poi_index] = 0.0
nom_bonly = model.expected_data(bonly_pars, include_auxdata=False)

nom_sb = model.expected_data(nompars, include_auxdata=False)

init_pars = model.config.suggested_init()
par_bounds = model.config.suggested_bounds()

print(init_pars)

bestfit_pars = pyhf.infer.mle.fit(data, model, init_pars, par_bounds)
bestfit_cts = model.expected_data(bestfit_pars, include_auxdata=False)
```

```
[1.0, 1.0, 1.0]
```

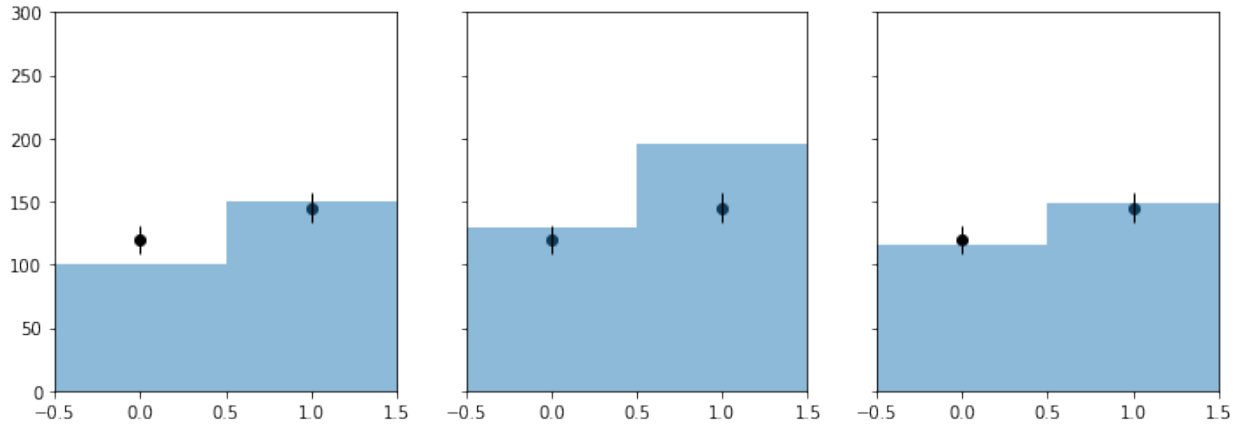
[7]:
```
f, axarr = plt.subplots(1, 3, sharey=True)
f.set_size_inches(12, 4)

plot_histo(axarr[0], binning, nom_bonly)
plot_data(axarr[0], binning, my_observed_counts)
axarr[0].set_xlim(binning[1:])

plot_histo(axarr[1], binning, nom_sb)
plot_data(axarr[1], binning, my_observed_counts)
axarr[1].set_xlim(binning[1:])

plot_histo(axarr[2], binning, bestfit_cts)
plot_data(axarr[2], binning, my_observed_counts)
axarr[2].set_xlim(binning[1:])

plt.ylim(0, 300);
```



[8]:
```
##  DUMMY 2D thing


def signal(m1, m2):
    massscale = 150.0
```

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```
    minmass = 100.0
    countscale = 2000

    effective_mass = np.sqrt(m1 ** 2 + m2 ** 2)
    return [countscale * np.exp(-(effective_mass - minmass) / massscale), 0]


def CLs(m1, m2):
    signal_counts = signal(m1, m2)
    pdf = uncorrelated_background(
        signal_counts, source['bindata']['bkg'], source['bindata']['bkgerr']
    )
    try:
        cls_obs, cls_exp_set = pyhf.infer.hypotest(
            1.0, data, pdf, init_pars, par_bounds, return_expected_set=True
        )
        return cls_obs, cls_exp_set, True
    except AssertionError:
        print(f'fit failed for mass points ({m1}, {m2})')
        return None, None, False
```

[9]:
```
nx, ny = 15, 15
grid = grid_x, grid_y = np.mgrid[
    100 : 1000 : complex(0, nx), 100 : 1000 : complex(0, ny)
]
X = grid.T.reshape(nx * ny, 2)
results = [CLs(m1, m2) for m1, m2 in X]
```

[10]:
```
X = np.array([x for x, (_, _, success) in zip(X, results) if success])
yobs = np.array([obs for obs, exp, success in results if success]).flatten()
yexp = [
    np.array([exp[i] for obs, exp, success in results if success]).flatten()
    for i in range(5)
]
```

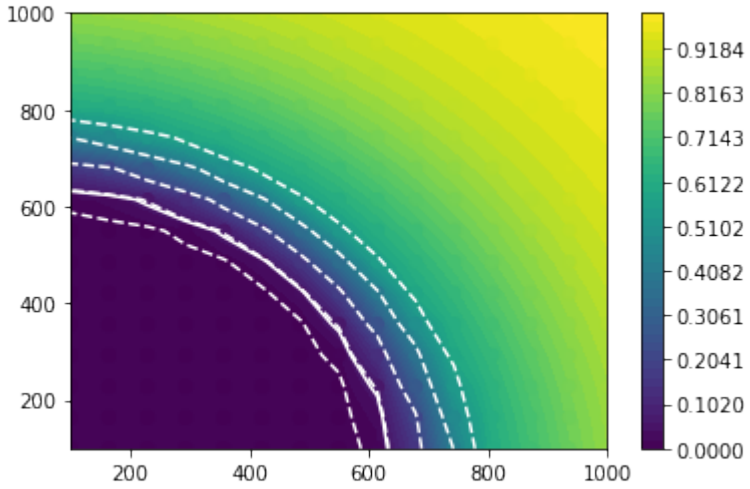
[11]:
```
int_obs = griddata(X, yobs, (grid_x, grid_y), method='linear')

int_exp = [griddata(X, yexp[i], (grid_x, grid_y), method='linear') for i in range(5)]

plt.contourf(grid_x, grid_y, int_obs, levels=np.linspace(0, 1))
plt.colorbar()

plt.contour(grid_x, grid_y, int_obs, levels=[0.05], colors='w')
for level in int_exp:
    plt.contour(grid_x, grid_y, level, levels=[0.05], colors='w', linestyles='dashed')

plt.scatter(X[:, 0], X[:, 1], c=yobs, vmin=0, vmax=1);
```



[12]:
```
sb.glue("number_2d_successpoints", len(X))
```

Data type cannot be displayed: application/scrapbook.scrap.json+json

6.6 Multibin Coupled HistoSys

[1]:
```
%pylab inline
```

```
Populating the interactive namespace from numpy and matplotlib
```

[2]:
```
import logging
import json

import pyhf
from pyhf import Model

logging.basicConfig(level=logging.INFO)
```

[3]:
```
def prep_data(sourcedata):
    spec = {
        "channels": [
            {
                "name": "signal",
                "samples": [
                    {
                        "name": "signal",
                        "data": sourcedata["signal"]["bindata"]["sig"],
                        "modifiers": [
                            {"name": "mu", "type": "normfactor", "data": None}
                        ],
                    },
                    {
```

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```
                    "name": "bkg1",
                    "data": sourcedata["signal"]["bindata"]["bkg1"],
                    "modifiers": [
                        {
                            "name": "coupled_histosys",
                            "type": "histosys",
                            "data": {
                                "lo_data": sourcedata["signal"]["bindata"][
                                    "bkg1_dn"
                                ],
                                "hi_data": sourcedata["signal"]["bindata"][
                                    "bkg1_up"
                                ],
                            },
                        }
                    ],
                },
                {
                    "name": "bkg2",
                    "data": sourcedata["signal"]["bindata"]["bkg2"],
                    "modifiers": [
                        {
                            "name": "coupled_histosys",
                            "type": "histosys",
                            "data": {
                                "lo_data": sourcedata["signal"]["bindata"][
                                    "bkg2_dn"
                                ],
                                "hi_data": sourcedata["signal"]["bindata"][
                                    "bkg2_up"
                                ],
                            },
                        }
                    ],
                },
            ],
        },
        {
            "name": "control",
            "samples": [
                {
                    "name": "background",
                    "data": sourcedata["control"]["bindata"]["bkg1"],
                    "modifiers": [
                        {
                            "name": "coupled_histosys",
                            "type": "histosys",
                            "data": {
                                "lo_data": sourcedata["control"]["bindata"][
                                    "bkg1_dn"
                                ],
                                "hi_data": sourcedata["control"]["bindata"][
```

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```
                                    "bkg1_up"
                                ],
                            },
                        }
                    ],
                }
            ],
        },
    ]
}
pdf = Model(spec)
data = []
for c in pdf.spec["channels"]:
    data += sourcedata[c["name"]]["bindata"]["data"]
data = data + pdf.config.auxdata
return data, pdf
```

[4]:
```
validation_datadir = "../../validation/data"
```

[5]:
```
source = json.load(open(validation_datadir + "/2bin_2channel_coupledhisto.json"))

data, pdf = prep_data(source["channels"])

print(data)

init_pars = pdf.config.suggested_init()
par_bounds = pdf.config.suggested_bounds()

unconpars = pyhf.infer.mle.fit(data, pdf, init_pars, par_bounds)
print(f"parameters post unconstrained fit: {unconpars}")

conpars = pyhf.infer.mle.fixed_poi_fit(0.0, data, pdf, init_pars, par_bounds)
print(f"parameters post constrained fit: {conpars}")

pdf.expected_data(conpars)
```

```
[170.0, 220.0, 110.0, 105.0, 0.0]
parameters post unconstrained fit: [1.53170588e-12 2.21657891e+00]
parameters post constrained fit: [0.         2.21655133]
```

[5]:
```
array([116.08275666, 133.24826999, 183.24826999,  98.08967672,
         2.21655133])
```

[6]:
```
def plot_results(test_mus, cls_obs, cls_exp, poi_tests, test_size=0.05):
    plt.plot(poi_tests, cls_obs, c="k")
    for i, c in zip(range(5), ["grey", "grey", "grey", "grey", "grey"]):
        plt.plot(poi_tests, cls_exp[i], c=c)
    plt.plot(poi_tests, [test_size] * len(test_mus), c="r")
    plt.ylim(0, 1)
```

[7]:
```
def invert_interval(test_mus, cls_obs, cls_exp, test_size=0.05):
    crossing_test_stats = {"exp": [], "obs": None}
```

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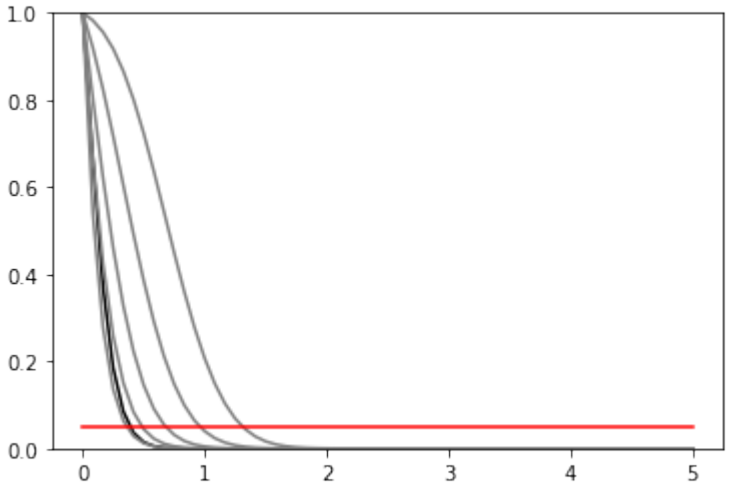
```
    for cls_exp_sigma in cls_exp:
        crossing_test_stats["exp"].append(
            np.interp(
                test_size, list(reversed(cls_exp_sigma)), list(reversed(test_mus))
            )
        )
    crossing_test_stats["obs"] = np.interp(
        test_size, list(reversed(cls_obs)), list(reversed(test_mus))
    )
    return crossing_test_stats
```

[8]:
```
poi_tests = np.linspace(0, 5, 61)
tests = [
    pyhf.infer.hypotest(
        poi_test, data, pdf, init_pars, par_bounds, return_expected_set=True
    )
    for poi_test in poi_tests
]
cls_obs = np.array([test[0] for test in tests]).flatten()
cls_exp = [np.array([test[1][i] for test in tests]).flatten() for i in range(5)]
```

[9]:
```
print("\n")
plot_results(poi_tests, cls_obs, cls_exp, poi_tests)
invert_interval(poi_tests, cls_obs, cls_exp)
```

[9]:
```
{'exp': [0.3654675198094938,
  0.4882076670368835,
  0.683262284467055,
  0.9650584704888153,
  1.3142329292131938],
 'obs': 0.3932476110375604}
```



[1]:
```
import numpy as np
import matplotlib.pyplot as plt
import pyhf
```

[2]:
```
np.random.seed(0)
plt.rcParams.update({"font.size": 14})
```

6.7 Running Monte Carlo simulations (toys)

Finding the (expected) significance can involve costly Monte Carlo calculations ("toys"). The asymptotic approximation described in the paper by Cowan, Cranmer, Gross, Vitells: *Asymptotic formulae for likelihood-based tests of new physics* [arXiv:1007.1727] provides an alternative to these computationally expensive toy calculations.

This notebook demonstrates a reproduction of one of the key plots in the paper using `pyhf`.

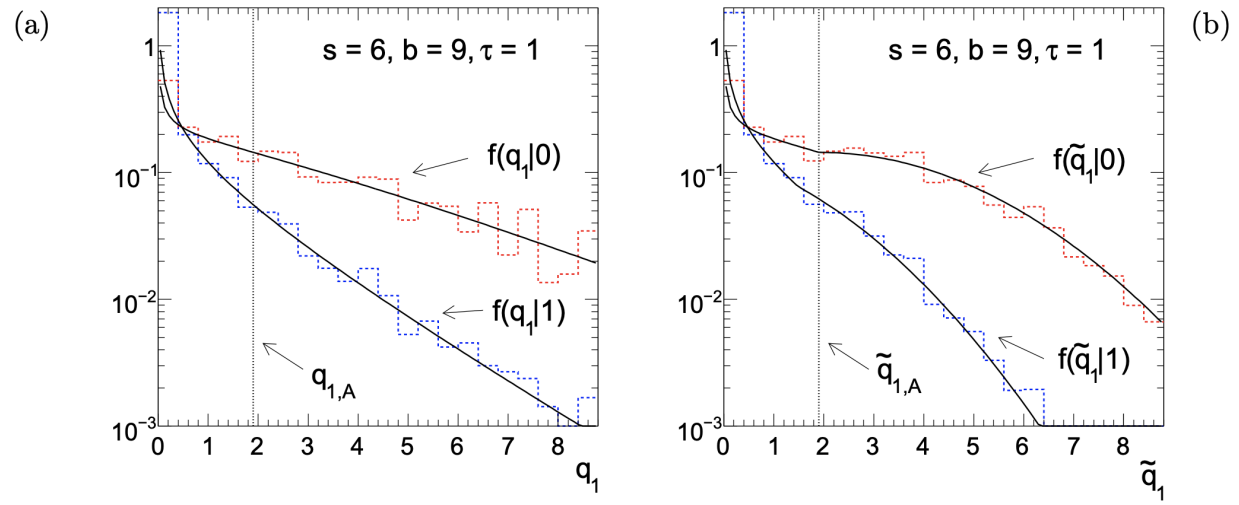


Figure 5: (a) The pdfs $f(q_1|1)$ and $f(q_1|0)$ for the counting experiment. The solid curves show the formulae from the text, and the histograms are from Monte Carlo using $s = 6$, $b = 9$, $\tau = 1$. (b) The same set of histograms with the alternative statistic $\tilde{q}_1$. The oscillatory structure evident in the histograms is a consequence of the discreteness of the data. The vertical line indicates the Asimov value of the test statistic corresponding to $\mu' = 0$.

6.7.1 Counting Experiment

Consider a counting experiment where one observes n events, following a Poisson distribution with expectation value

$$E[n] = \mu s + b$$

with s expected signal events and b expected background events, and signal strength parameter μ. Follow up in the paper to understand more of the math behind this as the notation is being introduced here. What we will show is the distribution of the (alternative) test statistic q_1 ($\tilde{q}_1$) calculated under the assumption of the nominal signal model ($\mu = 1$) for data corresponding to the strength parameter of the background-only ($\mu' = 0$) and signal+background ($\mu' = 1$) model hypotheses. For the rest of this notebook, we'll refer to the background-like model $\mu' = 0$ and the signal-like model $\mu' = 1$.

The first thing we will do is set up the `pyhf` model with $s = 6$ signal events and $b = 9$ background events (adding a Poisson uncertainty on the background).

[3]:
```
signal = 6
background = 9
background_uncertainty = 3
model = pyhf.simplemodels.uncorrelated_background(
    [signal], [background], [background_uncertainty]
)
print(f"Channels: {model.config.channels}")
print(f"Samples: {model.config.samples}")
print(f"Parameters: {model.config.parameters}")
```

```
Channels: ['singlechannel']
Samples: ['background', 'signal']
Parameters: ['mu', 'uncorr_bkguncrt']
```

This is a single channel with two samples: `signal` and `background`. `mu` here is the signal strength. Next, we need to define the background-like and signal-like p.d.f.s.

[4]:
```
# mu' = 0: background-like
pars_bkg = model.config.suggested_init()
pars_bkg[model.config.poi_index] = 0.0
print(f"Background parameters: {list(zip(model.config.parameters, pars_bkg))}")

# mu' = 1: signal-like
pars_sig = model.config.suggested_init()
pars_sig[model.config.poi_index] = 1.0
print(f"Signal parameters: {list(zip(model.config.parameters, pars_sig))}")

# make the pdfs
pdf_bkg = model.make_pdf(pyhf.tensorlib.astensor(pars_bkg))
pdf_sig = model.make_pdf(pyhf.tensorlib.astensor(pars_sig))
```

```
Background parameters: [('mu', 0.0), ('uncorr_bkguncrt', 1.0)]
Signal parameters: [('mu', 1.0), ('uncorr_bkguncrt', 1.0)]
```

Notice that the parameter of interest, μ' is set to zero for background-like models and to one for signal-like models.

Running Toys by Hand

Now that we've built our pdfs, we can go ahead and randomly (Monte Carlo) sample them. In this case, we want to "run 10,000 pseudo-experiments" (or "throw toys" as particle physicists would say). This means to draw $n = 10000$ samples from the models:

[5]:
```
# note: pdf.sample takes in a "shape" N=(10000,) given the number of samples
n_samples = 10000

# mu' = 0
mc_bkg = pdf_bkg.sample((n_samples,))
# mu' = 1
mc_sig = pdf_sig.sample((n_samples,))

print(mc_bkg.shape)
print(mc_sig.shape)
```

```
(10000, 2)
(10000, 2)
```

You'll notice that the shape for `mc_bkg` and `mc_sig` is not the input shape we passed in `(10000,)` but rather `(10000, 2)`! Why is that? The HistFactory model is a product of many separate pdfs: Poissons representing the main model, and Gaussians representing the auxiliary measurements. In `pyhf`, this is represented under the hood as a `Simultaneous <https://scikit-hep.org/pyhf/_generated/pyhf.probability.Simultaneous.html>`__ pdf of the main model and the auxiliary model — hence the second dimension.

We can now calculate the test statistic distributions for $\tilde{q}_1$ given the background-like and signal-like models. This inference step (running the toys) will take some time:

[6]:
```
init_pars = model.config.suggested_init()
par_bounds = model.config.suggested_bounds()
fixed_params = model.config.suggested_fixed()

qtilde_bkg = pyhf.tensorlib.astensor(
    [
        pyhf.infer.test_statistics.qmu_tilde(
            1.0, mc, model, init_pars, par_bounds, fixed_params
        )
        for mc in mc_bkg
    ]
)
qtilde_sig = pyhf.tensorlib.astensor(
    [
        pyhf.infer.test_statistics.qmu_tilde(
            1.0, mc, model, init_pars, par_bounds, fixed_params
        )
        for mc in mc_sig
    ]
)
```

Running Toys using Calculators

However, as you can see, a lot of this is somewhat cumbersome as you need to carry around two pieces of information: one for background-like and one for signal-like. Instead, `pyhf` provides a statistics calculator API that both simplifies and harmonizes some of this work for you.

This calculator API allows you to:

- compute a test statistic for the observed data
- provide distributions of that test statistic under various hypotheses

These provided distributions additionally have extra functionality to compute a p-value for the observed test statistic.

We will create a toy-based calculator and evaluate the model $(\mu = 1)$ for data simulated under background-like hypothesis $(\mu' = 0)$ and under the signal-like hypothesis $(\mu' = 1)$. This will compute $\tilde{q}_1$ for both values of μ'.

[7]:
```
toy_calculator_qtilde = pyhf.infer.utils.create_calculator(
    "toybased",
    model.expected_data(pars_sig),
    model,
    ntoys=n_samples,
```

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```
    test_stat="qtilde",
)
qtilde_sig, qtilde_bkg = toy_calculator_qtilde.distributions(1.0)
```

To compute q_1, we just need to alleviate the bounds to allow for μ (the parameter of interest) to go below zero. Right now, it is set to the default for `normfactor` which is `[0,10]` — a very sensible default most of the time. But if the $\hat{\mu}$ (the maximum likelihood estimator for μ) for our model is truly negative, then we should allow the fit to scan negative μ values as well.

[8]:
```
qmu_bounds = model.config.suggested_bounds()
print(f"Old bounds: {qmu_bounds}")
qmu_bounds[model.config.poi_index] = (-10, 10)
print(f"New bounds: {qmu_bounds}")
```

```
Old bounds: [(0, 10), (1e-10, 10.0)]
New bounds: [(-10, 10), (1e-10, 10.0)]
```

And then run the toys

[9]:
```
toy_calculator_qmu = pyhf.infer.utils.create_calculator(
    "toybased",
    model.expected_data(model.config.suggested_init()),
    model,
    par_bounds=qmu_bounds,
    ntoys=n_samples,
    test_stat="q",
)
qmu_sig, qmu_bkg = toy_calculator_qmu.distributions(1.0)
```

```
Signal-like:   0%|          | 0/10000 [00:00<?, ?toy/s]/Users/jovyan/pyhf/src/pyhf/
↪tensor/numpy_backend.py:253: RuntimeWarning: invalid value encountered in log
  return n * np.log(lam) - lam - gammaln(n + 1.0)
```

Now that we've ran the toys, we can make the key plots .

[10]:
```
fig, axes = plt.subplots(nrows=1, ncols=2)
for ax in axes:
    ax.set_xticks(np.arange(0, 10))
ax0, ax1 = axes.flatten()

bins = np.linspace(0, 10, 26)

ax0.hist(
    qmu_sig.samples,
    bins=bins,
    histtype="step",
    density=True,
    label="$f(q_1|1)$ signal-like",
    linewidth=2,
)
ax0.hist(
```

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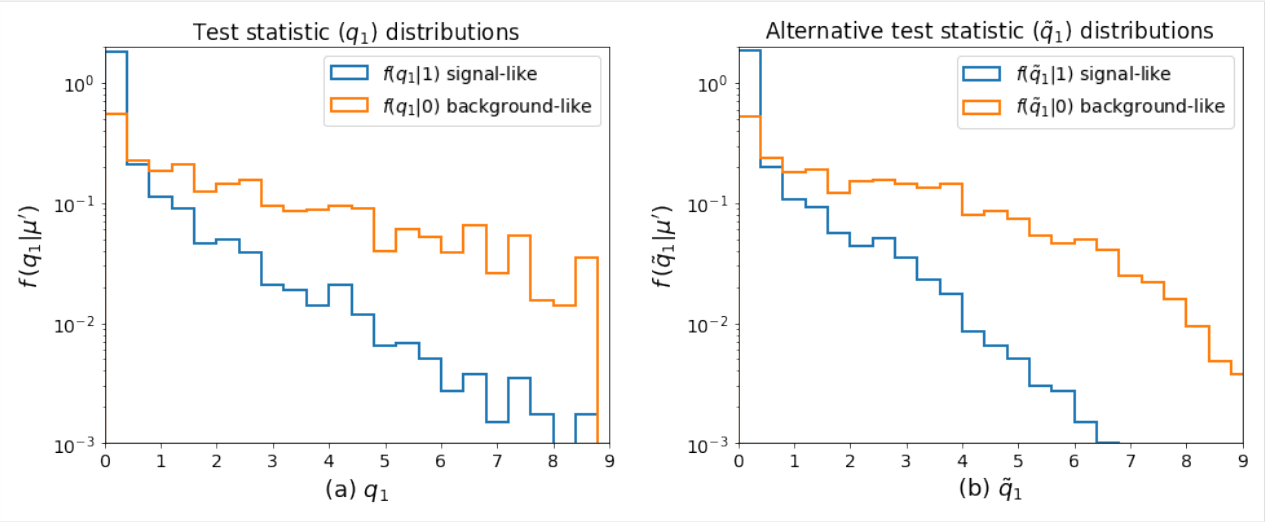
```
    qmu_bkg.samples,
    bins=bins,
    histtype="step",
    density=True,
    label="$f(q_1|0)$ background-like",
    linewidth=2,
)
ax0.set_xlabel(r"(a) $q_1$", fontsize=18)
ax0.set_ylabel(r"$f\,(q_1|\mu')$", fontsize=18)
ax0.set_title(r"Test statistic $(q_1)$ distributions")
ax0.legend()

ax1.hist(
    qtilde_sig.samples,
    bins=bins,
    histtype="step",
    density=True,
    label=r"$f(\tilde{q}_1|1)$ signal-like",
    linewidth=2,
)
ax1.hist(
    qtilde_bkg.samples,
    bins=bins,
    histtype="step",
    density=True,
    label=r"$f(\tilde{q}_1|0)$ background-like",
    linewidth=2,
)
ax1.set_xlabel(r"(b) $\tilde{q}_1$", fontsize=18)
ax1.set_ylabel(r"$f\,(\tilde{q}_1|\mu')$", fontsize=18)
ax1.set_title(r"Alternative test statistic $(\tilde{q}_1)$ distributions")
ax1.legend()


plt.setp(axes, xlim=(0, 9), ylim=(1e-3, 2), yscale="log")
fig.set_size_inches(14, 6)
fig.tight_layout(pad=2.0)
```



[1]:
```
from pathlib import Path

import numpy as np
import matplotlib.pyplot as plt

import pyhf
import pyhf.readxml
from pyhf.contrib.viz import brazil

import base64
from IPython.core.display import display, HTML
from ipywidgets import interact, fixed
```

6.8 Binned HEP Statistical Analysis in Python

6.8.1 HistFactory

HistFactory is a popular framework to analyze binned event data and commonly used in High Energy Physics. At its core it is a template for building a statistical model from individual binned distribution ('Histograms') and variations on them ('Systematics') that represent auxiliary measurements (for example an energy scale of the detector which affects the shape of a distribution)

6.8.2 pyhf

`pyhf` is a work-in-progress standalone implementation of the HistFactory p.d.f. template and an implementation of the test statistics and asymptotic formulae described in the paper by Cowan, Cranmer, Gross, Vitells: *Asymptotic formulae for likelihood-based tests of new physics* [arXiv:1007.1727].

Models can be defined using JSON specification, but existing models based on the XML + ROOT file scheme are readable as well.

6.8.3 The Demo

The input data for the statistical analysis was built generated using the containerized workflow engine yadage (see demo from KubeCon 2018 [youtube]). Similarly to Binder this utilizes modern container technology for reproducible science. Below you see the execution graph leading up to the model input data at the bottom.

[2]:
```
anim = base64.b64encode(open('workflow.gif', 'rb').read()).decode('ascii')
HTML(f'<img src="{anim}">')
```

[2]:
```
<IPython.core.display.HTML object>
```

6.8.4 Read in the Model from XML and ROOT

The ROOT files are read using scikit-hep's uproot module.

[3]:
```
spec = pyhf.readxml.parse('meas.xml', Path.cwd())
workspace = pyhf.Workspace(spec)
```

From the `meas.xml` spec, we construct a probability density function (p.d.f). As the model includes systematics, it will be a simultaneous joint p.d.f. of the main model (poisson) and constraint model. The latter is defined by the implied "auxiliary measurements".

[4]:
```
pdf = workspace.model(measurement_name='meas')
data = workspace.data(pdf)
# what is the measurement?
workspace.get_measurement(measurement_name='meas')
```

[4]:
```
{'name': 'meas',
 'config': {'poi': 'SigXsecOverSM',
  'parameters': [{'name': 'lumi',
    'auxdata': [1.0],
    'bounds': [[0.5, 1.5]],
    'inits': [1.0],
    'sigmas': [0.1]},
   {'name': 'SigXsecOverSM',
    'bounds': [[0.0, 3.0]],
    'inits': [1.0],
    'fixed': False}]}}
```

The p.d.f is build from one data-drived "qcd" (or multijet) estimate and two Monte Carlo-based background samples and is parametrized by five parameters: One parameter of interest `SigXsecOverSM` and four *nuisance parameters* that affect the shape of the two Monte Carlo background estimates (both weight-only and shape systematics)

[5]:
```
print(f'Samples:\n {pdf.config.samples}')
print(f'Parameters:\n {pdf.config.parameters}')
```

```
Samples:
 ['mc1', 'mc2', 'qcd', 'signal']
Parameters:
 ['SigXsecOverSM', 'lumi', 'mc1_shape_conv', 'mc1_weight_var1', 'mc2_shape_conv', 'mc2_
↪weight_var1']
```

[6]:
```
par_name_dict = {k: v["slice"].start for k, v in pdf.config.par_map.items()}
all_par_settings = {
```

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```
    n[0]: tuple(m)
    for n, m in zip(
        sorted(reversed(list(par_name_dict.items())), key=lambda x: x[1]),
        pdf.config.suggested_bounds(),
    )
}
default_par_settings = {n[0]: sum(tuple(m)) / 2.0 for n, m in all_par_settings.items()}
```

[7]:
```
def get_mc_counts(pars):
    deltas, factors = pdf._modifications(pars)
    allsum = pyhf.tensorlib.concatenate(
        deltas + [pyhf.tensorlib.astensor(pdf.nominal_rates)]
    )
    nom_plus_delta = pyhf.tensorlib.sum(allsum, axis=0)
    nom_plus_delta = pyhf.tensorlib.reshape(
        nom_plus_delta, (1,) + pyhf.tensorlib.shape(nom_plus_delta)
    )
    allfac = pyhf.tensorlib.concatenate(factors + [nom_plus_delta])
    return pyhf.tensorlib.product(allfac, axis=0)


animate_plot_pieces = None


def init_plot(fig, ax, par_settings):
    global animate_plot_pieces

    nbins = sum(list(pdf.config.channel_nbins.values()))
    x = np.arange(nbins)
    data = np.zeros(nbins)
    items = []
    for i in [3, 2, 1, 0]:
        items.append(ax.bar(x, data, 1, alpha=1.0))
    animate_plot_pieces = (
        items,
        ax.scatter(
            x, workspace.data(pdf, include_auxdata=False), c="k", alpha=1.0, zorder=99
        ),
    )


def animate(ax=None, fig=None, **par_settings):
    global animate_plot_pieces
    items, obs = animate_plot_pieces
    pars = pyhf.tensorlib.astensor(pdf.config.suggested_init())
    for k, v in par_settings.items():
        pars[par_name_dict[k]] = v

    mc_counts = get_mc_counts(pars)
    rectangle_collection = zip(*map(lambda x: x.patches, items))

    for rectangles, binvalues in zip(rectangle_collection, mc_counts[:, 0].T):
```

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```
        offset = 0
        for sample_index in [3, 2, 1, 0]:
            rect = rectangles[sample_index]
            binvalue = binvalues[sample_index]
            rect.set_y(offset)
            rect.set_height(binvalue)
            offset += rect.get_height()

    fig.canvas.draw()


def plot(ax=None, order=[3, 2, 1, 0], **par_settings):
    pars = pyhf.tensorlib.astensor(pdf.config.suggested_init())
    for k, v in par_settings.items():
        pars[par_name_dict[k]] = v

    mc_counts = get_mc_counts(pars)
    bottom = None
    # nb: bar_data[0] because evaluating only one parset
    for i, sample_index in enumerate(order):
        data = mc_counts[sample_index][0]
        x = np.arange(len(data))
        ax.bar(x, data, 1, bottom=bottom, alpha=1.0)
        bottom = data if i == 0 else bottom + data
    ax.scatter(
        x, workspace.data(pdf, include_auxdata=False), c="k", alpha=1.0, zorder=99
    )
```

6.8.5 Interactive Exploration of a HistFactory Model

One advantage of a pure-python implementation of Histfactory is the ability to explore the pdf interactively within the setting of a notebook. Try moving the sliders and oberserve the effect on the samples. For example changing the parameter of interest `SigXsecOverSM` (or μ) controls the overall normalization of the (BSM) signal sample (μ=0 for background-only and μ=1 for the nominal signal-plus-background hypothesis)

[8]:
```
%matplotlib notebook
fig, ax = plt.subplots(1, 1)
fig.set_size_inches(10, 5)
ax.set_ylim(0, 1.5 * np.max(workspace.data(pdf, include_auxdata=False)))

init_plot(fig, ax, default_par_settings)
interact(animate, fig=fixed(fig), ax=fixed(ax), **all_par_settings);
```

```
<IPython.core.display.Javascript object>
```

```
<IPython.core.display.HTML object>
```

```
interactive(children=(FloatSlider(value=1.0, description='lumi', max=1.5, min=0.5),␣
↪FloatSlider(value=1.5, des...
```

[9]:
```
nominal = pdf.config.suggested_init()
background_only = pdf.config.suggested_init()
```

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```
background_only[pdf.config.poi_index] = 0.0
best_fit = pyhf.infer.mle.fit(data, pdf)
```

```
/srv/conda/envs/notebook/lib/python3.7/site-packages/pyhf/tensor/numpy_backend.py:334:␣
↪RuntimeWarning: invalid value encountered in log
  return n * np.log(lam) - lam - gammaln(n + 1.0)
```

6.8.6 Fitting

We can now fit the statistical model to the observed data. The best fit of the signal strength is close to the background-only hypothesis.

[10]:
```
fig, (ax1, ax2, ax3) = plt.subplots(1, 3, sharey=True, sharex=True)
fig.set_size_inches(18, 4)
ax1.set_ylim(0, 1.5 * np.max(workspace.data(pdf, include_auxdata=False)))
ax1.set_title('nominal signal + background μ = 1')
plot(ax=ax1, **{k: nominal[v] for k, v in par_name_dict.items()})

ax2.set_title('nominal background-only μ = 0')
plot(ax=ax2, **{k: background_only[v] for k, v in par_name_dict.items()})

ax3.set_title(f'best fit μ = {best_fit[pdf.config.poi_index]:.3g}')
plot(ax=ax3, **{k: best_fit[v] for k, v in par_name_dict.items()});
```

```
<IPython.core.display.Javascript object>
```

```
<IPython.core.display.HTML object>
```

6.8.7 Interval Estimation (Computing Upper Limits on μ)

A common task in the statistical evaluation of High Energy Physics data analyses is the estimation of confidence intervals of parameters of interest. The general strategy is to perform a series of hypothesis tests and then *invert* the tests in order to obtain an interval with the correct coverage properties.

A common figure of merit is a modified p-value, CLs. Here we compute an upper limit based on a series of CLs tests.

[11]:
```
mu_tests = np.linspace(0, 1, 16)
obs_limit, exp_limits, (poi_tests, tests) = pyhf.infer.intervals.upperlimit(
    data, pdf, mu_tests, level=0.05, return_results=True
)
```

[12]:
```
fig, ax = plt.subplots()
fig.set_size_inches(7, 5)

ax.set_title("Hypothesis Tests")
artists = brazil.plot_results(mu_tests, tests, test_size=0.05, ax=ax)
```

```
<IPython.core.display.Javascript object>
```

```
<IPython.core.display.HTML object>
```

[13]:
```
print(f"Observed upper limit: {obs_limit:.3f}\n")
for i, n_sigma in enumerate(np.arange(-2, 3)):
    print(
        "Expected Limit{}: {:.3f}".format(
            "" if n_sigma == 0 else f"({n_sigma} )", exp_limits[i]
        )
    )
```

```
Observed upper limit: 0.630

Expected Limit(-2 ): 0.297
Expected Limit(-1 ): 0.393
Expected Limit: 0.546
Expected Limit(1 ): 0.762
Expected Limit(2 ): 1.000
```

CHAPTER

SEVEN

OUTREACH

We are always interested in talking about `pyhf`. See the abstract and a list of previously given presentations and feel free to invite us to your next conference/workshop/meeting!

7.1 Abstract

> The HistFactory p.d.f. template [CERN-OPEN-2012-016] is per-se independent of its implementation in ROOT and it is useful to be able to run statistical analysis outside of the ROOT, RooFit, RooStats framework. pyhf is a pure-python implementation of that statistical model for multi-bin histogram-based analysis and its interval estimation is based on the asymptotic formulas of "Asymptotic formulae for likelihood-based tests of new physics" [1007.1727]. pyhf supports modern computational graph libraries such as TensorFlow, PyTorch, and JAX in order to make use of features such as auto-differentiation and GPU acceleration.

```
The HistFactory p.d.f. template
\href{https://cds.cern.ch/record/1456844}{[CERN-OPEN-2012-016]} is
per-se independent of its implementation in ROOT and it is useful to be
able to run statistical analysis outside of the ROOT, RooFit, RooStats
framework. pyhf is a pure-python implementation of that statistical
model for multi-bin histogram-based analysis and its interval
estimation is based on the asymptotic formulas of "Asymptotic formulae
for likelihood-based tests of new physics"
\href{https://arxiv.org/abs/1007.1727}{[arXiv:1007.1727]}. pyhf
supports modern computational graph libraries such as TensorFlow,
PyTorch, and JAX in order to make use of features such as
auto-differentiation and GPU acceleration.
```

7.2 Presentations

This list will be updated with talks given on `pyhf`:

- Matthew Feickert. pyhf: pure-Python implementation of HistFactory with tensors and automatic differentiation. Tools for High Energy Physics and Cosmology 2020 Workshop, Nov 2020. URL: https://indico.cern.ch/event/955391/contributions/4075505/, doi:10.5281/zenodo.4246056.
- Matthew Feickert. pyhf: a pure Python statistical fitting library with tensors and autograd. 19th Python in Science Conference (SciPy 2020), July 2020. URL: http://conference.scipy.org/proceedings/scipy2020/slides.html, doi:10.25080/Majora-342d178e-023.

- Lukas Heinrich. Likelihoods associated with statistical fits used in searches for new physics on HEPData and use of RECAST. (Internal) ATLAS Weekly Meeting, Nov 2019. URL: https://indico.cern.ch/event/864395/contributions/3642165/.
- Matthew Feickert. Likelihood preservation and statistical reproduction of searches for new physics. CHEP 2019, Nov 2019. URL: https://indico.cern.ch/event/773049/contributions/3476143/.
- Lukas Heinrich. Traditional inference with machine learning tools. 1st Pan-European Advanced School on Statistics in High Energy Physics, Oct 2019. URL: https://indico.desy.de/indico/event/22731/session/4/contribution/19.
- Giordon Stark. Likelihood Preservation and Reproduction. West Coast LHC Jamboree 2019, Oct 2019. URL: https://indico.cern.ch/event/848030/contributions/3616614/.
- Lukas Heinrich. HEP in the Cloud Computing and Open Science Era. EP-IT Data science seminar, Oct 2019. URL: https://indico.cern.ch/event/840837/.
- Matthew Feickert. pyhf: pure-Python implementation of HistFactory. PyHEP 2019 Workshop, Oct 2019. URL: https://indico.cern.ch/event/833895/contributions/3577824/.
- Giordon Stark. New techniques for use of public likelihoods for reinterpretation of search results. 27th International Conference on Supersymmetry and Unification of Fundamental Interactions (SUSY2019), May 2019. URL: https://indico.cern.ch/event/746178/contributions/3396797/.
- Lukas Heinrich. pyhf: Full Run-2 ATLAS likelihoods. (Internal) Joint Machine Learning & Statistics Fora Meeting, May 2019. URL: https://indico.cern.ch/event/817483/contributions/3412907/.
- Lukas Heinrich. Gaussian Process Shape Estimation and Systematics. (Internal) Joint Machine Learning & Statistics Fora Meeting, Dec 2018. URL: https://indico.cern.ch/event/777561/contributions/3234669/.
- Matthew Feickert, Lukas Heinrich, Giordon Stark, and Kyle Cranmer. pyhf: a pure Python implementation of HistFactory with tensors and autograd. DIANA Meeting - pyhf, October 2018. URL: https://indico.cern.ch/event/759480/.
- Matthew Feickert, Lukas Heinrich, Giordon Stark, and Kyle Cranmer. pyhf: pure-Python implementation of HistFactory models with autograd. 2018 US LHC Users Association Meeting, October 2018. URL: https://indico.fnal.gov/event/17566/session/0/contribution/99.
- Matthew Feickert, Lukas Heinrich, Giordon Stark, and Kyle Cranmer. pyhf: pure-Python implementation of HistFactory models with autograd. (Internal) 3rd ATLAS Machine Learning Workshop, October 2018. URL: https://indico.cern.ch/event/735932/contributions/3136879/.
- Matthew Feickert, Lukas Heinrich, Giordon Stark, and Kyle Cranmer. pyhf: pure-Python implementation of HistFactory models with autograd. (Internal) Joint Machine Learning & Statistics Fora Meeting, September 2018. URL: https://indico.cern.ch/event/757657/contributions/3141134/.
- Lukas Heinrich, Matthew Feickert, Giordon Stark, and Kyle Cranmer. pyhf: A standalone HistFactory Implementation. (Re)interpreting the results of new physics searches at the LHC Workshop, May 2018. URL: https://indico.cern.ch/event/702612/contributions/2958658/.

7.3 Tutorials

This list will be updated with tutorials and schools given on `pyhf`:

- Giordon Stark. ATLAS Exotics + SUSY Workshop 2020 pyhf Tutorial. ATLAS Exotics + SUSY Workshop 2020, September 2020. URL: https://pyhf.github.io/tutorial-ATLAS-SUSY-Exotics-2020/introduction.html.
- Matthew Feickert. pyhf: Accelerating analyses and preserving likelihoods. PyHEP 2020 Workshop (pyhf v0.4.4), Jul 2020. URL: https://indico.cern.ch/event/882824/contributions/3931292/.
- Lukas Heinrich. pyhf tutorial. (Internal) ATLAS Induction Day + Software Tutorial (pyhf v0.4.4), Jul 2020. URL: https://indico.cern.ch/event/892952/contributions/3853306/.
- Lukas Heinrich. Introduction to pyhf. (Internal) ATLAS Induction Day + Software Tutorial (pyhf v0.1.2), Oct 2019. URL: https://indico.cern.ch/event/831761/contributions/3484275/.

7.4 Posters

This list will be updated with posters presented on `pyhf`:

- Lukas Heinrich, Matthew Feickert, Giordon Stark, and Kyle Cranmer. pyhf: auto-differentiable binned statistical models. 19th International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2019), March 2019. URL: https://indico.cern.ch/event/708041/contributions/3272095/.
- Matthew Feickert, Lukas Heinrich, Giordon Stark, and Kyle Cranmer. pyhf: a pure Python statistical fitting library for High Energy Physics with tensors and autograd. July 2019. 18th Scientific Computing with Python Conference (SciPy 2019). URL: http://conference.scipy.org/proceedings/scipy2019/slides.html, doi:10.25080/Majora-7ddc1dd1-019.
- Matthew Feickert, Lukas Heinrich, Giordon Stark, and Kyle Cranmer. pyhf: pure Python implementation of HistFactory. November 2019. 24th International Conference on computing in High Energy & Nuclear Physics (CHEP 2019). URL: https://indico.cern.ch/event/773049/contributions/3476180/.

7.5 In the Media

This list will be updated with media publications featuring `pyhf`:

- Sabine Kraml. LHC reinterpreters think long-term. *CERN Courier Volume 61, Number 3, May/June 2021*, April 2021. https://cds.cern.ch/record/2765233. URL: https://cerncourier.com/a/lhc-reinterpreters-think-long-term/.
- Stephanie Melchor. ATLAS releases 'full orchestra' of analysis instruments. *Symmetry Magazine*, January 2021. URL: https://www.symmetrymagazine.org/article/atlas-releases-full-orchestra-of-analysis-instruments.
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CHAPTER

EIGHT

INSTALLATION

To install, we suggest first setting up a virtual environment

```
# Python3
python3 -m venv pyhf
```

and activating it

```
source pyhf/bin/activate
```

8.1 Install latest stable release from PyPI...

8.1.1 ... with NumPy backend

```
python -m pip install pyhf
```

8.1.2 ... with TensorFlow backend

```
python -m pip install pyhf[tensorflow]
```

8.1.3 ... with PyTorch backend

```
python -m pip install pyhf[torch]
```

8.1.4 ... with JAX backend

```
python -m pip install pyhf[jax]
```

8.1.5 ... with all backends

```
python -m pip install pyhf[backends]
```

8.1.6 ... with xml import/export functionality

```
python -m pip install pyhf[xmlio]
```

8.2 Install latest development version from GitHub...

8.2.1 ... with NumPy backend

```
python -m pip install --upgrade "git+https://github.com/scikit-hep/pyhf.git#egg=pyhf"
```

8.2.2 ... with TensorFlow backend

```
python -m pip install --upgrade "git+https://github.com/scikit-hep/pyhf.git
↪#egg=pyhf[tensorflow]"
```

8.2.3 ... with PyTorch backend

```
python -m pip install --upgrade "git+https://github.com/scikit-hep/pyhf.git
↪#egg=pyhf[torch]"
```

8.2.4 ... with JAX backend

```
python -m pip install --upgrade "git+https://github.com/scikit-hep/pyhf.git#egg=pyhf[jax]
↪"
```

8.2.5 ... with all backends

```
python -m pip install --upgrade "git+https://github.com/scikit-hep/pyhf.git
↪#egg=pyhf[backends]"
```

8.2.6 ... with xml import/export functionality

```
python -m pip install --upgrade "git+https://github.com/scikit-hep/pyhf.git
↪#egg=pyhf[xmlio]"
```

8.3 Updating pyhf

Rerun the installation command. As the upgrade flag (`-U`, `--upgrade`) is used then the libraries will be updated.

CHAPTER

NINE

DEVELOPING

9.1 Developer Environment

To develop, we suggest using virtual environments together with `pip` or using pipenv. Once the environment is activated, clone the repo from GitHub

```
git clone https://github.com/scikit-hep/pyhf.git
```

and install all necessary packages for development

```
python -m pip install --upgrade --editable .[complete]
```

Then setup the Git pre-commit hook for Black by running

```
pre-commit install
```

as the `rev` gets updated through time to track changes of different hooks, simply run

```
pre-commit autoupdate
```

to have pre-commit install the new version.

9.2 Testing

9.2.1 Data Files

A function-scoped fixture called `datadir` exists for a given test module which will automatically copy files from the associated test modules data directory into a temporary directory for the given test execution. That is, for example, if a test was defined in `test_schema.py`, then data files located in `test_schema/` will be copied to a temporary directory whose path is made available by the `datadir` fixture. Therefore, one can do:

```
def test_patchset(datadir):
    data_file = open(datadir.join("test.txt"))
    ...
```

which will load the copy of `text.txt` in the temporary directory. This also works for parameterizations as this will effectively sandbox the file modifications made.

9.2.2 TestPyPI

pyhf tests packaging and distributing by publishing each commit to master to TestPyPI. In addition, installation of the latest test release from TestPyPI can be tested by first installing pyhf normally, to ensure all dependencies are installed from PyPI, and then upgrading pyhf to a dev release from TestPyPI

```
python -m pip install pyhf
python -m pip install --upgrade --extra-index-url https://test.pypi.org/simple/ --pre␣
↪pyhf
```

Note: This adds TestPyPI as an additional package index to search when installing. PyPI will still be the default package index pip will attempt to install from for all dependencies, but if a package has a release on TestPyPI that is a more recent release then the package will be installed from TestPyPI instead. Note that dev releases are considered pre-releases, so 0.1.2 is a "newer" release than 0.1.2.dev3.

9.3 Publishing

Publishing to PyPI and TestPyPI is automated through the PyPA's PyPI publish GitHub Action and the pyhf Tag Creator GitHub Actions workflow. A release can be created from any PR created by a core developer by adding a bumpversion tag to it that corresponds to the release type: major, minor, patch. Once the PR is tagged with the label, the GitHub Actions bot will post a comment with information on the actions it will take once the PR is merged. When the PR has been reviewed, approved, and merged, the Tag Creator workflow will automatically create a new release with bump2version and then deploy the release to PyPI.

9.4 Context Files and Archive Metadata

The .zenodo.json and codemeta.json files have the version number automatically updated through bump2version, though their additional metadata should be checked periodically by the dev team (probably every release). The codemeta.json file can be generated automatically **from a PyPI install** of pyhf using codemetapy

```
codemetapy --no-extras pyhf > codemeta.json
```

though the author metadata will still need to be checked and revised by hand. The .zenodo.json is currently generated by hand, so it is worth using codemeta.json as a guide to edit it.

9.5 Release Checklist

As part of the release process a checklist is required to be completed to make sure steps aren't missed. There is a GitHub Issue template for this that the developer in charge of the release should step through and update if needed.

CHAPTER

TEN

FAQ

Frequently Asked Questions about `pyhf` and its use.

10.1 Questions

10.1.1 Where can I ask questions about `pyhf` use?

If you have a question about the use of `pyhf` not covered in the documentation, please ask a question on the GitHub Discussions.

If you believe you have found a bug in `pyhf`, please report it in the GitHub Issues.

10.1.2 How can I get updates on `pyhf`?

If you're interested in getting updates from the `pyhf` dev team and release announcements you can join the `pyhf-announcements` mailing list.

10.1.3 Is it possible to set the backend from the CLI?

Yes. Use the `--backend` option for `pyhf cls` to specify a tensor backend. The default backend is NumPy. For more information see `pyhf cls --help`.

10.1.4 Does `pyhf` support Python 2?

No. Like the rest of the Python community, as of January 2020 the latest releases of `pyhf` no longer support Python 2. The last release of `pyhf` that was compatible with Python 2.7 is v0.3.4, which can be installed with

```
python -m pip install pyhf~=0.3
```

10.1.5 I only have access to Python 2. How can I use pyhf?

It is recommended that pyhf is used as a standalone step in any analysis, and its environment need not be the same as the rest of the analysis. As Python 2 is not supported it is suggested that you setup a Python 3 runtime on whatever machine you're using. If you're using a cluster, talk with your system administrators to get their help in doing so. If you are unable to get a Python 3 runtime, versioned Docker images of pyhf are distributed through Docker Hub.

Once you have Python 3 installed, see the *Installation* page to get started.

10.1.6 I validated my workspace by comparing pyhf and HistFactory, and while the expected CLs matches, the observed CLs is different. Why is this?

Make sure you're using the right test statistic (q or $\tilde{q}$) in both situations. In HistFactory, the asymptotics calculator, for example, will do something more involved for the observed CLs if you choose a different test statistic.

10.1.7 I ran validation to compare HistFitter and pyhf, but they don't match exactly. Why not?

pyhf is validated against HistFactory. HistFitter makes some particular implementation choices that pyhf doesn't reproduce. Instead of trying to compare pyhf and HistFitter you should try to validate them both against HistFactory.

10.1.8 How is pyhf typeset?

As you may have guessed from this page, pyhf is typeset in all lowercase. This is largely historical, as the core developers had just always typed it that way and it seemed a bit too short of a library name to write as PyHF. When typesetting in LaTeX the developers recommend introducing the command

```
\newcommand{\pyhf}{\texttt{pyhf}}
```

If the journal you are publishing in requires you to use textsc for software names it is okay to instead use

```
\newcommand{\pyhf}{\textsc{pyhf}}
```

10.1.9 Why use Python?

As of the late 2010's Python is widely considered the lingua franca of machine learning libraries, and is sufficiently high-level and expressive for physicists of various computational skill backgrounds to use. Using Python as the language for development allows for the distribution of the software — as both source files and binary distributions — through the Python Package Index (PyPI) and Conda-forge, which significantly lowers the barrier for use as compared to C++. Additionally, a 2017 DIANA/HEP study [faq-1] demonstrated the graph structure and automatic differentiation abilities of machine learning frameworks allowed them to be quite effective tools for statistical fits. As the frameworks considered in this study (TensorFlow, PyTorch, MXNet) all provided low-level Python APIs to the libraries this made Python an obvious choice for a common high-level control language. Given all these considerations, Python was chosen as the development language.

10.1.10 How did pyhf get started?

In 2017 Lukas Heinrich was discussing with colleauge Holger Schulz how it would be convienent to share and produce statistical results from LHC experiements if they were able to be created with tools that didn't require the large C++ dependencies and tooling expertise as . Around the same time that Lukas began thinking on these ideas, Matthew Feickert was working on a DIANA/HEP fellowship with Kyle Cranmer (co-author of) to study if the graph structure and automatic differentiation abilities of machine learning frameworks would allow them to be effective tools for statistical fits. Lukas would give helpful friendly advice on Matthew's project and one night[1] over dinner in CERN's R1 cafeteria the two were discussing the idea of implementing in Python using machine learning libraries to drive the computation. Continuing the discussion in Lukas's office, Lukas showed Matthew that the core statistical machinery could be implemented rather succinctly, and that night proceeded to do so and dubbed the project pyhf.

Matthew joined him on the project to begin development and by April 2018 Giordon Stark had learned about the project and began making contributions, quickly becoming the third core developer. The first physics paper to use pyhf followed closely in October 2018 [faq-2], making Lukas and Holger's original conversations a reality. pyhf was founded on the ideas of open contributions and community software and continues in that mission today as a Scikit-HEP project, with an open invitation for community contributions and new developers.

10.2 Troubleshooting

- `import torch` or `import pyhf` causes a `Segmentation fault (core dumped)`

  This is may be the result of a conflict with the NVIDIA drivers that you have installed on your machine. Try uninstalling and completely removing all of them from your machine

  ```
  # On Ubuntu/Debian
  sudo apt-get purge nvidia*
  ```

  and then installing the latest versions.

10.2.1 Footnotes

10.2.2 Bibliography

[1] 24 January, 2018

CHAPTER

ELEVEN

TRANSLATIONS

One key goal of pyhf is to provide seamless translations between other statistical frameworks and pyhf. This page details the various ways to translate from a tool you might already be using as part of an existing analysis to pyhf. Many of these solutions involve extracting out the HistFactory workspace and then running pyhf xml2json which provides a single JSON workspace that can be loaded directly into pyhf.

11.1 HistFitter

In order to go from HistFitter to pyhf, the first step is to extract out the HistFactory workspaces. Assuming you have an existing configuration file, config.py, you likely run an exclusion fit like so:

```
HistFitter.py -f -D "before,after,corrMatrix" -F excl config.py
```

The name of output workspace files depends on four parameters you define in your config.py:

- analysisName is from configMgr.analysisName
- prefix is defined in configMgr.addFitConfig({prefix})
- measurementName is the first measurement you define via fitConfig.addMeasurement(name={measurementName},...)
- channelName are the names of channels you define via fitConfig.addChannel("cuts", [{channelName}], ...)
- cachePath is where HistFitter stores the cached histograms, defined by configMgr.histCacheFile which defaults to data/{analysisName}.root

To dump the HistFactory workspace, you will modify the above to skip the fit -f and plotting -D so you end up with

```
HistFitter.py -wx -F excl config.py
```

The -w flag tells HistFitter to (re)create the HistFactory workspace stored in results/{analysisName}/{prefix}_combined_{measurementName}.root. The -x flag tells HistFitter to dump the XML files into config/{analysisName}/, with the top-level file being {prefix}.xml and all other files being {prefix}_{channelName}_cuts.xml.

Typically, prefix = 'FitConfig' and measurementName = 'NormalMeasurement'. For example, if the following exists in your config.py

```
from configManager import configMgr

# ...
configMgr.analysisName = "3b_tag21.2.27-1_RW_ExpSyst_36100_multibin_bkg"
```

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```
configMgr.histCacheFile = f"cache/{configMgr.analysisName:s}.root"
# ...
fitConfig = configMgr.addFitConfig("Excl")
# ...
channel = fitConfig.addChannel("cuts", ["SR_0L"], 1, 0.5, 1.5)
# ...
meas1 = fitConfig.addMeasurement(name="DefaultMeasurement", lumi=1.0, lumiErr=0.029)
meas1.addPOI("mu_SIG1")
# ...
meas2 = fitConfig.addMeasurement(name="DefaultMeasurement", lumi=1.0, lumiErr=0.029)
meas2.addPOI("mu_SIG2")
```

Then, you expect the following files to be made:

- `config/3b_tag21.2.27-1_RW_ExpSyst_36100_multibin_bkg/Excl.xml`
- `config/3b_tag21.2.27-1_RW_ExpSyst_36100_multibin_bkg/Excl_SR_0L_cuts.xml`
- `cache/3b_tag21.2.27-1_RW_ExpSyst_36100_multibin_bkg.root`
- `results/3b_tag21.2.27-1_RW_ExpSyst_36100_multibin_bkg/Excl_combined_DefaultMeasurement.root`

These are all the files you need in order to use pyhf xml2json. At this point, you could run

```
pyhf xml2json config/3b_tag21.2.27-1_RW_ExpSyst_36100_multibin_bkg/Excl.xml
```

which will read all of the XML files and load the histogram data from the histogram cache.

The `HistFactory` workspace in `results/` contains all of the information necessary to rebuild the XML files again. For debugging purposes, the `pyhf` developers will often ask for your workspace file, which means `results/3b_tag21.2.27-1_RW_ExpSyst_36100_multibin_bkg/Excl_combined_DefaultMeasurement.root`. If you want to generate the XML, you can open this file in `ROOT` and run `DefaultMeasurement->PrintXML()` which puts all of the XML files into the current directory you are in.

11.2 TRExFitter

Note: For more details on this section, please refer to the ATLAS-internal TRExFitter documentation.

In order to go from `TRExFitter` to `pyhf`, the good news is that the `RooWorkspace` files (`XML` and `ROOT`) are already made for you. For a given configuration which looks like

```
Job: "pyhf_example"
Label: "..."
```

You can expect some files to be made after the `n/h` and `w` steps:

- `pyhf_example/RooStats/pyhf_example.xml`
- `pyhf_example/RooStats/pyhf_example_Signal_region.xml`
- `pyhf_example/Histograms/pyhf_example_Signal_region_histos.root`

These are all the files you need in order to use pyhf xml2json. At this point, you could run

```
pyhf xml2json pyhf_example/RooStats/pyhf_example.xml
```

which will read all of the XML files and load the histogram data from the histogram cache.

Warning: There are a few caveats one needs to be aware of with this conversion:

- Uncorrelated shape systematics cannot be pruned, see Issue #662.
- Custom expressions for normalization factors cannot be used, see Issue #850.

CHAPTER

TWELVE

COMMAND LINE API

12.1 pyhf

Top-level CLI entrypoint.

```
pyhf [OPTIONS] COMMAND [ARGS]...
```

CHAPTER

THIRTEEN

PYTHON API

13.1 Top-Level

tensorlib	NumPy backend for pyhf
optimizer	Optimizer that uses scipy.optimize.minimize().
get_backend	Get the current backend and the associated optimizer
set_backend	Set the backend and the associated optimizer
readxml	
writexml	
compat	Compatibility functions for translating between ROOT and pyhf

13.1.1 pyhf.tensorlib

pyhf.**tensorlib = <pyhf.tensor.numpy_backend.numpy_backend object>**
NumPy backend for pyhf

13.1.2 pyhf.optimizer

pyhf.**optimizer = <pyhf.optimize.scipy_optimizer object>**
Optimizer that uses scipy.optimize.minimize().

13.1.3 pyhf.get_backend

pyhf.**get_backend**(*default=False*)
Get the current backend and the associated optimizer

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> backend, optimizer = pyhf.get_backend()
>>> backend
<pyhf.tensor.numpy_backend.numpy_backend object at 0x...>
>>> optimizer
<pyhf.optimize.scipy_optimizer object at 0x...>
```

Parameters **default** (bool) – Return the default backend or not

Returns backend, optimizer

13.1.4 pyhf.set_backend

pyhf.**set_backend**(*backend*, *custom_optimizer=None*, *precision=None*, *default=False*)
Set the backend and the associated optimizer

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> pyhf.tensorlib.name
'tensorflow'
>>> pyhf.tensorlib.precision
'64b'
>>> pyhf.set_backend(b"pytorch", precision="32b")
>>> pyhf.tensorlib.name
'pytorch'
>>> pyhf.tensorlib.precision
'32b'
>>> pyhf.set_backend(pyhf.tensor.numpy_backend())
>>> pyhf.tensorlib.name
'numpy'
>>> pyhf.tensorlib.precision
'64b'
```

Parameters

- **backend** (str or *pyhf.tensor* backend) – One of the supported pyhf backends: NumPy, TensorFlow, PyTorch, and JAX
- **custom_optimizer** (*pyhf.optimize* optimizer) – Optional custom optimizer defined by the user
- **precision** (str) – Floating point precision to use in the backend: 64b or 32b. Default is backend dependent.
- **default** (bool) – Set the backend as the default backend additionally

Returns None

13.1.5 pyhf.readxml

Description

Functions

clear_filecache()	
dedupe_parameters(parameters)	
extract_error(hist)	Determine the bin uncertainties for a histogram.
import_root_histogram(rootdir, filename, ...)	
parse(configfile, rootdir[, track_progress])	
process_channel(channelxml, rootdir[, ...])	
process_data(sample, rootdir, inputfile, ...)	
process_measurements(toplvl[, ...])	For a given XML structure, provide a parsed dictionary adhering to defs.json/#definitions/measurement.
process_sample(sample, rootdir, inputfile, ...)	

pyhf.readxml.clear_filecache

pyhf.readxml.**clear_filecache**()

pyhf.readxml.dedupe_parameters

pyhf.readxml.**dedupe_parameters**(*parameters*)

pyhf.readxml.extract_error

pyhf.readxml.**extract_error**(*hist*)

Determine the bin uncertainties for a histogram.

If *fSumw2* is not filled, then the histogram must have been filled with no weights and *.Sumw2()* was never called. The bin uncertainties are then Poisson, and so the *sqrt(entries)*.

Parameters **hist** (uproot.behaviors.TH1.TH1) – The histogram

Returns The uncertainty for each bin in the histogram

Return type list

pyhf.readxml.import_root_histogram

pyhf.readxml.**import_root_histogram**(*rootdir*, *filename*, *path*, *name*, *filecache=None*)

pyhf.readxml.parse

pyhf.readxml.**parse**(*configfile*, *rootdir*, *track_progress=False*)

pyhf.readxml.process_channel

pyhf.readxml.**process_channel**(*channelxml*, *rootdir*, *track_progress=False*)

pyhf.readxml.process_data

pyhf.readxml.**process_data**(*sample*, *rootdir*, *inputfile*, *histopath*)

pyhf.readxml.process_measurements

pyhf.readxml.**process_measurements**(*toplvl*, *other_parameter_configs=None*)

For a given XML structure, provide a parsed dictionary adhering to defs.json/#definitions/measurement.

Parameters

- **toplvl** (xml.etree.ElementTree) – The top-level XML document to parse.
- **other_parameter_configs** (list) – A list of other parameter configurations from other non-top-level XML documents to incorporate into the resulting measurement object.

Returns A measurement object.

Return type dict

pyhf.readxml.process_sample

pyhf.readxml.**process_sample**(*sample*, *rootdir*, *inputfile*, *histopath*, *channelname*, *track_progress=False*)

13.1.6 pyhf.writexml

Description

Functions

build_channel(spec, channelspec, obsspec)	
build_data(obsspec, channelname)	
build_measurement(measurementspec, modifiertypes)	Build the XML measurement specification for a given measurement adhering to defs.json/#definitions/measurement.

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Table 3 – continued from previous page

build_modifier(spec, modifierspec, ...)	
build_sample(spec, samplespec, channelname)	
indent(elem[, level])	

pyhf.writexml.build_channel

pyhf.writexml.**build_channel**(*spec*, *channelspec*, *obsspec*)

pyhf.writexml.build_data

pyhf.writexml.**build_data**(*obsspec*, *channelname*)

pyhf.writexml.build_measurement

pyhf.writexml.**build_measurement**(*measurementspec*, *modifiertypes*)

Build the XML measurement specification for a given measurement adhering to defs.json/#definitions/measurement.

Parameters

- **measurementspec** (dict) – The measurements specification from a *Workspace*.
- **modifiertypes** (dict) – A mapping from modifier name (str) to modifier type (str).

Returns The XML measurement specification.

Return type xml.etree.cElementTree.Element

pyhf.writexml.build_modifier

pyhf.writexml.**build_modifier**(*spec*, *modifierspec*, *channelname*, *samplename*, *sampledata*)

pyhf.writexml.build_sample

pyhf.writexml.**build_sample**(*spec*, *samplespec*, *channelname*)

pyhf.writexml.indent

pyhf.writexml.**indent**(*elem*, *level=0*)

13.1.7 pyhf.compat

Description

Compatibility functions for translating between ROOT and pyhf

Functions

interpret_rootname(rootname)	Interprets a ROOT-generated name as best as possible.
paramset_to_rootnames(paramset)	Generates parameter names for parameters in the set as ROOT would do.

pyhf.compat.interpret_rootname

pyhf.compat.**interpret_rootname**(*rootname*)

Interprets a ROOT-generated name as best as possible.

Possible properties of a ROOT parameter are:

- "constrained": bool representing if parameter is a member of a constrained paramset.
- "is_scalar": bool representing if parameter is a member of a scalar paramset.
- "name": The name of the param set.
- "element": The index in a non-scalar param set.

It is possible that some of the parameter names might not be determinable and will then hold the string value "n/a".

Parameters **rootname** (str) – The ROOT-generated name of the parameter.

Returns The interpreted key-value pairs.

Return type dict

Example

```
>>> import pyhf
>>> interpreted_name = pyhf.compat.interpret_rootname("gamma_foo_0")
>>> pyhf.compat.interpret_rootname("gamma_foo_0")
{'constrained': 'n/a', 'is_scalar': False, 'name': 'foo', 'element': 0}
>>> pyhf.compat.interpret_rootname("alpha_foo")
{'constrained': True, 'is_scalar': True, 'name': 'foo', 'element': 'n/a'}
>>> pyhf.compat.interpret_rootname("Lumi")
{'constrained': False, 'is_scalar': True, 'name': 'lumi', 'element': 'n/a'}
```

pyhf.compat.paramset_to_rootnames

pyhf.compat.**paramset_to_rootnames**(*paramset*)

Generates parameter names for parameters in the set as ROOT would do.

Parameters **paramset** (pyhf.paramsets.paramset) – The parameter set.

Returns The generated parameter names (for the non-scalar/scalar case) respectively.

Return type List[str] or str

Example

pyhf parameter names and then the converted names for ROOT:

- "lumi" -> "Lumi"
- unconstrained scalar parameter "foo" -> "foo"
- constrained scalar parameter "foo" -> "alpha_foo"
- non-scalar parameters "foo" -> "gamma_foo_i"

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.parameters
['mu', 'uncorr_bkguncrt']
>>> pyhf.compat.paramset_to_rootnames(model.config.param_set("mu"))
'mu'
>>> pyhf.compat.paramset_to_rootnames(model.config.param_set("uncorr_bkguncrt"))
['gamma_uncorr_bkguncrt_0', 'gamma_uncorr_bkguncrt_1']
```

13.2 Probability Distribution Functions (PDFs)

Normal	The Normal distribution with mean loc and standard deviation scale.
Poisson	The Poisson distribution with rate parameter rate.
Independent	A probability density corresponding to the joint distribution of a batch of identically distributed random variables.
Simultaneous	A probability density corresponding to the joint distribution of multiple non-identical component distributions

13.2.1 Normal

class pyhf.probability.**Normal**(*loc*, *scale*)

Bases: pyhf.probability._SimpleDistributionMixin

The Normal distribution with mean `loc` and standard deviation `scale`.

Example

```
>>> import pyhf
>>> means = pyhf.tensorlib.astensor([5, 8])
>>> stds = pyhf.tensorlib.astensor([1, 0.5])
>>> pyhf.probability.Normal(means, stds)
<pyhf.probability.Normal object at 0x...>
```

__init__(*loc*, *scale*)

Parameters

- **loc** (tensor or float) – The mean of the Normal distribution
- **scale** (tensor or float) – The standard deviation of the Normal distribution

Methods

expected_data()

The expectation value of the Normal distribution.

Example

```
>>> import pyhf
>>> means = pyhf.tensorlib.astensor([5, 8])
>>> stds = pyhf.tensorlib.astensor([1, 0.5])
>>> normals = pyhf.probability.Normal(means, stds)
>>> normals.expected_data()
array([5., 8.])
```

Returns The mean of the Normal distribution (which is the `loc`)

Return type Tensor

13.2.2 Poisson

class pyhf.probability.**Poisson**(*rate*)

Bases: pyhf.probability._SimpleDistributionMixin

The Poisson distribution with rate parameter `rate`.

Example

```
>>> import pyhf
>>> rates = pyhf.tensorlib.astensor([5, 8])
>>> pyhf.probability.Poisson(rates)
<pyhf.probability.Poisson object at 0x...>
```

__init__(*rate*)

Parameters **rate** (tensor or float) – The mean of the Poisson distribution (the expected number of events)

Methods

expected_data()
The expectation value of the Poisson distribution.

Example

```
>>> import pyhf
>>> rates = pyhf.tensorlib.astensor([5, 8])
>>> poissons = pyhf.probability.Poisson(rates)
>>> poissons.expected_data()
array([5., 8.])
```

Returns The mean of the Poisson distribution (which is the rate)

Return type Tensor

13.2.3 Independent

class pyhf.probability.**Independent**(*batched_pdf*, *batch_size=None*)
Bases: pyhf.probability._SimpleDistributionMixin

A probability density corresponding to the joint distribution of a batch of identically distributed random variables.

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> rates = pyhf.tensorlib.astensor([10.0, 10.0])
>>> poissons = pyhf.probability.Poisson(rates)
>>> independent = pyhf.probability.Independent(poissons)
>>> independent.sample()
array([10, 11])
```

__init__(*batched_pdf*, *batch_size=None*)

Parameters

- **batched_pdf** (pyhf.probability distribution) – The batch of pdfs of the same type (e.g. Poisson)
- **batch_size** (int) – The size of the batch

Methods

log_prob(*value*)

The log of the probability density function at the given value. As the distribution is a joint distribution of the same type, this is the sum of the log probabilities of each of the distributions the compose the joint.

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> rates = pyhf.tensorlib.astensor([10.0, 10.0])
>>> poissons = pyhf.probability.Poisson(rates)
>>> independent = pyhf.probability.Independent(poissons)
>>> values = pyhf.tensorlib.astensor([8.0, 9.0])
>>> independent.log_prob(values)
-4.262483801927939
>>> broadcast_value = pyhf.tensorlib.astensor([11.0])
>>> independent.log_prob(broadcast_value)
-4.347743645878765
```

Parameters **value** (tensor or float) – The value at which to evaluate the distribution

Returns The value of $\log(f\,(x|\theta))$ for $x =$value

Return type Tensor

13.2.4 Simultaneous

class pyhf.probability.**Simultaneous**(*pdfobjs*, *tensorview*, *batch_size=None*)

Bases: object

A probability density corresponding to the joint distribution of multiple non-identical component distributions

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> from pyhf.tensor.common import _TensorViewer
>>> random.seed(0)
>>> poissons = pyhf.probability.Poisson(pyhf.tensorlib.astensor([1.,100.]))
>>> normals = pyhf.probability.Normal(pyhf.tensorlib.astensor([1.,100.]), pyhf.
↪tensorlib.astensor([1.,2.]))
>>> tv = _TensorViewer([[0,2],[1,3]])
```

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```
>>> sim = pyhf.probability.Simultaneous([poissons,normals], tv)
>>> sim.sample((4,))
array([[  2.        ,   1.3130677 , 101.        ,  98.29180852],
       [  1.        ,  -1.55298982,  97.        , 101.30723719],
       [  1.        ,   1.8644362 , 118.        ,  98.51566996],
       [  0.        ,   3.26975462,  99.        ,  97.09126865]])
```

__init__(*pdfobjs*, *tensorview*, *batch_size=None*)

Construct a simultaneous pdf.

Parameters

- **pdfobjs** (Distribution) – The constituent pdf objects
- **tensorview** (_TensorViewer) – The _TensorViewer defining the data composition
- **batch_size** (int) – The size of the batch

Methods

static _joint_logpdf(*terms*, *batch_size=None*)

expected_data()

The expectation value of the probability density function.

Returns The expectation value of the distribution $\mathrm{E}\left[f(\theta)\right]$

Return type Tensor

log_prob(*value*)

The log of the probability density function at the given value.

Parameters **value** (tensor) – The observed value

Returns The value of $\log(f\left(x|\theta\right))$ for $x =$value

Return type Tensor

sample(*sample_shape=()*)

The collection of values sampled from the probability density function.

Parameters **sample_shape** (tuple) – The shape of the sample to be returned

Returns The values $x \sim f(\theta)$ where x has shape sample_shape

Return type Tensor

13.3 Making Models from PDFs

Model	The main pyhf model class.
_ModelConfig	Configuration for the *Model*.
Workspace	A JSON-serializable object that is built from an object that follows the workspace.json schema.
PatchSet	A way to store a collection of patches (*Patch*).
Patch	A way to store a patch definition as part of a patchset (*PatchSet*).

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Table 6 – continued from previous page

simplemodels.uncorrelated_background	Construct a simple single channel *Model* with a *shapesys* modifier representing an uncorrelated background uncertainty.
simplemodels.correlated_background	Construct a simple single channel *Model* with a *histosys* modifier representing a background with a fully correlated bin-by-bin uncertainty.

13.3.1 Model

class pyhf.pdf.**Model**(*spec*, *modifier_set=None*, *batch_size=None*, *validate=True*, ***config_kwargs*)

Bases: object

The main pyhf model class.

__init__(*spec*, *modifier_set=None*, *batch_size=None*, *validate=True*, ***config_kwargs*)

Construct a HistFactory Model.

Parameters

- **spec** (jsonable) – The HistFactory JSON specification
- **batch_size** (None or int) – Number of simultaneous (batched) Models to compute.
- **config_kwargs** – Possible keyword arguments for the model configuration

Returns The Model instance.

Return type model (*Model*)

Attributes

nominal_rates

Nominal value of bin rates of the main model.

Methods

_modifications(*pars*)

constraint_logpdf(*auxdata*, *pars*)

Compute the log value of the constraint pdf.

Parameters

- **auxdata** (tensor) – The auxiliary measurement data
- **pars** (tensor) – The parameter values

Returns The log density value

Return type Tensor

expected_actualdata(*pars*)

Compute the expected value of the main model.

Parameters **pars** (tensor) – The parameter values

Returns The expected data of the main model (no auxiliary data)

Return type Tensor

expected_auxdata(*pars*)
Compute the expected value of the auxiliary measurements.

Parameters **pars** (tensor) – The parameter values

Returns The expected data of the auxiliary pdf

Return type Tensor

expected_data(*pars*, *include_auxdata=True*)
Compute the expected value of the main model

Parameters **pars** (tensor) – The parameter values

Returns The expected data of the main and auxiliary model

Return type Tensor

logpdf(*pars*, *data*)
Compute the log value of the full density.

Parameters

- **pars** (tensor) – The parameter values
- **data** (tensor) – The measurement data

Returns The log density value

Return type Tensor

mainlogpdf(*maindata*, *pars*)
Compute the log value of the main term.

Parameters

- **maindata** (tensor) – The main measurement data
- **pars** (tensor) – The parameter values

Returns The log density value

Return type Tensor

make_pdf(*pars*)
Construct a pdf object for a given set of parameter values.

Parameters **pars** (tensor) – The model parameters

Returns A distribution object implementing the main measurement pdf of HistFactory

Return type pdf

pdf(*pars*, *data*)
Compute the density at a given observed point in data space of the full model.

Parameters

- **pars** (tensor) – The parameter values
- **data** (tensor) – The measurement data

Returns The density value

Return type Tensor

13.3.2 _ModelConfig

class pyhf.pdf.**_ModelConfig**(*spec*, ***config_kwargs*)

Bases: pyhf.mixins._ChannelSummaryMixin

Configuration for the *Model*.

Note: *_ModelConfig* should not be called directly. It should instead by accessed through the `config` attribute of *Model*.

__init__(*spec*, ***config_kwargs*)

Parameters **spec** (jsonable) – The HistFactory JSON specification.

Methods

_create_and_register_paramsets(*required_paramsets*)

par_names()

The names of the parameters in the model including binned-parameter indexing.

Returns Names of the model parameters.

Return type list

Example

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.par_names()
['mu', 'uncorr_bkguncrt[0]', 'uncorr_bkguncrt[1]']
```

par_slice(*name*)

The slice of the model parameter tensor corresponding to the model parameter `name`.

Returns Slice of the model parameter tensor.

Return type slice

Example

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.par_slice("uncorr_bkguncrt")
slice(1, 3, None)
```

param_set(*name*)

The `paramset` for the model parameter `name`.

Returns Corresponding `paramset`.

Return type `paramsets`

Example

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> param_set = model.config.param_set("uncorr_bkguncrt")
>>> param_set.pdf_type
'poisson'
```

set_auxinfo(*auxdata*, *auxdata_order*)
Sets a group of configuration data for the constraint terms.

set_parameters(*_required_paramsets*)
Evaluate the required parameters for the model configuration.

set_poi(*name*)
Set the model parameter of interest to be model parameter `name`.

Example

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.set_poi("mu")
>>> model.config.poi_name
'mu'
```

suggested_bounds()
Return suggested parameter bounds for the model.

Returns Suggested bounds on model parameters.

Return type `list`

Example

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.suggested_bounds()
[(0, 10), (1e-10, 10.0), (1e-10, 10.0)]
```

suggested_fixed()
Identify the fixed parameters in the model.

Returns A list of booleans, `True` for fixed and `False` for not fixed.

Return type `list`

Example

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.suggested_fixed()
[False, False, False]
```

Something like the following to build `fixed_vals` appropriately:

```
fixed_pars = model.config.suggested_fixed()
inits = model.config.suggested_init()
fixed_vals = [
    (index, init)
    for index, (init, is_fixed) in enumerate(zip(inits, fixed_pars))
    if is_fixed
]
```

suggested_init()

Return suggested initial parameter values for the model.

Returns Suggested initial model parameters.

Return type list

Example

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.suggested_init()
[1.0, 1.0, 1.0]
```

13.3.3 Workspace

class pyhf.workspace.**Workspace**(*spec*, ***config_kwargs*)

Bases: pyhf.mixins._ChannelSummaryMixin, dict

A JSON-serializable object that is built from an object that follows the `workspace.json` schema.

__init__(*spec*, ***config_kwargs*)

Workspaces hold the model, data and measurements.

Attributes

valid_joins = ['none', 'outer', 'left outer', 'right outer']

Methods

_prune_and_rename(*prune_modifiers=None*, *prune_modifier_types=None*, *prune_samples=None*, *prune_channels=None*, *prune_measurements=None*, *rename_modifiers=None*, *rename_samples=None*, *rename_channels=None*, *rename_measurements=None*)

Return a new, pruned, renamed workspace specification. This will not modify the original workspace.

Pruning removes pieces of the workspace whose name or type matches the user-provided lists. The pruned, renamed workspace must also be a valid workspace.

A workspace is composed of many named components, such as channels and samples, as well as types of systematics (e.g. *histosys*). Components can be removed (pruned away) filtering on name or be renamed according to the provided `dict` mapping. Additionally, modifiers of specific types can be removed (pruned away).

This function also handles specific peculiarities, such as renaming/removing a channel which needs to rename/remove the corresponding *observation*.

Parameters

- **prune_modifiers** – A `str` or a `list` of modifiers to prune.
- **prune_modifier_types** – A `str` or a `list` of modifier types to prune.
- **prune_samples** – A `str` or a `list` of samples to prune.
- **prune_channels** – A `str` or a `list` of channels to prune.
- **prune_measurements** – A `str` or a `list` of measurements to prune.
- **rename_modifiers** – A `dict` mapping old modifier name to new modifier name.
- **rename_samples** – A `dict` mapping old sample name to new sample name.
- **rename_channels** – A `dict` mapping old channel name to new channel name.
- **rename_measurements** – A `dict` mapping old measurement name to new measurement name.

Returns A new workspace object with the specified components removed or renamed

Return type *Workspace*

Raises ***InvalidWorkspaceOperation*** – An item name to prune or rename does not exist in the workspace.

classmethod build(*model*, *data*, *name='measurement'*)

Build a workspace from model and data.

Parameters

- **model** (`Model`) – A model to store into a workspace
- **data** (`tensor`) – A array holding observations to store into a workspace
- **name** (`str`) – The name of the workspace measurement

Returns A new workspace object

Return type *Workspace*

classmethod combine(*left*, *right*, *join='none'*, *merge_channels=False*)

Return a new workspace specification that is the combination of the two workspaces.

The new workspace must also be a valid workspace. A combination of workspaces is done by combining the set of:

- channels,
- observations, and
- measurements

between the two workspaces. If the two workspaces have modifiers that follow the same naming convention, then correlations across the two workspaces may be possible. In particular, the *lumi* modifier will be fully-correlated.

If the two workspaces have the same measurement (with the same POI), those measurements will get merged.

Raises ***InvalidWorkspaceOperation*** – The workspaces have common channel names, incompatible measurements, or incompatible schema versions.

Parameters

- **left** (Workspace) – A workspace
- **right** (Workspace) – Another workspace
- **join** (str) – How to join the two workspaces. Pick from “none”, “outer”, “left outer”, or “right outer”.
- **merge_channels** (bool) – Whether or not to merge channels when performing the combine. This is only done with “outer”, “left outer”, and “right outer” options.

Returns A new combined workspace object

Return type *Workspace*

data(*model*, *include_auxdata=True*)

Return the data for the supplied model with or without auxiliary data from the model.

The model is needed as the order of the data depends on the order of the channels in the model.

Raises **KeyError** – Invalid or missing channel

Parameters

- **model** (Model) – A model object adhering to the schema model.json
- **include_auxdata** (bool) – Whether to include auxiliary data from the model or not

Returns data

Return type list

get_measurement(*measurement_name=None*, *measurement_index=None*)

Get a measurement object.

The following logic is used:

1. if the measurement name is given, find the measurement for the given name
2. if the measurement index is given, return the measurement at that index
3. if there are measurements but none of the above have been specified, return the 0th measurement

Raises ***InvalidMeasurement*** – If the measurement was not found

Parameters

- **measurement_name** (str) – The name of the measurement to use
- **measurement_index** (int) – The index of the measurement to use

Returns A measurement object adhering to the schema defs.json#/definitions/measurement

Return type dict

model(*measurement_name=None*, *measurement_index=None*, *patches=None*, ***config_kwargs*)
Create a model object with/without patches applied.

See *pyhf.workspace.Workspace.get_measurement()* and *pyhf.pdf.Model* for possible keyword arguments.

Parameters

- **measurement_name** (str) – The name of the measurement to use in *get_measurement()*.
- **measurement_index** (int) – The index of the measurement to use in *get_measurement()*.
- **patches** (list of jsonpatch.JsonPatch or *pyhf.patchset.Patch*) – A list of patches to apply to the model specification.
- **config_kwargs** – Possible keyword arguments for the model configuration. See *Model* for more details.
- **poi_name** (str or None) – Specify this keyword argument to override the default parameter of interest specified in the measurement. Set to None for a POI-less model.

Returns A model object adhering to the schema model.json

Return type *Model*

prune(*modifiers=None*, *modifier_types=None*, *samples=None*, *channels=None*, *measurements=None*)
Return a new, pruned workspace specification. This will not modify the original workspace.

The pruned workspace must also be a valid workspace.

Parameters

- **modifiers** – A str or a list of modifiers to prune.
- **modifier_types** – A str or a list of modifier types to prune.
- **samples** – A str or a list of samples to prune.
- **channels** – A str or a list of channels to prune.
- **measurements** – A str or a list of measurements to prune.

Returns A new workspace object with the specified components removed

Return type *Workspace*

Raises ***InvalidWorkspaceOperation*** – An item name to prune does not exist in the workspace.

rename(*modifiers=None*, *samples=None*, *channels=None*, *measurements=None*)
Return a new workspace specification with certain elements renamed.

This will not modify the original workspace. The renamed workspace must also be a valid workspace.

Parameters

- **modifiers** – A dict mapping old modifier name to new modifier name.
- **samples** – A dict mapping old sample name to new sample name.
- **channels** – A dict mapping old channel name to new channel name.
- **measurements** – A dict mapping old measurement name to new measurement name.

Returns A new workspace object with the specified components renamed

Return type *Workspace*

Raises ***InvalidWorkspaceOperation*** – An item name to rename does not exist in the workspace.

classmethod sorted(*workspace*)

Return a new workspace specification that is sorted.

Parameters **workspace** (Workspace) – A workspace to sort

Returns A new sorted workspace object

Return type *Workspace*

13.3.4 PatchSet

class pyhf.patchset.**PatchSet**(*spec*, ***config_kwargs*)

Bases: object

A way to store a collection of patches (*Patch*).

It contains *metadata* about the PatchSet itself:

- a high-level *description* of what the patches represent or the analysis it is for
- a list of *references* where the patchset is sourced from (e.g. hepdata)
- a list of *digests* corresponding to the background-only workspace the patchset was made for
- the *labels* of the dimensions of the phase-space for what the patches cover

In addition to the above metadata, the PatchSet object behaves like a:

- smart list allowing you to iterate over all the patches defined
- smart dictionary allowing you to access a patch by the patch name or the patch values

The below example shows various ways one can interact with a *PatchSet* object.

Example

```
>>> import pyhf
>>> patchset = pyhf.PatchSet({
...     "metadata": {
...         "references": { "hepdata": "ins1234567" },
...         "description": "example patchset",
...         "digests": { "md5": "098f6bcd4621d373cade4e832627b4f6" },
...         "labels": ["x", "y"]
...     },
...     "patches": [
...         {
```

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```
...             "metadata": {
...                 "name": "patch_name_for_2100x_800y",
...                 "values": [2100, 800]
...             },
...             "patch": [
...                 {
...                     "op": "add",
...                     "path": "/foo/0/bar",
...                     "value": {
...                         "foo": [1.0]
...                     }
...                 }
...             ]
...         }
...     ],
...     "version": "1.0.0"
... })
...
>>> patchset.version
'1.0.0'
>>> patchset.references
{'hepdata': 'ins1234567'}
>>> patchset.description
'example patchset'
>>> patchset.digests
{'md5': '098f6bcd4621d373cade4e832627b4f6'}
>>> patchset.labels
['x', 'y']
>>> patchset.patches
[<pyhf.patchset.Patch object 'patch_name_for_2100x_800y(2100, 800)' at 0x...>]
>>> patchset['patch_name_for_2100x_800y']
<pyhf.patchset.Patch object 'patch_name_for_2100x_800y(2100, 800)' at 0x...>
>>> patchset[(2100,800)]
<pyhf.patchset.Patch object 'patch_name_for_2100x_800y(2100, 800)' at 0x...>
>>> patchset[[2100,800]]
<pyhf.patchset.Patch object 'patch_name_for_2100x_800y(2100, 800)' at 0x...>
>>> patchset[2100,800]
<pyhf.patchset.Patch object 'patch_name_for_2100x_800y(2100, 800)' at 0x...>
>>> for patch in patchset:
...     print(patch.name)
...
patch_name_for_2100x_800y
>>> len(patchset)
1
```

__init__(*spec*, ***config_kwargs*)

Construct a PatchSet.

Parameters

- **spec** (jsonable) – The patchset JSON specification
- **config_kwargs** – Possible keyword arguments for the patchset validation

Returns The PatchSet instance.

Return type patchset (*PatchSet*)

Attributes

description
The description in the PatchSet metadata

digests
The digests in the PatchSet metadata

labels
The labels in the PatchSet metadata

metadata
The metadata of the PatchSet

patches
The patches in the PatchSet

references
The references in the PatchSet metadata

version
The version of the PatchSet

Methods

apply(*spec*, *key*)
Apply the patch associated with the key to the background-only workspace specificatiom.

Parameters

- **spec** (*Workspace*) – The workspace specification to verify the patchset against.
- **key** (`str` or `tuple` of `int`/`float`) – The key to look up the associated patch - either a name or a set of values.

Raises

- *InvalidPatchLookup* – if the provided patch name is not in the patchset
- *PatchSetVerificationError* – if the patchset cannot be verified against the workspace specification

Returns The background-only workspace with the patch applied.

Return type workspace (*Workspace*)

verify(*spec*)
Verify the patchset digests against a background-only workspace specification. Verified if no exception was raised.

Parameters **spec** (*Workspace*) – The workspace specification to verify the patchset against.

Raises *PatchSetVerificationError* – if the patchset cannot be verified against the workspace specification

Returns None

13.3.5 Patch

class pyhf.patchset.**Patch**(*spec*)

Bases: jsonpatch.JsonPatch

A way to store a patch definition as part of a patchset (*PatchSet*).

It contains *metadata* about the Patch itself:

- a descriptive *name*
- a list of the *values* for each dimension in the phase-space the associated *PatchSet* is defined for, see *labels*

In addition to the above metadata, the Patch object behaves like the underlying jsonpatch.JsonPatch.

__init__(*spec*)

Construct a Patch.

Parameters **spec** (jsonable) – The patch JSON specification

Returns The Patch instance.

Return type patch (*Patch*)

Attributes

metadata

The metadata of the patch

name

The name of the patch

operations = mappingproxy({'remove': <class 'jsonpatch.RemoveOperation'>, 'add': <class 'jsonpatch.AddOperation'>, 'replace': <class 'jsonpatch.ReplaceOperation'>, 'move': <class 'jsonpatch.MoveOperation'>, 'test': <class 'jsonpatch.TestOperation'>, 'copy': <class 'jsonpatch.CopyOperation'>})

A JSON Patch is a list of Patch Operations.

```
>>> patch = JsonPatch([
...     {'op': 'add', 'path': '/foo', 'value': 'bar'},
...     {'op': 'add', 'path': '/baz', 'value': [1, 2, 3]},
...     {'op': 'remove', 'path': '/baz/1'},
...     {'op': 'test', 'path': '/baz', 'value': [1, 3]},
...     {'op': 'replace', 'path': '/baz/0', 'value': 42},
...     {'op': 'remove', 'path': '/baz/1'},
... ])
>>> doc = {}
>>> result = patch.apply(doc)
>>> expected = {'foo': 'bar', 'baz': [42]}
>>> result == expected
True
```

JsonPatch object is iterable, so you can easily access each patch statement in a loop:

```
>>> lpatch = list(patch)
>>> expected = {'op': 'add', 'path': '/foo', 'value': 'bar'}
>>> lpatch[0] == expected
```

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```
True
>>> lpatch == patch.patch
True
```

Also JsonPatch could be converted directly to `bool` if it contains any operation statements:

```
>>> bool(patch)
True
>>> bool(JsonPatch([]))
False
```

This behavior is very handy with `make_patch()` to write more readable code:

```
>>> old = {'foo': 'bar', 'numbers': [1, 3, 4, 8]}
>>> new = {'baz': 'qux', 'numbers': [1, 4, 7]}
>>> patch = make_patch(old, new)
>>> if patch:
...     # document have changed, do something useful
...     patch.apply(old)
{...}
```

values
The values of the associated labels for the patch

Methods

13.3.6 pyhf.simplemodels.uncorrelated_background

pyhf.simplemodels.**uncorrelated_background**(*signal*, *bkg*, *bkg_uncertainty*, *batch_size=None*)
Construct a simple single channel *Model* with a *shapesys* modifier representing an uncorrelated background uncertainty.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.schema
'model.json'
>>> model.config.channels
['singlechannel']
>>> model.config.samples
['background', 'signal']
>>> model.config.parameters
['mu', 'uncorr_bkguncrt']
>>> model.expected_data(model.config.suggested_init())
array([ 62.        ,  63.        , 277.77777778,  55.18367347])
```

Parameters

- **signal** (list) – The data in the signal sample
- **bkg** (list) – The data in the background sample
- **bkg_uncertainty** (list) – The statistical uncertainty on the background sample counts
- **batch_size** (None or int) – Number of simultaneous (batched) Models to compute

Returns The statistical model adhering to the `model.json` schema

Return type *Model*

13.3.7 pyhf.simplemodels.correlated_background

pyhf.simplemodels.**correlated_background**(*signal*, *bkg*, *bkg_up*, *bkg_down*, *batch_size=None*)

Construct a simple single channel *Model* with a *histosys* modifier representing a background with a fully correlated bin-by-bin uncertainty.

Parameters

- **signal** (list) – The data in the signal sample.
- **bkg** (list) – The data in the background sample.
- **bkg_up** (list) – The background sample under an upward variation corresponding to $\alpha = +1$.
- **bkg_down** (list) – The background sample under a downward variation corresponding to $\alpha = -1$.
- **batch_size** (None or int) – Number of simultaneous (batched) Models to compute.

Returns The statistical model adhering to the `model.json` schema.

Return type *Model*

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.correlated_background(
...     signal=[12.0, 11.0],
...     bkg=[50.0, 52.0],
...     bkg_up=[45.0, 57.0],
...     bkg_down=[55.0, 47.0],
... )
>>> model.schema
'model.json'
>>> model.config.channels
['single_channel']
>>> model.config.samples
['background', 'signal']
>>> model.config.parameters
['correlated_bkg_uncertainty', 'mu']
>>> model.expected_data(model.config.suggested_init())
array([62., 63.,  0.])
```

13.4 Backends

The computational backends that `pyhf` provides interfacing for the vector-based calculations.

numpy_backend.numpy_backend	NumPy backend for pyhf
pytorch_backend.pytorch_backend	PyTorch backend for pyhf
tensorflow_backend.tensorflow_backend	TensorFlow backend for pyhf
jax_backend.jax_backend	JAX backend for pyhf

13.4.1 numpy_backend

class pyhf.tensor.numpy_backend.**numpy_backend**(***kwargs*)

Bases: `object`

NumPy backend for pyhf

__init__(***kwargs*)

Attributes

name

precision

dtypemap

default_do_grad

Methods

_setup()

Run any global setups for the numpy lib.

abs(*tensor*)

astensor(*tensor_in*, *dtype='float'*)

Convert to a NumPy array.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> tensor
array([[1., 2., 3.],
       [4., 5., 6.]])
>>> type(tensor)
<class 'numpy.ndarray'>
```

Parameters **tensor_in** (*Number or Tensor*) – Tensor object

Returns A multi-dimensional, fixed-size homogeneous array.

Return type *numpy.ndarray*

boolean_mask(*tensor*, *mask*)

clip(*tensor_in*, *min_value*, *max_value*)
Clips (limits) the tensor values to be within a specified min and max.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> a = pyhf.tensorlib.astensor([-2, -1, 0, 1, 2])
>>> pyhf.tensorlib.clip(a, -1, 1)
array([-1., -1.,  0.,  1.,  1.])
```

Parameters

- **tensor_in** (tensor) – The input tensor object
- **min_value** (scalar or tensor or None) – The minimum value to be cliped to
- **max_value** (scalar or tensor or None) – The maximum value to be cliped to

Returns A clipped *tensor*

Return type NumPy ndarray

concatenate(*sequence*, *axis=0*)
Join a sequence of arrays along an existing axis.

Parameters

- **sequence** – sequence of tensors
- **axis** – dimension along which to concatenate

Returns the concatenated tensor

Return type output

conditional(*predicate*, *true_callable*, *false_callable*)
Runs a callable conditional on the boolean value of the evaluation of a predicate

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> tensorlib = pyhf.tensorlib
>>> a = tensorlib.astensor([4])
>>> b = tensorlib.astensor([5])
>>> tensorlib.conditional((a < b)[0], lambda: a + b, lambda: a - b)
array([9.])
```

Parameters

- **predicate** (scalar) – The logical condition that determines which callable to evaluate

- **true_callable** (callable) – The callable that is evaluated when the predicate evaluates to true
- **false_callable** (callable) – The callable that is evaluated when the predicate evaluates to false

Returns The output of the callable that was evaluated

Return type NumPy ndarray

divide(*tensor_in_1*, *tensor_in_2*)

einsum(*subscripts*, **operands*)

Evaluates the Einstein summation convention on the operands.

Using the Einstein summation convention, many common multi-dimensional array operations can be represented in a simple fashion. This function provides a way to compute such summations. The best way to understand this function is to try the examples below, which show how many common NumPy functions can be implemented as calls to einsum.

Parameters

- **subscripts** – str, specifies the subscripts for summation
- **operands** – list of array_like, these are the tensors for the operation

Returns the calculation based on the Einstein summation convention

Return type tensor

erf(*tensor_in*)

The error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> pyhf.tensorlib.erf(a)
array([-0.99532227, -0.84270079,  0.        ,  0.84270079,  0.99532227])
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the error function at the given points.

Return type NumPy ndarray

erfinv(*tensor_in*)

The inverse of the error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> pyhf.tensorlib.erfinv(pyhf.tensorlib.erf(a))
array([-2., -1.,  0.,  1.,  2.])
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the inverse of the error function at the given points.

Return type NumPy ndarray

exp(*tensor_in*)

gather(*tensor*, *indices*)

isfinite(*tensor*)

log(*tensor_in*)

normal(*x*, *mu*, *sigma*)

The probability density function of the Normal distribution evaluated at `x` given parameters of mean of `mu` and standard deviation of `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> pyhf.tensorlib.normal(0.5, 0., 1.)
0.3520653267642995
>>> values = pyhf.tensorlib.astensor([0.5, 2.0])
>>> means = pyhf.tensorlib.astensor([0., 2.3])
>>> sigmas = pyhf.tensorlib.astensor([1., 0.8])
>>> pyhf.tensorlib.normal(values, means, sigmas)
array([0.35206533, 0.46481887])
```

Parameters

- **x** (tensor or float) – The value at which to evaluate the Normal distribution p.d.f.
- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns Value of Normal(x|mu, sigma)

Return type NumPy float

normal_cdf(*x*, *mu=0*, *sigma=1*)

The cumulative distribution function for the Normal distribution

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> pyhf.tensorlib.normal_cdf(0.8)
0.7881446014166034
>>> values = pyhf.tensorlib.astensor([0.8, 2.0])
>>> pyhf.tensorlib.normal_cdf(values)
array([0.7881446 , 0.97724987])
```

Parameters

- **x** (tensor or float) – The observed value of the random variable to evaluate the CDF for
- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns The CDF

Return type NumPy float

normal_dist(*mu*, *sigma*)

The Normal distribution with mean `mu` and standard deviation `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> means = pyhf.tensorlib.astensor([5, 8])
>>> stds = pyhf.tensorlib.astensor([1, 0.5])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> normals = pyhf.tensorlib.normal_dist(means, stds)
>>> normals.log_prob(values)
array([-1.41893853, -2.22579135])
```

Parameters

- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns The Normal distribution class

Return type Normal distribution

normal_logpdf(*x*, *mu*, *sigma*)

ones(*shape*, *dtype='float'*)

outer(*tensor_in_1*, *tensor_in_2*)

poisson(*n*, *lam*)

The continuous approximation, using $n! = \Gamma(n+1)$, to the probability mass function of the Poisson distribution evaluated at `n` given the parameter `lam`.

Note: Though the p.m.f of the Poisson distribution is not defined for $\lambda = 0$, the limit as $\lambda \to 0$ is still defined, which gives a degenerate p.m.f. of

$$\lim_{\lambda \to 0} \text{Pois}(n|\lambda) = \begin{cases} 1, & n = 0, \\ 0, & n > 0 \end{cases}$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> pyhf.tensorlib.poisson(5., 6.)
0.16062314104797995
>>> values = pyhf.tensorlib.astensor([5., 9.])
>>> rates = pyhf.tensorlib.astensor([6., 8.])
>>> pyhf.tensorlib.poisson(values, rates)
array([0.16062314, 0.12407692])
```

Parameters

- **n** (tensor or float) – The value at which to evaluate the approximation to the Poisson distribution p.m.f. (the observed number of events)
- **lam** (tensor or float) – The mean of the Poisson distribution p.m.f. (the expected number of events)

Returns Value of the continuous approximation to Poisson(n|lam)

Return type NumPy float

poisson_dist(*rate*)

The Poisson distribution with rate parameter rate.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> rates = pyhf.tensorlib.astensor([5, 8])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> poissons = pyhf.tensorlib.poisson_dist(rates)
>>> poissons.log_prob(values)
array([-1.74030218, -2.0868536 ])
```

Parameters **rate** (tensor or float) – The mean of the Poisson distribution (the expected number of events)

Returns The Poisson distribution class

Return type Poisson distribution

poisson_logpdf(*n*, *lam*)

power(*tensor_in_1*, *tensor_in_2*)

product(*tensor_in*, *axis=None*)

ravel(*tensor*)
Return a flattened view of the tensor, not a copy.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> pyhf.tensorlib.ravel(tensor)
array([1., 2., 3., 4., 5., 6.])
```

Parameters **tensor** (*Tensor*) – Tensor object

Returns A flattened array.

Return type *numpy.ndarray*

reshape(*tensor*, *newshape*)

shape(*tensor*)

simple_broadcast(**args*)
Broadcast a sequence of 1 dimensional arrays.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> pyhf.tensorlib.simple_broadcast(
...   pyhf.tensorlib.astensor([1]),
...   pyhf.tensorlib.astensor([2, 3, 4]),
...   pyhf.tensorlib.astensor([5, 6, 7]))
[array([1., 1., 1.]), array([2., 3., 4.]), array([5., 6., 7.])]
```

Parameters **args** (*Array of Tensors*) – Sequence of arrays

Returns The sequence broadcast together.

Return type list of Tensors

sqrt(*tensor_in*)

stack(*sequence*, *axis=0*)

sum(*tensor_in*, *axis=None*)

tile(*tensor_in*, *repeats*)
Repeat tensor data along a specific dimension

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> a = pyhf.tensorlib.astensor([[1.0], [2.0]])
>>> pyhf.tensorlib.tile(a, (1, 2))
array([[1., 1.],
       [2., 2.]])
```

Parameters

- **tensor_in** (tensor) – The tensor to be repeated
- **repeats** (tensor) – The tuple of multipliers for each dimension

Returns The tensor with repeated axes

Return type NumPy ndarray

to_numpy(*tensor_in*)

Return the input tensor as it already is a numpy.ndarray. This API exists only for pyhf.tensorlib compatibility.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> tensor
array([[1., 2., 3.],
       [4., 5., 6.]])
>>> numpy_ndarray = pyhf.tensorlib.to_numpy(tensor)
>>> numpy_ndarray
array([[1., 2., 3.],
       [4., 5., 6.]])
>>> type(numpy_ndarray)
<class 'numpy.ndarray'>
```

Parameters **tensor_in** (tensor) – The input tensor object.

Returns The tensor converted to a NumPy ndarray.

Return type numpy.ndarray

tolist(*tensor_in*)

where(*mask*, *tensor_in_1*, *tensor_in_2*)

zeros(*shape*, *dtype='float'*)

13.4.2 pytorch_backend

class pyhf.tensor.pytorch_backend.**pytorch_backend**(***kwargs*)

Bases: object

PyTorch backend for pyhf

__init__(***kwargs*)

Attributes

name

precision

dtypemap

default_do_grad

Methods

_setup()

Run any global setups for the pytorch lib.

abs(*tensor*)

astensor(*tensor_in*, *dtype='float'*)

Convert to a PyTorch Tensor.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> tensor
tensor([[1., 2., 3.],
        [4., 5., 6.]])
>>> type(tensor)
<class 'torch.Tensor'>
```

Parameters **tensor_in** (*Number or Tensor*) – Tensor object

Returns A multi-dimensional matrix containing elements of a single data type.

Return type torch.Tensor

boolean_mask(*tensor*, *mask*)

clip(*tensor_in*, *min_value*, *max_value*)

Clips (limits) the tensor values to be within a specified min and max.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> a = pyhf.tensorlib.astensor([-2, -1, 0, 1, 2])
>>> pyhf.tensorlib.clip(a, -1, 1)
tensor([-1., -1.,  0.,  1.,  1.])
```

Parameters

- **tensor_in** (tensor) – The input tensor object
- **min_value** (scalar or tensor or None) – The minimum value to be cliped to
- **max_value** (scalar or tensor or None) – The maximum value to be cliped to

Returns A clipped *tensor*

Return type PyTorch tensor

concatenate(*sequence*, *axis=0*)
Join a sequence of arrays along an existing axis.

Parameters

- **sequence** – sequence of tensors
- **axis** – dimension along which to concatenate

Returns the concatenated tensor

Return type output

conditional(*predicate*, *true_callable*, *false_callable*)
Runs a callable conditional on the boolean value of the evaluation of a predicate

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> tensorlib = pyhf.tensorlib
>>> a = tensorlib.astensor([4])
>>> b = tensorlib.astensor([5])
>>> tensorlib.conditional((a < b)[0], lambda: a + b, lambda: a - b)
tensor([9.])
```

Parameters

- **predicate** (scalar) – The logical condition that determines which callable to evaluate
- **true_callable** (callable) – The callable that is evaluated when the predicate evaluates to true
- **false_callable** (callable) – The callable that is evaluated when the predicate evaluates to false

Returns The output of the callable that was evaluated

Return type PyTorch Tensor

divide(*tensor_in_1*, *tensor_in_2*)

einsum(*subscripts*, **operands*)

This function provides a way of computing multilinear expressions (i.e. sums of products) using the Einstein summation convention.

Parameters

- **subscripts** – str, specifies the subscripts for summation
- **operands** – list of array_like, these are the tensors for the operation

Returns the calculation based on the Einstein summation convention

Return type tensor

erf(*tensor_in*)

The error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> pyhf.tensorlib.erf(a)
tensor([-0.9953, -0.8427,  0.0000,  0.8427,  0.9953])
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the error function at the given points.

Return type PyTorch Tensor

erfinv(*tensor_in*)

The inverse of the error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> pyhf.tensorlib.erfinv(pyhf.tensorlib.erf(a))
tensor([-2.0000, -1.0000,  0.0000,  1.0000,  2.0000])
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the inverse of the error function at the given points.

Return type PyTorch Tensor

exp(*tensor_in*)

gather(*tensor*, *indices*)

isfinite(*tensor*)

log(*tensor_in*)

normal(*x*, *mu*, *sigma*)

The probability density function of the Normal distribution evaluated at `x` given parameters of mean of `mu` and standard deviation of `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> pyhf.tensorlib.normal(0.5, 0., 1.)
tensor(0.3521)
>>> values = pyhf.tensorlib.astensor([0.5, 2.0])
>>> means = pyhf.tensorlib.astensor([0., 2.3])
>>> sigmas = pyhf.tensorlib.astensor([1., 0.8])
>>> pyhf.tensorlib.normal(values, means, sigmas)
tensor([0.3521, 0.4648])
```

Parameters

- **x** (`tensor` or `float`) – The value at which to evaluate the Normal distribution p.d.f.
- **mu** (`tensor` or `float`) – The mean of the Normal distribution
- **sigma** (`tensor` or `float`) – The standard deviation of the Normal distribution

Returns Value of Normal(x|mu, sigma)

Return type PyTorch FloatTensor

normal_cdf(*x*, *mu=0.0*, *sigma=1.0*)

The cumulative distribution function for the Normal distribution

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> pyhf.tensorlib.normal_cdf(0.8)
tensor(0.7881)
>>> values = pyhf.tensorlib.astensor([0.8, 2.0])
>>> pyhf.tensorlib.normal_cdf(values)
tensor([0.7881, 0.9772])
```

Parameters

- **x** (`tensor` or `float`) – The observed value of the random variable to evaluate the CDF for
- **mu** (`tensor` or `float`) – The mean of the Normal distribution
- **sigma** (`tensor` or `float`) – The standard deviation of the Normal distribution

Returns The CDF

Return type PyTorch FloatTensor

normal_dist(*mu*, *sigma*)

The Normal distribution with mean `mu` and standard deviation `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> means = pyhf.tensorlib.astensor([5, 8])
>>> stds = pyhf.tensorlib.astensor([1, 0.5])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> normals = pyhf.tensorlib.normal_dist(means, stds)
>>> normals.log_prob(values)
tensor([-1.4189, -2.2258])
```

Parameters

- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns The Normal distribution class

Return type PyTorch Normal distribution

normal_logpdf(*x*, *mu*, *sigma*)

ones(*shape*, *dtype='float'*)

outer(*tensor_in_1*, *tensor_in_2*)

Outer product of the input tensors.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> a = pyhf.tensorlib.astensor([1.0, 2.0, 3.0])
>>> b = pyhf.tensorlib.astensor([1.0, 2.0, 3.0, 4.0])
>>> pyhf.tensorlib.outer(a, b)
tensor([[ 1.,  2.,  3.,  4.],
        [ 2.,  4.,  6.,  8.],
        [ 3.,  6.,  9., 12.]])
```

Parameters

- **tensor_in_1** (tensor) – 1-D input tensor.
- **tensor_in_2** (tensor) – 1-D input tensor.

Returns The outer product.

Return type PyTorch tensor

poisson(*n*, *lam*)

The continuous approximation, using $n! = \Gamma(n+1)$, to the probability mass function of the Poisson distribution evaluated at `n` given the parameter `lam`.

Note: Though the p.m.f of the Poisson distribution is not defined for $\lambda = 0$, the limit as $\lambda \to 0$ is still defined, which gives a degenerate p.m.f. of

$$\lim_{\lambda \to 0} \text{Pois}(n|\lambda) = \begin{cases} 1, & n = 0, \\ 0, & n > 0 \end{cases}$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> pyhf.tensorlib.poisson(5., 6.)
tensor(0.1606)
>>> values = pyhf.tensorlib.astensor([5., 9.])
>>> rates = pyhf.tensorlib.astensor([6., 8.])
>>> pyhf.tensorlib.poisson(values, rates)
tensor([0.1606, 0.1241])
```

Parameters

- **n** (tensor or float) – The value at which to evaluate the approximation to the Poisson distribution p.m.f. (the observed number of events)
- **lam** (tensor or float) – The mean of the Poisson distribution p.m.f. (the expected number of events)

Returns Value of the continuous approximation to Poisson(n|lam)

Return type PyTorch FloatTensor

poisson_dist(*rate*)

The Poisson distribution with rate parameter rate.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> rates = pyhf.tensorlib.astensor([5, 8])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> poissons = pyhf.tensorlib.poisson_dist(rates)
>>> poissons.log_prob(values)
tensor([-1.7403, -2.0869])
```

Parameters **rate** (tensor or float) – The mean of the Poisson distribution (the expected number of events)

Returns The Poisson distribution class

Return type PyTorch Poisson distribution

poisson_logpdf(*n*, *lam*)

power(*tensor_in_1*, *tensor_in_2*)

product(*tensor_in*, *axis=None*)

ravel(*tensor*)
Return a flattened view of the tensor, not a copy.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> pyhf.tensorlib.ravel(tensor)
tensor([1., 2., 3., 4., 5., 6.])
```

Parameters **tensor** (*Tensor*) – Tensor object

Returns A flattened array.

Return type *torch.Tensor*

reshape(*tensor*, *newshape*)

shape(*tensor*)

simple_broadcast(**args*)
Broadcast a sequence of 1 dimensional arrays.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> pyhf.tensorlib.simple_broadcast(
...   pyhf.tensorlib.astensor([1]),
...   pyhf.tensorlib.astensor([2, 3, 4]),
...   pyhf.tensorlib.astensor([5, 6, 7]))
[tensor([1., 1., 1.]), tensor([2., 3., 4.]), tensor([5., 6., 7.])]
```

Parameters **args** (*Array of Tensors*) – Sequence of arrays

Returns The sequence broadcast together.

Return type list of Tensors

sqrt(*tensor_in*)

stack(*sequence*, *axis=0*)

sum(*tensor_in*, *axis=None*)

tile(*tensor_in*, *repeats*)
Repeat tensor data along a specific dimension

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> a = pyhf.tensorlib.astensor([[1.0], [2.0]])
>>> pyhf.tensorlib.tile(a, (1, 2))
tensor([[1., 1.],
        [2., 2.]])
```

Parameters

- **tensor_in** (tensor) – The tensor to be repeated
- **repeats** (tensor) – The tuple of multipliers for each dimension

Returns The tensor with repeated axes

Return type PyTorch tensor

to_numpy(*tensor_in*)

Convert the PyTorch tensor to a numpy.ndarray.

Example

```
>>> import pyhf
>>> pyhf.set_backend("pytorch")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> tensor
tensor([[1., 2., 3.],
        [4., 5., 6.]])
>>> numpy_ndarray = pyhf.tensorlib.to_numpy(tensor)
>>> numpy_ndarray
array([[1., 2., 3.],
       [4., 5., 6.]])
>>> type(numpy_ndarray)
<class 'numpy.ndarray'>
```

Parameters **tensor_in** (tensor) – The input tensor object.

Returns The tensor converted to a NumPy ndarray.

Return type numpy.ndarray

tolist(*tensor_in*)

where(*mask*, *tensor_in_1*, *tensor_in_2*)

zeros(*shape*, *dtype='float'*)

13.4.3 tensorflow_backend

class pyhf.tensor.tensorflow_backend.**tensorflow_backend**(***kwargs*)

Bases: object

TensorFlow backend for pyhf

__init__(***kwargs*)

Attributes

name

precision

dtypemap

default_do_grad

Methods

_setup()

Run any global setups for the tensorflow lib.

abs(*tensor*)

astensor(*tensor_in*, *dtype='float'*)

Convert to a TensorFlow Tensor.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> tensor
<tf.Tensor: shape=(2, 3), dtype=float64, numpy=
array([[1., 2., 3.],
       [4., 5., 6.]])>
>>> type(tensor)
<class 'tensorflow.python.framework.ops.EagerTensor'>
```

Parameters **tensor_in** (*Number or Tensor*) – Tensor object

Returns A symbolic handle to one of the outputs of a *tf.Operation*.

Return type *tf.Tensor*

boolean_mask(*tensor*, *mask*)

clip(*tensor_in*, *min_value*, *max_value*)

Clips (limits) the tensor values to be within a specified min and max.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> a = pyhf.tensorlib.astensor([-2, -1, 0, 1, 2])
>>> t = pyhf.tensorlib.clip(a, -1, 1)
>>> print(t)
tf.Tensor([-1. -1.  0.  1.  1.], shape=(5,), dtype=float64)
```

Parameters

- **tensor_in** (tensor) – The input tensor object
- **min_value** (scalar or tensor or None) – The minimum value to be cliped to
- **max_value** (scalar or tensor or None) – The maximum value to be cliped to

Returns A clipped *tensor*

Return type TensorFlow Tensor

concatenate(*sequence*, *axis=0*)

Join a sequence of arrays along an existing axis.

Parameters

- **sequence** – sequence of tensors
- **axis** – dimension along which to concatenate

Returns the concatenated tensor

Return type output

conditional(*predicate*, *true_callable*, *false_callable*)

Runs a callable conditional on the boolean value of the evaluation of a predicate

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> tensorlib = pyhf.tensorlib
>>> a = tensorlib.astensor([4])
>>> b = tensorlib.astensor([5])
>>> t = tensorlib.conditional((a < b)[0], lambda: a + b, lambda: a - b)
>>> print(t)
tf.Tensor([9.], shape=(1,), dtype=float64)
```

Parameters

- **predicate** (scalar) – The logical condition that determines which callable to evaluate
- **true_callable** (callable) – The callable that is evaluated when the predicate evaluates to true
- **false_callable** (callable) – The callable that is evaluated when the predicate evaluates to false

Returns The output of the callable that was evaluated

Return type TensorFlow Tensor

divide(*tensor_in_1*, *tensor_in_2*)

einsum(*subscripts*, **operands*)

A generalized contraction between tensors of arbitrary dimension.

This function returns a tensor whose elements are defined by equation, which is written in a shorthand form inspired by the Einstein summation convention.

Parameters

- **subscripts** – str, specifies the subscripts for summation
- **operands** – list of array_like, these are the tensors for the operation

Returns the calculation based on the Einstein summation convention

Return type TensorFlow Tensor

erf(*tensor_in*)

The error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> t = pyhf.tensorlib.erf(a)
>>> print(t)
tf.Tensor([-0.99532227 -0.84270079  0.          0.84270079  0.99532227],␣
↪shape=(5,), dtype=float64)
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the error function at the given points.

Return type TensorFlow Tensor

erfinv(*tensor_in*)

The inverse of the error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> t = pyhf.tensorlib.erfinv(pyhf.tensorlib.erf(a))
>>> print(t)
tf.Tensor([-2. -1.  0.  1.  2.], shape=(5,), dtype=float64)
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the inverse of the error function at the given points.

Return type TensorFlow Tensor

exp(*tensor_in*)

gather(*tensor*, *indices*)

isfinite(*tensor*)

log(*tensor_in*)

normal(*x*, *mu*, *sigma*)

The probability density function of the Normal distribution evaluated at `x` given parameters of mean of `mu` and standard deviation of `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> t = pyhf.tensorlib.normal(0.5, 0., 1.)
>>> print(t)
tf.Tensor(0.3520653267642995, shape=(), dtype=float64)
>>> values = pyhf.tensorlib.astensor([0.5, 2.0])
>>> means = pyhf.tensorlib.astensor([0., 2.3])
>>> sigmas = pyhf.tensorlib.astensor([1., 0.8])
>>> t = pyhf.tensorlib.normal(values, means, sigmas)
>>> print(t)
tf.Tensor([0.35206533 0.46481887], shape=(2,), dtype=float64)
```

Parameters

- **x** (`tensor` or `float`) – The value at which to evaluate the Normal distribution p.d.f.
- **mu** (`tensor` or `float`) – The mean of the Normal distribution
- **sigma** (`tensor` or `float`) – The standard deviation of the Normal distribution

Returns Value of Normal(x|mu, sigma)

Return type TensorFlow Tensor

normal_cdf(*x*, *mu=0.0*, *sigma=1*)

Compute the value of cumulative distribution function for the Normal distribution at x.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> t = pyhf.tensorlib.normal_cdf(0.8)
>>> print(t)
tf.Tensor(0.7881446014166034, shape=(), dtype=float64)
>>> values = pyhf.tensorlib.astensor([0.8, 2.0])
>>> t = pyhf.tensorlib.normal_cdf(values)
>>> print(t)
tf.Tensor([0.7881446  0.97724987], shape=(2,), dtype=float64)
```

Parameters

- **x** (`tensor` or `float`) – The observed value of the random variable to evaluate the CDF for

- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns The CDF

Return type TensorFlow Tensor

normal_dist(*mu*, *sigma*)

Construct a Normal distribution with mean `mu` and standard deviation `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> means = pyhf.tensorlib.astensor([5, 8])
>>> stds = pyhf.tensorlib.astensor([1, 0.5])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> normals = pyhf.tensorlib.normal_dist(means, stds)
>>> t = normals.log_prob(values)
>>> print(t)
tf.Tensor([-1.41893853 -2.22579135], shape=(2,), dtype=float64)
```

Parameters

- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns The Normal distribution class

Return type TensorFlow Probability Normal distribution

normal_logpdf(*x*, *mu*, *sigma*)

The log of the probability density function of the Normal distribution evaluated at `x` given parameters of mean of `mu` and standard deviation of `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> t = pyhf.tensorlib.normal_logpdf(0.5, 0., 1.)
>>> print(t)
tf.Tensor(-1.0439385332046727, shape=(), dtype=float64)
>>> values = pyhf.tensorlib.astensor([0.5, 2.0])
>>> means = pyhf.tensorlib.astensor([0., 2.3])
>>> sigmas = pyhf.tensorlib.astensor([1., 0.8])
>>> t = pyhf.tensorlib.normal_logpdf(values, means, sigmas)
>>> print(t)
tf.Tensor([-1.04393853 -0.76610747], shape=(2,), dtype=float64)
```

Parameters

- **x** (tensor or float) – The value at which to evaluate the Normal distribution p.d.f.

- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns Value of log(Normal(x|mu, sigma))

Return type TensorFlow Tensor

ones(*shape*, *dtype='float'*)

outer(*tensor_in_1*, *tensor_in_2*)

poisson(*n*, *lam*)

The continuous approximation, using $n! = \Gamma(n+1)$, to the probability mass function of the Poisson distribution evaluated at `n` given the parameter `lam`.

Note: Though the p.m.f of the Poisson distribution is not defined for $\lambda = 0$, the limit as $\lambda \to 0$ is still defined, which gives a degenerate p.m.f. of

$$\lim_{\lambda \to 0} \text{Pois}(n|\lambda) = \begin{cases} 1, & n = 0, \\ 0, & n > 0 \end{cases}$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> t = pyhf.tensorlib.poisson(5., 6.)
>>> print(t)
tf.Tensor(0.1606231410479..., shape=(), dtype=float64)
>>> values = pyhf.tensorlib.astensor([5., 9.])
>>> rates = pyhf.tensorlib.astensor([6., 8.])
>>> t = pyhf.tensorlib.poisson(values, rates)
>>> print(t)
tf.Tensor([0.16062314 0.12407692], shape=(2,), dtype=float64)
```

Parameters

- **n** (tensor or float) – The value at which to evaluate the approximation to the Poisson distribution p.m.f. (the observed number of events)
- **lam** (tensor or float) – The mean of the Poisson distribution p.m.f. (the expected number of events)

Returns Value of the continuous approximation to Poisson(n|lam)

Return type TensorFlow Tensor

poisson_dist(*rate*)

Construct a Poisson distribution with rate parameter `rate`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> rates = pyhf.tensorlib.astensor([5, 8])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> poissons = pyhf.tensorlib.poisson_dist(rates)
>>> t = poissons.log_prob(values)
>>> print(t)
tf.Tensor([-1.74030218 -2.0868536 ], shape=(2,), dtype=float64)
```

Parameters **rate** (tensor or float) – The mean of the Poisson distribution (the expected number of events)

Returns The Poisson distribution class

Return type TensorFlow Probability Poisson distribution

poisson_logpdf(*n*, *lam*)

The log of the continuous approximation, using $n! = \Gamma(n+1)$, to the probability mass function of the Poisson distribution evaluated at n given the parameter lam.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> t = pyhf.tensorlib.poisson_logpdf(5., 6.)
>>> print(t)
tf.Tensor(-1.8286943966417..., shape=(), dtype=float64)
>>> values = pyhf.tensorlib.astensor([5., 9.])
>>> rates = pyhf.tensorlib.astensor([6., 8.])
>>> t = pyhf.tensorlib.poisson_logpdf(values, rates)
>>> print(t)
tf.Tensor([-1.8286944 -2.0868536], shape=(2,), dtype=float64)
```

Parameters

- **n** (tensor or float) – The value at which to evaluate the approximation to the Poisson distribution p.m.f. (the observed number of events)
- **lam** (tensor or float) – The mean of the Poisson distribution p.m.f. (the expected number of events)

Returns Value of the continuous approximation to log(Poisson(n|lam))

Return type TensorFlow Tensor

power(*tensor_in_1*, *tensor_in_2*)

product(*tensor_in*, *axis=None*)

ravel(*tensor*)

Return a flattened view of the tensor, not a copy.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> t_ravel = pyhf.tensorlib.ravel(tensor)
>>> print(t_ravel)
tf.Tensor([1. 2. 3. 4. 5. 6.], shape=(6,), dtype=float64)
```

Parameters **tensor** (*Tensor*) – Tensor object

Returns A flattened array.

Return type *tf.Tensor*

reshape(*tensor*, *newshape*)

shape(*tensor*)

simple_broadcast(**args*)
Broadcast a sequence of 1 dimensional arrays.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> b = pyhf.tensorlib.simple_broadcast(
...   pyhf.tensorlib.astensor([1]),
...   pyhf.tensorlib.astensor([2, 3, 4]),
...   pyhf.tensorlib.astensor([5, 6, 7]))
>>> print([str(t) for t in b])
['tf.Tensor([1. 1. 1.], shape=(3,), dtype=float64)',
 'tf.Tensor([2. 3. 4.], shape=(3,), dtype=float64)',
 'tf.Tensor([5. 6. 7.], shape=(3,), dtype=float64)']
```

Parameters **args** (*Array of Tensors*) – Sequence of arrays

Returns The sequence broadcast together.

Return type list of Tensors

sqrt(*tensor_in*)

stack(*sequence*, *axis=0*)

sum(*tensor_in*, *axis=None*)

tile(*tensor_in*, *repeats*)
Repeat tensor data along a specific dimension

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> a = pyhf.tensorlib.astensor([[1.0], [2.0]])
>>> t = pyhf.tensorlib.tile(a, (1, 2))
>>> print(t)
tf.Tensor(
[[1. 1.]
 [2. 2.]], shape=(2, 2), dtype=float64)
```

Parameters

- **tensor_in** (tensor) – The tensor to be repeated
- **repeats** (tensor) – The tuple of multipliers for each dimension

Returns The tensor with repeated axes

Return type TensorFlow Tensor

to_numpy(*tensor_in*)

Convert the TensorFlow tensor to a numpy.ndarray.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> print(tensor)
tf.Tensor(
[[1. 2. 3.]
 [4. 5. 6.]], shape=(2, 3), dtype=float64)
>>> numpy_ndarray = pyhf.tensorlib.to_numpy(tensor)
>>> numpy_ndarray
array([[1., 2., 3.],
       [4., 5., 6.]])
>>> type(numpy_ndarray)
<class 'numpy.ndarray'>
```

Parameters **tensor_in** (tensor) – The input tensor object.

Returns The tensor converted to a NumPy ndarray.

Return type numpy.ndarray

tolist(*tensor_in*)

where(*mask*, *tensor_in_1*, *tensor_in_2*)

Apply a boolean selection mask to the elements of the input tensors.

Example

```
>>> import pyhf
>>> pyhf.set_backend("tensorflow")
>>> t = pyhf.tensorlib.where(
...     pyhf.tensorlib.astensor([1, 0, 1], dtype='bool'),
...     pyhf.tensorlib.astensor([1, 1, 1]),
...     pyhf.tensorlib.astensor([2, 2, 2]),
... )
>>> print(t)
tf.Tensor([1. 2. 1.], shape=(3,), dtype=float64)
```

Parameters

- **mask** (*bool*) – Boolean mask (boolean or tensor object of booleans)
- **tensor_in_1** (*Tensor*) – Tensor object
- **tensor_in_2** (*Tensor*) – Tensor object

Returns The result of the mask being applied to the tensors.

Return type TensorFlow Tensor

zeros(*shape*, *dtype='float'*)

13.4.4 jax_backend

class pyhf.tensor.jax_backend.**jax_backend**(***kwargs*)

Bases: object

JAX backend for pyhf

__init__(***kwargs*)

Attributes

name

precision

dtypemap

default_do_grad

Methods

_setup()
Run any global setups for the jax lib.

abs(*tensor*)

astensor(*tensor_in*, *dtype='float'*)
Convert to a JAX ndarray.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> tensor
DeviceArray([[1., 2., 3.],
             [4., 5., 6.]], dtype=float64)
>>> type(tensor)
<class '...DeviceArray'>
```

Parameters **tensor_in** (*Number or Tensor*) – Tensor object

Returns A multi-dimensional, fixed-size homogeneous array.

Return type *jaxlib.xla_extension.DeviceArray*

boolean_mask(*tensor*, *mask*)

clip(*tensor_in*, *min_value*, *max_value*)

Clips (limits) the tensor values to be within a specified min and max.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> a = pyhf.tensorlib.astensor([-2, -1, 0, 1, 2])
>>> pyhf.tensorlib.clip(a, -1, 1)
DeviceArray([-1., -1.,  0.,  1.,  1.], dtype=float64)
```

Parameters

- **tensor_in** (tensor) – The input tensor object
- **min_value** (scalar or tensor or None) – The minimum value to be cliped to
- **max_value** (scalar or tensor or None) – The maximum value to be cliped to

Returns A clipped *tensor*

Return type JAX ndarray

concatenate(*sequence*, *axis=0*)

Join a sequence of arrays along an existing axis.

Parameters

- **sequence** – sequence of tensors
- **axis** – dimension along which to concatenate

Returns the concatenated tensor

Return type output

conditional(*predicate*, *true_callable*, *false_callable*)

Runs a callable conditional on the boolean value of the evaluation of a predicate

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> tensorlib = pyhf.tensorlib
>>> a = tensorlib.astensor([4])
>>> b = tensorlib.astensor([5])
>>> tensorlib.conditional((a < b)[0], lambda: a + b, lambda: a - b)
DeviceArray([9.], dtype=float64)
```

Parameters

- **predicate** (scalar) – The logical condition that determines which callable to evaluate
- **true_callable** (callable) – The callable that is evaluated when the predicate evaluates to true
- **false_callable** (callable) – The callable that is evaluated when the predicate evaluates to false

Returns The output of the callable that was evaluated

Return type JAX ndarray

divide(*tensor_in_1*, *tensor_in_2*)

einsum(*subscripts*, **operands*)

Evaluates the Einstein summation convention on the operands.

Using the Einstein summation convention, many common multi-dimensional array operations can be represented in a simple fashion. This function provides a way to compute such summations. The best way to understand this function is to try the examples below, which show how many common NumPy functions can be implemented as calls to einsum.

Parameters

- **subscripts** – str, specifies the subscripts for summation
- **operands** – list of array_like, these are the tensors for the operation

Returns the calculation based on the Einstein summation convention

Return type tensor

erf(*tensor_in*)

The error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> pyhf.tensorlib.erf(a)
DeviceArray([-0.99532227, -0.84270079,  0.        ,  0.84270079,
              0.99532227], dtype=float64)
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the error function at the given points.

Return type JAX ndarray

erfinv(*tensor_in*)
The inverse of the error function of complex argument.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> a = pyhf.tensorlib.astensor([-2., -1., 0., 1., 2.])
>>> pyhf.tensorlib.erfinv(pyhf.tensorlib.erf(a))
DeviceArray([-2., -1.,  0.,  1.,  2.], dtype=float64)
```

Parameters **tensor_in** (tensor) – The input tensor object

Returns The values of the inverse of the error function at the given points.

Return type JAX ndarray

exp(*tensor_in*)

gather(*tensor*, *indices*)

isfinite(*tensor*)

log(*tensor_in*)

normal(*x*, *mu*, *sigma*)
The probability density function of the Normal distribution evaluated at `x` given parameters of mean of `mu` and standard deviation of `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> pyhf.tensorlib.normal(0.5, 0., 1.)
DeviceArray(0.35206533, dtype=float64)
>>> values = pyhf.tensorlib.astensor([0.5, 2.0])
>>> means = pyhf.tensorlib.astensor([0., 2.3])
>>> sigmas = pyhf.tensorlib.astensor([1., 0.8])
>>> pyhf.tensorlib.normal(values, means, sigmas)
DeviceArray([0.35206533, 0.46481887], dtype=float64)
```

Parameters

- **x** (tensor or float) – The value at which to evaluate the Normal distribution p.d.f.
- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns Value of Normal(x|mu, sigma)

Return type JAX ndarray

normal_cdf(*x*, *mu=0*, *sigma=1*)
The cumulative distribution function for the Normal distribution

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> pyhf.tensorlib.normal_cdf(0.8)
DeviceArray(0.7881446, dtype=float64)
>>> values = pyhf.tensorlib.astensor([0.8, 2.0])
>>> pyhf.tensorlib.normal_cdf(values)
DeviceArray([0.7881446 , 0.97724987], dtype=float64)
```

Parameters

- **x** (tensor or float) – The observed value of the random variable to evaluate the CDF for
- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns The CDF

Return type JAX ndarray

normal_dist(*mu*, *sigma*)

The Normal distribution with mean `mu` and standard deviation `sigma`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> means = pyhf.tensorlib.astensor([5, 8])
>>> stds = pyhf.tensorlib.astensor([1, 0.5])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> normals = pyhf.tensorlib.normal_dist(means, stds)
>>> normals.log_prob(values)
DeviceArray([-1.41893853, -2.22579135], dtype=float64)
```

Parameters

- **mu** (tensor or float) – The mean of the Normal distribution
- **sigma** (tensor or float) – The standard deviation of the Normal distribution

Returns The Normal distribution class

Return type Normal distribution

normal_logpdf(*x*, *mu*, *sigma*)

ones(*shape*, *dtype='float'*)

outer(*tensor_in_1*, *tensor_in_2*)

poisson(*n*, *lam*)

The continuous approximation, using $n! = \Gamma(n+1)$, to the probability mass function of the Poisson distribution evaluated at `n` given the parameter `lam`.

Note: Though the p.m.f of the Poisson distribution is not defined for $\lambda = 0$, the limit as $\lambda \to 0$ is still defined, which gives a degenerate p.m.f. of

$$\lim_{\lambda \to 0} \text{Pois}(n|\lambda) = \begin{cases} 1, & n = 0, \\ 0, & n > 0 \end{cases}$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> pyhf.tensorlib.poisson(5., 6.)
DeviceArray(0.16062314, dtype=float64, weak_type=True)
>>> values = pyhf.tensorlib.astensor([5., 9.])
>>> rates = pyhf.tensorlib.astensor([6., 8.])
>>> pyhf.tensorlib.poisson(values, rates)
DeviceArray([0.16062314, 0.12407692], dtype=float64)
```

Parameters

- **n** (tensor or float) – The value at which to evaluate the approximation to the Poisson distribution p.m.f. (the observed number of events)
- **lam** (tensor or float) – The mean of the Poisson distribution p.m.f. (the expected number of events)

Returns Value of the continuous approximation to Poisson(n|lam)

Return type JAX ndarray

poisson_dist(*rate*)

The Poisson distribution with rate parameter rate.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> rates = pyhf.tensorlib.astensor([5, 8])
>>> values = pyhf.tensorlib.astensor([4, 9])
>>> poissons = pyhf.tensorlib.poisson_dist(rates)
>>> poissons.log_prob(values)
DeviceArray([-1.74030218, -2.0868536 ], dtype=float64)
```

Parameters **rate** (tensor or float) – The mean of the Poisson distribution (the expected number of events)

Returns The Poisson distribution class

Return type Poisson distribution

poisson_logpdf(*n*, *lam*)

power(*tensor_in_1*, *tensor_in_2*)

product(*tensor_in*, *axis=None*)

ravel(*tensor*)
Return a flattened view of the tensor, not a copy.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> pyhf.tensorlib.ravel(tensor)
DeviceArray([1., 2., 3., 4., 5., 6.], dtype=float64)
```

Parameters **tensor** (*Tensor*) – Tensor object

Returns A flattened array.

Return type *jaxlib.xla_extension.DeviceArray*

reshape(*tensor*, *newshape*)

shape(*tensor*)

simple_broadcast(**args*)
Broadcast a sequence of 1 dimensional arrays.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> pyhf.tensorlib.simple_broadcast(
...   pyhf.tensorlib.astensor([1]),
...   pyhf.tensorlib.astensor([2, 3, 4]),
...   pyhf.tensorlib.astensor([5, 6, 7]))
[DeviceArray([1., 1., 1.], dtype=float64), DeviceArray([2., 3., 4.],␣
↪dtype=float64), DeviceArray([5., 6., 7.], dtype=float64)]
```

Parameters **args** (*Array of Tensors*) – Sequence of arrays

Returns The sequence broadcast together.

Return type list of Tensors

sqrt(*tensor_in*)

stack(*sequence*, *axis=0*)

sum(*tensor_in*, *axis=None*)

tile(*tensor_in*, *repeats*)
Repeat tensor data along a specific dimension

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> a = pyhf.tensorlib.astensor([[1.0], [2.0]])
>>> pyhf.tensorlib.tile(a, (1, 2))
DeviceArray([[1., 1.],
             [2., 2.]], dtype=float64)
```

Parameters

- **tensor_in** (tensor) – The tensor to be repeated
- **repeats** (tensor) – The tuple of multipliers for each dimension

Returns The tensor with repeated axes

Return type JAX ndarray

to_numpy(*tensor_in*)

Convert the TensorFlow tensor to a numpy.ndarray.

Example

```
>>> import pyhf
>>> pyhf.set_backend("jax")
>>> tensor = pyhf.tensorlib.astensor([[1.0, 2.0, 3.0], [4.0, 5.0, 6.0]])
>>> tensor
DeviceArray([[1., 2., 3.],
             [4., 5., 6.]], dtype=float64)
>>> numpy_ndarray = pyhf.tensorlib.to_numpy(tensor)
>>> numpy_ndarray
array([[1., 2., 3.],
       [4., 5., 6.]])
>>> type(numpy_ndarray)
<class 'numpy.ndarray'>
```

Parameters **tensor_in** (tensor) – The input tensor object.

Returns The tensor converted to a NumPy ndarray.

Return type numpy.ndarray

tolist(*tensor_in*)

where(*mask*, *tensor_in_1*, *tensor_in_2*)

zeros(*shape*, *dtype='float'*)

13.5 Optimizers

mixins.OptimizerMixin	Mixin Class to build optimizers.
opt_scipy.scipy_optimizer	Optimizer that uses scipy.optimize.minimize().
opt_minuit.minuit_optimizer	Optimizer that minimizes via iminuit.Minuit.migrad().

13.5.1 OptimizerMixin

class pyhf.optimize.mixins.**OptimizerMixin**(***kwargs*)

Bases: object

Mixin Class to build optimizers.

__init__(***kwargs*)

Create an optimizer.

Parameters

- **maxiter** (int) – maximum number of iterations. Default is 100000.
- **verbose** (int) – verbose output level during minimization. Default is off (0).

Attributes

maxiter

verbose

Methods

_internal_minimize(*func*, *x0*, *do_grad=False*, *bounds=None*, *fixed_vals=None*, *options={}*, *par_names=None*)

_internal_postprocess(*fitresult*, *stitch_pars*, *return_uncertainties=False*)

Post-process the fit result.

Returns A modified version of the fit result.

Return type fitresult (scipy.optimize.OptimizeResult)

minimize(*objective*, *data*, *pdf*, *init_pars*, *par_bounds*, *fixed_vals=None*, *return_fitted_val=False*, *return_result_obj=False*, *return_uncertainties=False*, *return_correlations=False*, *do_grad=None*, *do_stitch=False*, ***kwargs*)

Find parameters that minimize the objective.

Parameters

- **objective** (func) – objective function
- **data** (list) – observed data
- **pdf** (Model) – The statistical model adhering to the schema model.json
- **init_pars** (list of float) – The starting values of the model parameters for minimization.

- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be (n, 2) for n model parameters.
- **fixed_vals** (list of list/tuple) – The pairs of index and constant value for a constant model parameter during minimization. Set to None to allow all parameters to float.
- **return_fitted_val** (bool) – Return bestfit value of the objective. Default is off (False).
- **return_result_obj** (bool) – Return scipy.optimize.OptimizeResult. Default is off (False).
- **return_uncertainties** (bool) – Return uncertainties on the fitted parameters. Default is off (False).
- **return_correlations** (bool) – Return correlations of the fitted parameters. Default is off (False).
- **do_grad** (bool) – enable autodifferentiation mode. Default depends on backend (pyhf.tensorlib.default_do_grad).
- **do_stitch** (bool) – enable splicing/stitching fixed parameter.
- **kwargs** – other options to pass through to underlying minimizer

Returns

- parameters (tensor): fitted parameters
- minimum (float): if return_fitted_val flagged, return minimized objective value
- result (scipy.optimize.OptimizeResult): if return_result_obj flagged

Return type Fitted parameters or tuple of results

13.5.2 scipy_optimizer

class pyhf.optimize.opt_scipy.**scipy_optimizer**(**args*, ***kwargs*)

Bases: *pyhf.optimize.mixins.OptimizerMixin*

Optimizer that uses scipy.optimize.minimize().

__init__(**args*, ***kwargs*)

Initialize the scipy_optimizer.

See *pyhf.optimize.mixins.OptimizerMixin* for other configuration options.

Parameters

- **tolerance** (float) – Tolerance for termination. See specific optimizer for detailed meaning. Default is None.
- **solver_options** (dict) – additional solver options. See scipy.optimize.show_options() for additional options of optimization solvers.

Attributes

name

tolerance

solver_options

maxiter

verbose

Methods

_get_minimizer(*objective_and_grad*, *init_pars*, *init_bounds*, *fixed_vals=None*, *do_grad=False*, *par_names=None*)

_minimize(*minimizer*, *func*, *x0*, *do_grad=False*, *bounds=None*, *fixed_vals=None*, *options={}*)

Same signature as `scipy.optimize.minimize()`.

Minimizer Options:

- maxiter (`int`): Maximum number of iterations. Default is `100000`.
- verbose (`bool`): Print verbose output during minimization. Default is `False`.
- method (`str`): Minimization routine. Default is `'SLSQP'`.
- tolerance (`float`): Tolerance for termination. See specific optimizer for detailed meaning. Default is `None`.
- solver_options (`dict`): additional solver options. See `scipy.optimize.show_options()` for additional options of optimization solvers.

Returns the fit result

Return type fitresult (scipy.optimize.OptimizeResult)

13.5.3 minuit_optimizer

class pyhf.optimize.opt_minuit.**minuit_optimizer**(**args*, ***kwargs*)

Bases: *pyhf.optimize.mixins.OptimizerMixin*

Optimizer that minimizes via `iminuit.Minuit.migrad()`.

__init__(**args*, ***kwargs*)

Create `iminuit.Minuit` optimizer.

Note: `errordef` should be 1.0 for a least-squares cost function and 0.5 for negative log-likelihood function. See page 37 of http://hep.fi.infn.it/minuit.pdf. This parameter is sometimes called `UP` in the `MINUIT` docs.

Parameters

- **errordef** (`float`) – See minuit docs. Default is `1.0`.
- **steps** (`int`) – Number of steps for the bounds. Default is `1000`.
- **strategy** (`int`) – See `iminuit.Minuit.strategy`. Default is `None`.

- **tolerance** (float) – Tolerance for termination. See specific optimizer for detailed meaning. Default is 0.1.

Attributes

name

errordef

steps

strategy

tolerance

maxiter

verbose

Methods

_get_minimizer(*objective_and_grad*, *init_pars*, *init_bounds*, *fixed_vals=None*, *do_grad=False*, *par_names=None*)

_minimize(*minimizer*, *func*, *x0*, *do_grad=False*, *bounds=None*, *fixed_vals=None*, *options={}*)

Same signature as scipy.optimize.minimize().

Note: an additional *minuit* is injected into the fitresult to get the underlying minimizer.

Minimizer Options:

- maxiter (int): Maximum number of iterations. Default is 100000.
- strategy (int): See iminuit.Minuit.strategy. Default is to configure in response to do_grad.
- tolerance (float): Tolerance for termination. See specific optimizer for detailed meaning. Default is 0.1.

Returns the fit result

Return type fitresult (scipy.optimize.OptimizeResult)

13.6 Modifiers

histosys
normfactor
normsys
shapefactor
shapesys

continues on next page

Table 9 – continued from previous page

staterror	

13.6.1 pyhf.modifiers.histosys

Description

Classes

histosys_builder(config)	Builder class for collecting histoys modifier data
histosys_combined(modifiers, pdfconfig, ...)	

histosys_builder

class pyhf.modifiers.histosys.**histosys_builder**(*config*)

Bases: object

Builder class for collecting histoys modifier data

__init__(*config*)

Methods

append(*key*, *channel*, *sample*, *thismod*, *defined_samp*)

collect(*thismod*, *nom*)

finalize()

histosys_combined

class pyhf.modifiers.histosys.**histosys_combined**(*modifiers*, *pdfconfig*, *builder_data*, *interpcode='code0'*, *batch_size=None*)

Bases: object

__init__(*modifiers*, *pdfconfig*, *builder_data*, *interpcode='code0'*, *batch_size=None*)

Attributes

name = 'histosys'

op_code = 'addition'

Methods

_precompute()

apply(*pars*)

Returns Shape (n_modifiers, n_global_samples, n_alphas, n_global_bin)

Return type modification tensor

Functions

required_parset(sample_data, modifier_data)	

pyhf.modifiers.histosys.required_parset

pyhf.modifiers.histosys.**required_parset**(*sample_data*, *modifier_data*)

13.6.2 pyhf.modifiers.normfactor

Description

Classes

normfactor_builder(config)	Builder class for collecting normfactor modifier data
normfactor_combined(modifiers, pdfconfig, ...)	

normfactor_builder

class pyhf.modifiers.normfactor.**normfactor_builder**(*config*)

Bases: object

Builder class for collecting normfactor modifier data

__init__(*config*)

Methods

append(*key*, *channel*, *sample*, *thismod*, *defined_samp*)

collect(*thismod*, *nom*)

finalize()

normfactor_combined

class pyhf.modifiers.normfactor.**normfactor_combined**(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Bases: object

__init__(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Attributes

name = 'normfactor'

op_code = 'multiplication'

Methods

_precompute()

apply(*pars*)

Returns Shape (n_modifiers, n_global_samples, n_alphas, n_global_bin)

Return type modification tensor

Functions

required_parset(sample_data, modifier_data)	

pyhf.modifiers.normfactor.required_parset

pyhf.modifiers.normfactor.**required_parset**(*sample_data*, *modifier_data*)

13.6.3 pyhf.modifiers.normsys

Description

Classes

normsys_builder(config)	Builder class for collecting normsys modifier data
normsys_combined(modifiers, pdfconfig, ...)	

normsys_builder

class pyhf.modifiers.normsys.**normsys_builder**(*config*)

Bases: object

Builder class for collecting normsys modifier data

__init__(*config*)

Methods

append(*key*, *channel*, *sample*, *thismod*, *defined_samp*)

collect(*thismod*, *nom*)

finalize()

normsys_combined

class pyhf.modifiers.normsys.**normsys_combined**(*modifiers*, *pdfconfig*, *builder_data*, *interpcode='code1'*, *batch_size=None*)

Bases: object

__init__(*modifiers*, *pdfconfig*, *builder_data*, *interpcode='code1'*, *batch_size=None*)

Attributes

name = 'normsys'

op_code = 'multiplication'

Methods

_precompute()

apply(*pars*)

Returns Shape (n_modifiers, n_global_samples, n_alphas, n_global_bin)

Return type modification tensor

Functions

required_parset(sample_data, modifier_data)

pyhf.modifiers.normsys.required_parset

pyhf.modifiers.normsys.**required_parset**(*sample_data*, *modifier_data*)

13.6.4 pyhf.modifiers.shapefactor

Description

Classes

shapefactor_builder(config)	Builder class for collecting shapefactor modifier data
shapefactor_combined(modifiers, pdfconfig, ...)	

shapefactor_builder

class pyhf.modifiers.shapefactor.**shapefactor_builder**(*config*)

Bases: object

Builder class for collecting shapefactor modifier data

__init__(*config*)

Methods

append(*key*, *channel*, *sample*, *thismod*, *defined_samp*)

collect(*thismod*, *nom*)

finalize()

shapefactor_combined

class pyhf.modifiers.shapefactor.**shapefactor_combined**(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Bases: object

__init__(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Parameters

- **modifiers** (list of tuple) – List of tuples of form (modifier, modifier_type).
- **pdfconfig** (*_ModelConfig*) – Configuration for the model.
- **builder_data** (dict) – Map of keys 'modifier_type/modifier' to the channels and bins they are applied to.
- **batch_size** (int) – The number of rows in the resulting tensor. If None defaults to 1.

Imagine a situation where we have 2 channels (SR, CR), 3 samples (sig1, bkg1, bkg2), and 2 *shapefactor* modifiers (coupled_shapefactor, uncoupled_shapefactor). Let's say this is the set-up:

```
SR(nbins=2)
  sig1 -> subscribes to normfactor
  bkg1 -> subscribes to coupled_shapefactor
CR(nbins=3)
  bkg2 -> subscribes to coupled_shapefactor, uncoupled_shapefactor
```

The `coupled_shapefactor` needs to have 3 nuisance parameters to account for the `CR`, with 2 of them shared in the `SR`. The `uncoupled_shapefactor` just has 3 nuisance parameters.

`self._parindices` will look like

```
[0, 1, 2, 3, 4, 5, 6]
```

`self._shapefactor_indices` will look like

```
[0, 1, 2, 3, 4, 5, 6]
[[1,2,3],[4,5,6]]
 ^^^^^^^          = coupled_shapefactor
         ^^^^^^^ = uncoupled_shapefactor
```

with the 0th par-index corresponding to the *normfactor*. Because the `SR` channel has 2 bins, and the `CR` channel has 3 bins (with `SR` before `CR`), `global_concatenated_bin_indices` looks like

```
[0, 1, 0, 1, 2]
^^^^^             = SR channel

      ^^^^^^^^^  = CR channel
```

So now we need to gather the corresponding *shapefactor* indices according to `global_concatenated_bin_indices`. Therefore `self._shapefactor_indices` now looks like

```
[[1, 2, 1, 2, 3], [4, 5, 4, 5, 6]]
```

and at that point can be used to compute the effect of *shapefactor*.

Attributes

name = 'shapefactor'

op_code = 'multiplication'

Methods

_precompute()

apply(*pars*)

Returns Shape (n_modifiers, n_global_samples, n_alphas, n_global_bin)

Return type modification tensor

Functions

required_parset(sample_data, modifier_data)	

pyhf.modifiers.shapefactor.required_parset

pyhf.modifiers.shapefactor.**required_parset**(*sample_data*, *modifier_data*)

13.6.5 pyhf.modifiers.shapesys

Description

Classes

shapesys_builder(config)	Builder class for collecting shapesys modifier data
shapesys_combined(modifiers, pdfconfig, ...)	

shapesys_builder

class pyhf.modifiers.shapesys.**shapesys_builder**(*config*)

Bases: object

Builder class for collecting shapesys modifier data

__init__(*config*)

Methods

append(*key*, *channel*, *sample*, *thismod*, *defined_samp*)

collect(*thismod*, *nom*)

finalize()

shapesys_combined

class pyhf.modifiers.shapesys.**shapesys_combined**(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Bases: object

__init__(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Attributes

name = 'shapesys'

op_code = 'multiplication'

Methods

_precompute()

_reindex_access_field(*pdfconfig*)

apply(*pars*)

Returns Shape (n_modifiers, n_global_samples, n_alphas, n_global_bin)

Return type modification tensor

Functions

required_parset(sample_data, modifier_data)	

pyhf.modifiers.shapesys.required_parset

pyhf.modifiers.shapesys.**required_parset**(*sample_data*, *modifier_data*)

13.6.6 pyhf.modifiers.staterror

Description

Classes

staterror_builder(config)	Builder class for collecting staterror modifier data
staterror_combined(modifiers, pdfconfig, ...)	

staterror_builder

class pyhf.modifiers.staterror.**staterror_builder**(*config*)

Bases: object

Builder class for collecting staterror modifier data

__init__(*config*)

Methods

append(*key*, *channel*, *sample*, *thismod*, *defined_samp*)

collect(*thismod*, *nom*)

finalize()

staterror_combined

class pyhf.modifiers.staterror.**staterror_combined**(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Bases: object

__init__(*modifiers*, *pdfconfig*, *builder_data*, *batch_size=None*)

Attributes

name = 'staterror'

op_code = 'multiplication'

Methods

_precompute()

_reindex_access_field(*pdfconfig*)

apply(*pars*)

Functions

required_parset(sigmas, fixed)	

pyhf.modifiers.staterror.required_parset

pyhf.modifiers.staterror.**required_parset**(*sigmas*, *fixed*)

13.7 Interpolators

code0	The piecewise-linear interpolation strategy.
code1	The piecewise-exponential interpolation strategy.
code2	The quadratic interpolation and linear extrapolation strategy.
code4	The polynomial interpolation and exponential extrapolation strategy.
code4p	The piecewise-linear interpolation strategy, with polynomial at $\lvert a\rvert < 1$.

13.7.1 code0

class pyhf.interpolators.**code0**(*histogramssets*, *subscribe=True*)

Bases: object

The piecewise-linear interpolation strategy.

$$\sigma_{sb}(\vec{\alpha}) = \sigma^0_{sb}(\vec{\alpha}) + \underbrace{\sum_{p \in \text{Syst}} I_{\text{lin.}}(\alpha_p; \sigma^0_{sb}, \sigma^+_{psb}, \sigma^-_{psb})}_{\text{deltas to calculate}}$$

with

$$I_{\text{lin.}}(\alpha; I^0, I^+, I^-) = \begin{cases} \alpha(I^+ - I^0) & \alpha \geq 0 \\ \alpha(I^0 - I^-) & \alpha < 0 \end{cases}$$

__init__(*histogramssets*, *subscribe=True*)

Piecewise-linear Interpolation.

Methods

_precompute()

_precompute_alphasets(*alphasets_shape*)

13.7.2 code1

class pyhf.interpolators.**code1**(*histogramssets*, *subscribe=True*)

Bases: object

The piecewise-exponential interpolation strategy.

$$\sigma_{sb}(\vec{\alpha}) = \sigma^0_{sb}(\vec{\alpha}) \underbrace{\prod_{p \in \text{Syst}} I_{\text{exp.}}(\alpha_p; \sigma^0_{sb}, \sigma^+_{psb}, \sigma^-_{psb})}_{\text{factors to calculate}}$$

with

$$I_{\text{exp.}}(\alpha; I^0, I^+, I^-) = \begin{cases} \left(\frac{I^+}{I^0}\right)^{\alpha} & \alpha \geq 0 \\ \left(\frac{I^-}{I^0}\right)^{-\alpha} & \alpha < 0 \end{cases}$$

__init__(*histogramssets*, *subscribe=True*)

Piecewise-Exponential Interpolation.

Methods

_precompute()

_precompute_alphasets(*alphasets_shape*)

13.7.3 code2

class pyhf.interpolators.**code2**(*histogramssets*, *subscribe=True*)

Bases: object

The quadratic interpolation and linear extrapolation strategy.

$$\sigma_{sb}(\vec{\alpha}) = \sigma_{sb}^{0}(\vec{\alpha}) + \underbrace{\sum_{p\in\text{Syst}} I_{\text{quad.|lin.}}(\alpha_p; \sigma_{sb}^{0}, \sigma_{psb}^{+}, \sigma_{psb}^{-})}_{\text{deltas to calculate}}$$

with

$$I_{\text{quad.|lin.}}(\alpha; I^0, I^+, I^-) = \begin{cases} (b+2a)(\alpha-1) & \alpha \geq 1 \\ a\alpha^2 + b\alpha & |\alpha| < 1 \\ (b-2a)(\alpha+1) & \alpha < -1 \end{cases}$$

and

$$a = \frac{1}{2}(I^+ + I^-) - I^0 \qquad \text{and} \qquad b = \frac{1}{2}(I^+ - I^-)$$

__init__(*histogramssets*, *subscribe=True*)

Quadratic Interpolation.

Methods

_precompute()

_precompute_alphasets(*alphasets_shape*)

13.7.4 code4

class pyhf.interpolators.**code4**(*histogramssets*, *subscribe=True*, *alpha0=1*)

Bases: object

The polynomial interpolation and exponential extrapolation strategy.

$$\sigma_{sb}(\vec{\alpha}) = \sigma_{sb}^{0}(\vec{\alpha}) \underbrace{\prod_{p\in\text{Syst}} I_{\text{poly|exp.}}(\alpha_p; \sigma_{sb}^{0}, \sigma_{psb}^{+}, \sigma_{psb}^{-}, \alpha_0)}_{\text{factors to calculate}}$$

with

$$I_{\text{poly|exp.}}(\alpha; I^0, I^+, I^-, \alpha_0) = \begin{cases} \left(\frac{I^+}{I^0}\right)^{\alpha} & \alpha \geq \alpha_0 \\ 1 + \sum_{i=1}^{6} a_i \alpha^i & |\alpha| < \alpha_0 \\ \left(\frac{I^-}{I^0}\right)^{-\alpha} & \alpha < -\alpha_0 \end{cases}$$

and the a_i are fixed by the boundary conditions

$$\sigma_{sb}(\alpha = \pm\alpha_0), \left.\frac{\mathrm{d}\sigma_{sb}}{\mathrm{d}\alpha}\right|_{\alpha=\pm\alpha_0}, \text{and } \left.\frac{\mathrm{d}^2\sigma_{sb}}{\mathrm{d}\alpha^2}\right|_{\alpha=\pm\alpha_0}.$$

Namely that $\sigma_{sb}(\vec{\alpha})$ is continuous, and its first- and second-order derivatives are continuous as well.

__init__(*histogramssets*, *subscribe=True*, *alpha0=1*)

Polynomial Interpolation.

Methods

_precompute()

_precompute_alphasets(*alphasets_shape*)

13.7.5 code4p

class pyhf.interpolators.**code4p**(*histogramssets*, *subscribe=True*)
Bases: object

The piecewise-linear interpolation strategy, with polynomial at $|a| < 1$.

$$\sigma_{sb}(\vec{\alpha}) = \sigma^0_{sb}(\vec{\alpha}) + \underbrace{\sum_{p \in \text{Syst}} I_{\text{lin.}}(\alpha_p; \sigma^0_{sb}, \sigma^+_{psb}, \sigma^-_{psb})}_{\text{deltas to calculate}}$$

__init__(*histogramssets*, *subscribe=True*)
Piecewise-Linear + Polynomial Interpolation.

Methods

_precompute()

_precompute_alphasets(*alphasets_shape*)

13.8 Inference

13.8.1 Test Statistics

test_statistics.q0	The test statistic, q_0, for discovery of a positive signal as defined in Equation (12) in [1007.1727], for $\mu = 0$.
test_statistics.qmu	The test statistic, q_μ, for establishing an upper limit on the strength parameter, μ, as defined in Equation (14) in [1007.1727]
test_statistics.qmu_tilde	The "alternative" test statistic, $\tilde{q}_\mu$, for establishing an upper limit on the strength parameter, μ, for models with bounded POI, as defined in Equation (16) in [1007.1727]
test_statistics.tmu	The test statistic, t_μ, for establishing a two-sided interval on the strength parameter, μ, as defined in Equation (8) in [1007.1727]
test_statistics.tmu_tilde	The test statistic, $\tilde{t}_\mu$, for establishing a two-sided interval on the strength parameter, μ, for models with bounded POI, as defined in Equation (11) in [1007.1727]
utils.get_test_stat	Get the test statistic function by name.

pyhf.infer.test_statistics.q0

pyhf.infer.test_statistics.**q0**(*mu*, *data*, *pdf*, *init_pars*, *par_bounds*, *fixed_params*, *return_fitted_pars=False*)

The test statistic, q_0, for discovery of a positive signal as defined in Equation (12) in [1007.1727], for $\mu = 0$.

$$q_0 = \begin{cases} -2\ln\lambda\left(0\right), & \hat{\mu} \geq 0, \\ 0, & \hat{\mu} < 0, \end{cases} \tag{13.1}$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [60, 65]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> test_mu = 0.0
>>> init_pars = model.config.suggested_init()
>>> par_bounds = model.config.suggested_bounds()
>>> fixed_params = model.config.suggested_fixed()
>>> pyhf.infer.test_statistics.q0(test_mu, data, model, init_pars, par_bounds,␣
↪fixed_params)
array(2.98339447)
```

Access the best-fit parameter tensors:

```
>>> pyhf.infer.test_statistics.q0(test_mu, data, model, init_pars, par_bounds,␣
↪fixed_params, return_fitted_pars = True)
(array(2.98339447), (array([0.        , 1.03050845, 1.12128752]), array([0.95260667,
↪ 0.99635345, 1.02140172])))
```

Parameters

- **mu** (*Number or Tensor*) – The signal strength parameter (must be set to zero)
- **data** (*Tensor*) – The data to be considered
- **pdf** (Model) – The HistFactory statistical model used in the likelihood ratio calculation
- **init_pars** (list of float) – The starting values of the model parameters for minimization.
- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.
- **fixed_params** (list of bool) – The flag to set a parameter constant to its starting value during minimization.
- **return_fitted_pars** (bool) – Return the best-fit parameter tensors the fixed-POI and unconstrained fits have converged on (i.e. $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$)

Returns

- The calculated test statistic, q_0
- The parameter tensors corresponding to the constrained and unconstrained best fit, $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$. Only returned if `return_fitted_pars` is `True`.

Return type Tuple of a Float and a Tuple of Tensors

pyhf.infer.test_statistics.qmu

pyhf.infer.test_statistics.**qmu**(*mu*, *data*, *pdf*, *init_pars*, *par_bounds*, *fixed_params*, *return_fitted_pars=False*)

The test statistic, q_μ, for establishing an upper limit on the strength parameter, μ, as defined in Equation (14) in [1007.1727]

$$q_\mu = \begin{cases} -2\ln\lambda\left(\mu\right), & \hat{\mu} < \mu, \\ 0, & \hat{\mu} > \mu \end{cases} \tag{13.2}$$

where $\lambda\left(\mu\right)$ is the profile likelihood ratio as defined in Equation (7)

$$\lambda\left(\mu\right) = \frac{L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}\right)}{L\left(\hat{\mu}, \hat{\boldsymbol{\theta}}\right)}.$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> test_mu = 1.0
>>> init_pars = model.config.suggested_init()
>>> par_bounds = model.config.suggested_bounds()
>>> par_bounds[model.config.poi_index] = [-10.0, 10.0]
>>> fixed_params = model.config.suggested_fixed()
>>> pyhf.infer.test_statistics.qmu(test_mu, data, model, init_pars, par_bounds,␣
↪fixed_params)
array(3.9549891)
```

Access the best-fit parameter tensors:

```
>>> pyhf.infer.test_statistics.qmu(test_mu, data, model, init_pars, par_bounds,␣
↪fixed_params, return_fitted_pars = True)
(array(3.9549891), (array([1.        , 0.97224597, 0.87553894]), array([-0.06679525,
↪  1.00555369,  0.96930896])))
```

Parameters

- **mu** (*Number or Tensor*) – The signal strength parameter
- **data** (*Tensor*) – The data to be considered
- **pdf** (Model) – The HistFactory statistical model used in the likelihood ratio calculation
- **init_pars** (list of float) – The starting values of the model parameters for minimization.
- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.

- **fixed_params** (list of bool) – The flag to set a parameter constant to its starting value during minimization.
- **return_fitted_pars** (bool) – Return the best-fit parameter tensors the fixed-POI and unconstrained fits have converged on (i.e. $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$)

Returns

- The calculated test statistic, q_μ
- The parameter tensors corresponding to the constrained and unconstrained best fit, $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$. Only returned if `return_fitted_pars` is `True`.

Return type Tuple of a Float and a Tuple of Tensors

pyhf.infer.test_statistics.qmu_tilde

pyhf.infer.test_statistics.**qmu_tilde**(*mu*, *data*, *pdf*, *init_pars*, *par_bounds*, *fixed_params*, *return_fitted_pars=False*)

The "alternative" test statistic, $\tilde{q}_\mu$, for establishing an upper limit on the strength parameter, μ, for models with bounded POI, as defined in Equation (16) in [1007.1727]

$$\tilde{q}_\mu = \begin{cases} -2\ln\tilde{\lambda}\left(\mu\right), & \hat{\mu} < \mu, \\ 0, & \hat{\mu} > \mu \end{cases} \tag{13.3}$$

where $\tilde{\lambda}\left(\mu\right)$ is the constrained profile likelihood ratio as defined in Equation (10)

$$\tilde{\lambda}\left(\mu\right) = \begin{cases} \frac{L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu)\right)}{L\left(\hat{\mu}, \hat{\hat{\boldsymbol{\theta}}}(0)\right)}, & \hat{\mu} < 0, \\ \frac{L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu)\right)}{L\left(\hat{\mu}, \hat{\boldsymbol{\theta}}\right)}, & \hat{\mu} \geq 0. \end{cases} \tag{13.4}$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> test_mu = 1.0
>>> init_pars = model.config.suggested_init()
>>> par_bounds = model.config.suggested_bounds()
>>> fixed_params = model.config.suggested_fixed()
>>> pyhf.infer.test_statistics.qmu_tilde(test_mu, data, model, init_pars, par_
↪bounds, fixed_params)
array(3.93824492)
```

Access the best-fit parameter tensors:

```
>>> pyhf.infer.test_statistics.qmu_tilde(test_mu, data, model, init_pars, par_
↪bounds, fixed_params, return_fitted_pars = True)
(array(3.93824492), (array([1.        , 0.97224597, 0.87553894]), array([0.        ,
↪ 1.0030512 , 0.96266961])))
```

Parameters

- **mu** (*Number or Tensor*) – The signal strength parameter
- **data** (tensor) – The data to be considered
- **pdf** (Model) – The statistical model adhering to the schema model.json
- **init_pars** (list of float) – The starting values of the model parameters for minimization.
- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.
- **fixed_params** (list of bool) – The flag to set a parameter constant to its starting value during minimization.
- **return_fitted_pars** (bool) – Return the best-fit parameter tensors the fixed-POI and unconstrained fits have converged on (i.e. $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$)

Returns

- The calculated test statistic, $\tilde{q}_\mu$
- The parameter tensors corresponding to the constrained and unconstrained best fit, $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$. Only returned if `return_fitted_pars` is `True`.

Return type Tuple of a Float and a Tuple of Tensors

pyhf.infer.test_statistics.tmu

pyhf.infer.test_statistics.**tmu**(*mu*, *data*, *pdf*, *init_pars*, *par_bounds*, *fixed_params*, *return_fitted_pars=False*)

The test statistic, t_μ, for establishing a two-sided interval on the strength parameter, μ, as defined in Equation (8) in [1007.1727]

$$t_\mu = -2\ln\lambda\left(\mu\right)$$

where $\lambda\left(\mu\right)$ is the profile likelihood ratio as defined in Equation (7)

$$\lambda\left(\mu\right) = \frac{L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}\right)}{L\left(\hat{\mu}, \hat{\boldsymbol{\theta}}\right)}.$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> test_mu = 1.0
>>> init_pars = model.config.suggested_init()
>>> par_bounds = model.config.suggested_bounds()
>>> par_bounds[model.config.poi_index] = [-10.0, 10.0]
```

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```
>>> fixed_params = model.config.suggested_fixed()
>>> pyhf.infer.test_statistics.tmu(test_mu, data, model, init_pars, par_bounds,␣
↪fixed_params)
array(3.9549891)
```

Access the best-fit parameter tensors:

```
>>> pyhf.infer.test_statistics.tmu(test_mu, data, model, init_pars, par_bounds,␣
↪fixed_params, return_fitted_pars = True)
(array(3.9549891), (array([1.        , 0.97224597, 0.87553894]), array([-0.06679525,
↪  1.00555369,  0.96930896])))
```

Parameters

- **mu** (*Number or Tensor*) – The signal strength parameter
- **data** (*Tensor*) – The data to be considered
- **pdf** (Model) – The statistical model adhering to the schema model.json
- **init_pars** (list of float) – The starting values of the model parameters for minimization.
- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.
- **fixed_params** (list of bool) – The flag to set a parameter constant to its starting value during minimization.
- **return_fitted_pars** (bool) – Return the best-fit parameter tensors the fixed-POI and unconstrained fits have converged on (i.e. $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$)

Returns

- The calculated test statistic, t_μ
- The parameter tensors corresponding to the constrained and unconstrained best fit, $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$. Only returned if `return_fitted_pars` is `True`.

Return type Tuple of a Float and a Tuple of Tensors

pyhf.infer.test_statistics.tmu_tilde

pyhf.infer.test_statistics.**tmu_tilde**(*mu*, *data*, *pdf*, *init_pars*, *par_bounds*, *fixed_params*, *return_fitted_pars=False*)

The test statistic, $\tilde{t}_\mu$, for establishing a two-sided interval on the strength parameter, μ, for models with bounded POI, as defined in Equation (11) in [1007.1727]

$$\tilde{t}_\mu = -2\ln\tilde{\lambda}\left(\mu\right)$$

where $\tilde{\lambda}\left(\mu\right)$ is the constrained profile likelihood ratio as defined in Equation (10)

$$\tilde{\lambda}\left(\mu\right) = \begin{cases} \frac{L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu)\right)}{L\left(\hat{\mu}, \hat{\hat{\boldsymbol{\theta}}}(0)\right)}, & \hat{\mu} < 0, \\ \frac{L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu)\right)}{L\left(\hat{\mu}, \hat{\boldsymbol{\theta}}\right)}, & \hat{\mu} \geq 0. \end{cases} \tag{13.5}$$

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> test_mu = 1.0
>>> init_pars = model.config.suggested_init()
>>> par_bounds = model.config.suggested_bounds()
>>> fixed_params = model.config.suggested_fixed()
>>> pyhf.infer.test_statistics.tmu_tilde(test_mu, data, model, init_pars, par_
↪bounds, fixed_params)
array(3.93824492)
```

Access the best-fit parameter tensors:

```
>>> pyhf.infer.test_statistics.tmu_tilde(test_mu, data, model, init_pars, par_
↪bounds, fixed_params, return_fitted_pars = True)
(array(3.93824492), (array([1.        , 0.97224597, 0.87553894]), array([0.        ,
↪ 1.0030512 , 0.96266961])))
```

Parameters

- **mu** (*Number or Tensor*) – The signal strength parameter
- **data** (tensor) – The data to be considered
- **pdf** (Model) – The statistical model adhering to the schema model.json
- **init_pars** (list of float) – The starting values of the model parameters for minimization.
- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.
- **fixed_params** (list of bool) – The flag to set a parameter constant to its starting value during minimization.
- **return_fitted_pars** (bool) – Return the best-fit parameter tensors the fixed-POI and unconstrained fits have converged on (i.e. $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$)

Returns

- The calculated test statistic, $\tilde{t}_{\mu}$
- The parameter tensors corresponding to the constrained and unconstrained best fit, $\mu, \hat{\hat{\theta}}$ and $\hat{\mu}, \hat{\theta}$. Only returned if `return_fitted_pars` is `True`.

Return type Tuple of a Float and a Tuple of Tensors

pyhf.infer.utils.get_test_stat

pyhf.infer.utils.**get_test_stat**(*name*)

Get the test statistic function by name. The following test statistics are supported:

- *q0()*
- *qmu()*
- *qmu_tilde()*

Example

```
>>> from pyhf.infer import utils, test_statistics
>>> utils.get_test_stat("q0")
<function q0 at 0x...>
>>> utils.get_test_stat("q0") == test_statistics.q0
True
>>> utils.get_test_stat("q")
<function qmu at 0x...>
>>> utils.get_test_stat("q") == test_statistics.qmu
True
>>> utils.get_test_stat("qtilde")
<function qmu_tilde at 0x...>
>>> utils.get_test_stat("qtilde") == test_statistics.qmu_tilde
True
```

Parameters **name** (str) – The name of the test statistic to retrieve

Returns The test statistic function

Return type callable

13.8.2 Calculators

calculators.generate_asimov_data	Compute Asimov Dataset (expected yields at best-fit values) for a given POI value.
calculators.HypoTestFitResults	Fitted model parameters of the fits in *AsymptoticCalculator.teststatistic*
calculators.AsymptoticTestStatDistribution	The distribution the test statistic in the asymptotic case.
calculators.EmpiricalDistribution	The empirical distribution of the test statistic.
calculators.AsymptoticCalculator	The Asymptotic Calculator.
calculators.ToyCalculator	The Toy-based Calculator.
utils.create_calculator	Creates a calculator object of the specified *calctype*.

pyhf.infer.calculators.generate_asimov_data

pyhf.infer.calculators.**generate_asimov_data**(*asimov_mu*, *data*, *pdf*, *init_pars*, *par_bounds*, *fixed_params*, *return_fitted_pars=False*)

Compute Asimov Dataset (expected yields at best-fit values) for a given POI value.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> pyhf.infer.calculators.generate_asimov_data(mu_test, data, model, None, None,␣
↪None)
array([ 60.61229858,  56.52802479, 270.06832542,  48.31545488])
```

It is possible to access the Asimov parameters as well:

```
>>> pyhf.infer.calculators.generate_asimov_data(
...     mu_test, data, model, None, None, None,
...     return_fitted_pars = True
... )
(array([ 60.61229858,  56.52802479, 270.06832542,  48.31545488]), array([1.        ,
↪ 0.97224597, 0.87553894]))
```

Parameters

- **asimov_mu** (float) – The value for the parameter of interest to be used.
- **data** (tensor) – The observed data.
- **pdf** (Model) – The statistical model adhering to the schema model.json.
- **init_pars** (tensor of float) – The starting values of the model parameters for minimization.
- **par_bounds** (tensor) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be (n, 2) for n model parameters.
- **fixed_params** (tensor of bool) – The flag to set a parameter constant to its starting value during minimization.
- **return_fitted_pars** (bool) – Return the best-fit parameter values for the given asimov_mu.

Returns

- The Asimov dataset.
- The Asimov parameters. Only returned if return_fitted_pars is True.

Return type A Tensor or a Tuple of two Tensors

HypoTestFitResults

class pyhf.infer.calculators.**HypoTestFitResults**(*asimov_pars: Tensor*, *free_fit_to_data: Tensor*, *free_fit_to_asimov: Tensor*, *fixed_poi_fit_to_data: Tensor*, *fixed_poi_fit_to_asimov: Tensor*)

Bases: object

Fitted model parameters of the fits in *AsymptoticCalculator.teststatistic*

__init__(*asimov_pars: Tensor*, *free_fit_to_data: Tensor*, *free_fit_to_asimov: Tensor*, *fixed_poi_fit_to_data: Tensor*, *fixed_poi_fit_to_asimov: Tensor*) → None

Attributes

asimov_pars: Tensor

free_fit_to_data: Tensor

free_fit_to_asimov: Tensor

fixed_poi_fit_to_data: Tensor

fixed_poi_fit_to_asimov: Tensor

Methods

AsymptoticTestStatDistribution

class pyhf.infer.calculators.**AsymptoticTestStatDistribution**(*shift*, *cutoff=- inf*)

Bases: object

The distribution the test statistic in the asymptotic case.

Note: These distributions are in $-\hat{\mu}/\sigma$ space. In the ROOT implementation the same sigma is assumed for both hypotheses and p-values etc are computed in that space. This assumption is necessarily valid, but we keep this for compatibility reasons.

In the $-\hat{\mu}/\sigma$ space, the test statistic (i.e. $\hat{\mu}/\sigma$) is normally distributed with unit variance and its mean at the $-\mu'$, where μ' is the true poi value of the hypothesis.

__init__(*shift*, *cutoff=- inf*)

Asymptotic test statistic distribution.

Parameters **shift** (float) – The displacement of the test statistic distribution.

Returns The asymptotic distribution of test statistic.

Return type *AsymptoticTestStatDistribution*

Methods

cdf(*value*)

Compute the value of the cumulative distribution function for a given value of the test statistic.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> bkg_dist = pyhf.infer.calculators.AsymptoticTestStatDistribution(0.0)
>>> bkg_dist.cdf(0.0)
0.5
```

Parameters **value** (float) – The test statistic value.

Returns The integrated probability to observe a test statistic less than or equal to the observed value.

Return type Float

expected_value(*nsigma*)

Return the expected value of the test statistic.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> bkg_dist = pyhf.infer.calculators.AsymptoticTestStatDistribution(0.0)
>>> n_sigma = pyhf.tensorlib.astensor([-2, -1, 0, 1, 2])
>>> bkg_dist.expected_value(n_sigma)
array([-2., -1.,  0.,  1.,  2.])
```

Parameters **nsigma** (int or tensor) – The number of standard deviations.

Returns The expected value of the test statistic.

Return type Float

pvalue(*value*)

The p-value for a given value of the test statistic corresponding to signal strength μ and Asimov strength μ' as defined in Equations (59) and (57) of [1007.1727]

$$p_\mu = 1 - F\left(q_\mu|\mu'\right) = 1 - \Phi\left(\sqrt{q_\mu} - \frac{(\mu - \mu')}{\sigma}\right)$$

with Equation (29)

$$\frac{(\mu - \mu')}{\sigma} = \sqrt{\Lambda} = \sqrt{q_{\mu,A}}$$

given the observed test statistics q_μ and $q_{\mu,A}$.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> bkg_dist = pyhf.infer.calculators.AsymptoticTestStatDistribution(0.0)
>>> bkg_dist.pvalue(0.0)
array(0.5)
```

Parameters **value** (float) – The test statistic value.

Returns The integrated probability to observe a value at least as large as the observed one.

Return type Tensor

EmpiricalDistribution

class pyhf.infer.calculators.**EmpiricalDistribution**(*samples*)

Bases: object

The empirical distribution of the test statistic.

Unlike *AsymptoticTestStatDistribution* where the distribution for the test statistic is normally distributed, the p-values etc are computed from the sampled distribution.

__init__(*samples*)

Empirical distribution.

Parameters **samples** (tensor) – The test statistics sampled from the distribution.

Returns The empirical distribution of the test statistic.

Return type *EmpiricalDistribution*

Methods

expected_value(*nsigma*)

Return the expected value of the test statistic.

Examples

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> mean = pyhf.tensorlib.astensor([5])
>>> std = pyhf.tensorlib.astensor([1])
>>> normal = pyhf.probability.Normal(mean, std)
>>> samples = normal.sample((100,))
>>> dist = pyhf.infer.calculators.EmpiricalDistribution(samples)
>>> dist.expected_value(nsigma=1)
6.15094381209...
```

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> init_pars = model.config.suggested_init()
>>> par_bounds = model.config.suggested_bounds()
>>> fixed_params = model.config.suggested_fixed()
>>> mu_test = 1.0
>>> pdf = model.make_pdf(pyhf.tensorlib.astensor(init_pars))
>>> samples = pdf.sample((100,))
>>> dist = pyhf.infer.calculators.EmpiricalDistribution(
...     pyhf.tensorlib.astensor(
...         [
...             pyhf.infer.test_statistics.qmu_tilde(
...                 mu_test, sample, model, init_pars, par_bounds, fixed_params
...             )
...             for sample in samples
...         ]
...     )
... )
>>> n_sigma = pyhf.tensorlib.astensor([-2, -1, 0, 1, 2])
>>> dist.expected_value(n_sigma)
array([0.00000000e+00, 0.00000000e+00, 5.53671231e-04, 8.29987137e-01,
       2.99592664e+00])
```

Parameters **nsigma** (int or tensor) – The number of standard deviations.

Returns The expected value of the test statistic.

Return type Float

pvalue(*value*)

Compute the p-value for a given value of the test statistic.

Examples

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> mean = pyhf.tensorlib.astensor([5])
>>> std = pyhf.tensorlib.astensor([1])
>>> normal = pyhf.probability.Normal(mean, std)
>>> samples = normal.sample((100,))
>>> dist = pyhf.infer.calculators.EmpiricalDistribution(samples)
>>> dist.pvalue(7)
array(0.02)
```

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> init_pars = model.config.suggested_init()
>>> par_bounds = model.config.suggested_bounds()
>>> fixed_params = model.config.suggested_fixed()
>>> mu_test = 1.0
>>> pdf = model.make_pdf(pyhf.tensorlib.astensor(init_pars))
>>> samples = pdf.sample((100,))
>>> test_stat_dist = pyhf.infer.calculators.EmpiricalDistribution(
...     pyhf.tensorlib.astensor(
...         [pyhf.infer.test_statistics.qmu_tilde(mu_test, sample, model, init_
↪pars, par_bounds, fixed_params) for sample in samples]
...     )
... )
>>> test_stat_dist.pvalue(test_stat_dist.samples[9])
array(0.3)
```

Parameters **value** (float) – The test statistic value.

Returns The integrated probability to observe a value at least as large as the observed one.

Return type Tensor

AsymptoticCalculator

class pyhf.infer.calculators.**AsymptoticCalculator**(*data*, *pdf*, *init_pars=None*, *par_bounds=None*, *fixed_params=None*, *test_stat='qtilde'*, *calc_base_dist='normal'*)

Bases: object

The Asymptotic Calculator.

__init__(*data*, *pdf*, *init_pars=None*, *par_bounds=None*, *fixed_params=None*, *test_stat='qtilde'*, *calc_base_dist='normal'*)

Asymptotic Calculator.

Parameters

- **data** (tensor) – The observed data.
- **pdf** (Model) – The statistical model adhering to the schema model.json.
- **init_pars** (tensor of float) – The starting values of the model parameters for minimization.
- **par_bounds** (tensor) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be (n, 2) for n model parameters.
- **fixed_params** (tensor of bool) – The flag to set a parameter constant to its starting value during minimization.
- **test_stat** (str) – The test statistic to use as a numerical summary of the data: 'qtilde', 'q', or 'q0'.

- `'qtilde'`: (default) performs the calculation using the alternative test statistic, $\tilde{q}_\mu$, as defined under the Wald approximation in Equation (62) of [1007.1727] (*qmu_tilde()*).
- `'q'`: performs the calculation using the test statistic q_μ (*qmu()*).
- `'q0'`: performs the calculation using the discovery test statistic q_0 (*q0()*).

- **calc_base_dist** (`str`) – The statistical distribution, `'normal'` or `'clipped_normal'`, to use for calculating the p-values.
  - `'normal'`: (default) use the full Normal distribution in $\hat{\mu}/\sigma$ space. Note that expected limits may correspond to unphysical test statistics from scenarios with the expected $\hat{\mu} > \mu$.
  - `'clipped_normal'`: use a clipped Normal distribution in $\hat{\mu}/\sigma$ space to avoid expected limits that correspond to scenarios with the expected $\hat{\mu} > \mu$. This will properly cap the test statistic at `0`, as noted in Equation (14) and Equation (16) in [1007.1727].

  The choice of `calc_base_dist` only affects the p-values for expected limits, and the default value will be changed in a future release.

Returns The calculator for asymptotic quantities.

Return type *AsymptoticCalculator*

Methods

distributions(*poi_test*)

Probability distributions of the test statistic, as defined in § 3 of [1007.1727] under the Wald approximation, under the signal + background and background-only hypotheses.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> asymptotic_calculator = pyhf.infer.calculators.AsymptoticCalculator(data,␣
↪model, test_stat="qtilde")
>>> _ = asymptotic_calculator.teststatistic(mu_test)
>>> sig_plus_bkg_dist, bkg_dist = asymptotic_calculator.distributions(mu_test)
>>> sig_plus_bkg_dist.pvalue(mu_test), bkg_dist.pvalue(mu_test)
(array(0.00219262), array(0.15865525))
```

Parameters **poi_test** (`float` or `tensor`) – The value for the parameter of interest.

Returns The distributions under the hypotheses.

Return type Tuple (*AsymptoticTestStatDistribution*)

expected_pvalues(*sig_plus_bkg_distribution*, *bkg_only_distribution*)

Calculate the CL_s values corresponding to the median significance of variations of the signal strength from the background only hypothesis ($\mu = 0$) at $(-2, -1, 0, 1, 2)\sigma$.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> asymptotic_calculator = pyhf.infer.calculators.AsymptoticCalculator(
...     data, model, test_stat="qtilde"
... )
>>> _ = asymptotic_calculator.teststatistic(mu_test)
>>> sig_plus_bkg_dist, bkg_dist = asymptotic_calculator.distributions(mu_test)
>>> CLsb_exp_band, CLb_exp_band, CLs_exp_band = asymptotic_calculator.expected_
↪pvalues(sig_plus_bkg_dist, bkg_dist)
>>> CLs_exp_band
[array(0.00260626), array(0.01382005), array(0.06445321), array(0.23525644),␣
↪array(0.57303621)]
```

Parameters

- **sig_plus_bkg_distribution** (AsymptoticTestStatDistribution) – The distribution for the signal + background hypothesis.
- **bkg_only_distribution** (AsymptoticTestStatDistribution) – The distribution for the background-only hypothesis.

Returns The p-values for the test statistic corresponding to the CL_{s+b}, CL_b, and CL_s.

Return type Tuple (tensor)

pvalues(*teststat*, *sig_plus_bkg_distribution*, *bkg_only_distribution*)

Calculate the p-values for the observed test statistic under the signal + background and background-only model hypotheses.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> asymptotic_calculator = pyhf.infer.calculators.AsymptoticCalculator(
...     data, model, test_stat="qtilde"
... )
>>> q_tilde = asymptotic_calculator.teststatistic(mu_test)
>>> sig_plus_bkg_dist, bkg_dist = asymptotic_calculator.distributions(mu_test)
>>> CLsb, CLb, CLs = asymptotic_calculator.pvalues(q_tilde, sig_plus_bkg_dist,␣
↪bkg_dist)
```

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```
>>> CLsb, CLb, CLs
(array(0.02332502), array(0.4441594), array(0.05251497))
```

Parameters

- **teststat** (tensor) – The test statistic.
- **sig_plus_bkg_distribution** (AsymptoticTestStatDistribution) – The distribution for the signal + background hypothesis.
- **bkg_only_distribution** (AsymptoticTestStatDistribution) – The distribution for the background-only hypothesis.

Returns The p-values for the test statistic corresponding to the CL_{s+b}, CL_b, and CL_s.

Return type Tuple (tensor)

teststatistic(*poi_test*)

Compute the test statistic for the observed data under the studied model.

The fitted parameters of the five fits that are implicitly ran at every call of this method are afterwards accessible through `self.fitted_pars`, which is a *HypoTestFitResults* instance.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> asymptotic_calculator = pyhf.infer.calculators.AsymptoticCalculator(data,␣
↪model, test_stat="qtilde")
>>> asymptotic_calculator.teststatistic(mu_test)
array(0.14043184)
```

Access the best-fit parameters afterwards:

```
>>> asymptotic_calculator.fitted_pars
HypoTestFitResults(asimov_pars=array([0.        , 1.0030482 , 0.96264534]),␣
↪free_fit_to_data=array([0.        , 1.0030512 , 0.96266961]), free_fit_to_
↪asimov=array([0.        , 1.00304893, 0.96263365]), fixed_poi_fit_to_
↪data=array([1.        , 0.97224597, 0.87553894]), fixed_poi_fit_to_
↪asimov=array([1.        , 0.97276864, 0.87142047]))
```

E.g. the $\hat{\mu}$ and $\hat{\theta}$ fitted to the asimov dataset:

```
>>> asymptotic_calculator.fitted_pars.free_fit_to_asimov
array([0.        , 1.00304893, 0.96263365])
```

Parameters **poi_test** (float or tensor) – The value for the parameter of interest.

Returns The value of the test statistic.

Return type Tensor

ToyCalculator

class pyhf.infer.calculators.**ToyCalculator**(*data*, *pdf*, *init_pars=None*, *par_bounds=None*, *fixed_params=None*, *test_stat='qtilde'*, *ntoys=2000*, *track_progress=True*)

Bases: `object`

The Toy-based Calculator.

__init__(*data*, *pdf*, *init_pars=None*, *par_bounds=None*, *fixed_params=None*, *test_stat='qtilde'*, *ntoys=2000*, *track_progress=True*)

Toy-based Calculator.

Parameters

- **data** (`tensor`) – The observed data.
- **pdf** (`Model`) – The statistical model adhering to the schema `model.json`.
- **init_pars** (`tensor` of `float`) – The starting values of the model parameters for minimization.
- **par_bounds** (`tensor`) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.
- **fixed_params** (`tensor` of `bool`) – The flag to set a parameter constant to its starting value during minimization.
- **test_stat** (`str`) – The test statistic to use as a numerical summary of the data: `'qtilde'`, `'q'`, or `'q0'`. `'qtilde'` (default) performs the calculation using the alternative test statistic, $\tilde{q}_\mu$, as defined under the Wald approximation in Equation (62) of [1007.1727] (*qmu_tilde()*), `'q'` performs the calculation using the test statistic q_μ (*qmu()*), and `'q0'` performs the calculation using the discovery test statistic q_0 (*q0()*).
- **ntoys** (`int`) – Number of toys to use (how many times to sample the underlying distributions).
- **track_progress** (`bool`) – Whether to display the *tqdm* progress bar or not (outputs to *stderr*).

Returns The calculator for toy-based quantities.

Return type *ToyCalculator*

Methods

distributions(*poi_test*, *track_progress=None*)

Probability distributions of the test statistic value under the signal + background and background-only hypotheses.

These distributions are produced by generating pseudo-data ("toys") with the nuisance parameters set to their conditional maximum likelihood estimators at the corresponding value of the parameter of interest for each hypothesis, following the joint recommendations of the ATLAS and CMS experiments in *Procedure for the LHC Higgs boson search combination in Summer 2011*.

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> toy_calculator = pyhf.infer.calculators.ToyCalculator(
...     data, model, ntoys=100, track_progress=False
... )
>>> sig_plus_bkg_dist, bkg_dist = toy_calculator.distributions(mu_test)
>>> sig_plus_bkg_dist.pvalue(mu_test), bkg_dist.pvalue(mu_test)
(array(0.14), array(0.79))
```

Parameters

- **poi_test** (float or tensor) – The value for the parameter of interest.
- **track_progress** (bool) – Whether to display the *tqdm* progress bar or not (outputs to *stderr*)

Returns The distributions under the hypotheses.

Return type Tuple (*EmpiricalDistribution*)

expected_pvalues(*sig_plus_bkg_distribution*, *bkg_only_distribution*)

Calculate the CL_s values corresponding to the median significance of variations of the signal strength from the background only hypothesis $(\mu = 0)$ at $(-2, -1, 0, 1, 2)\sigma$.

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> toy_calculator = pyhf.infer.calculators.ToyCalculator(
...     data, model, ntoys=100, track_progress=False
... )
>>> sig_plus_bkg_dist, bkg_dist = toy_calculator.distributions(mu_test)
>>> CLsb_exp_band, CLb_exp_band, CLs_exp_band = toy_calculator.expected_
↪pvalues(sig_plus_bkg_dist, bkg_dist)
>>> CLs_exp_band
[array(0.), array(0.), array(0.08403955), array(0.21892596), array(0.86072977)]
```

Parameters

- **sig_plus_bkg_distribution** (EmpiricalDistribution) – The distribution for the signal + background hypothesis.
- **bkg_only_distribution** (EmpiricalDistribution) – The distribution for the background-only hypothesis.

Returns The p-values for the test statistic corresponding to the CL_{s+b}, CL_b, and CL_s.

Return type Tuple (tensor)

pvalues(*teststat*, *sig_plus_bkg_distribution*, *bkg_only_distribution*)

Calculate the p-values for the observed test statistic under the signal + background and background-only model hypotheses.

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> toy_calculator = pyhf.infer.calculators.ToyCalculator(
...     data, model, ntoys=100, track_progress=False
... )
>>> q_tilde = toy_calculator.teststatistic(mu_test)
>>> sig_plus_bkg_dist, bkg_dist = toy_calculator.distributions(mu_test)
>>> CLsb, CLb, CLs = toy_calculator.pvalues(q_tilde, sig_plus_bkg_dist, bkg_
↪dist)
>>> CLsb, CLb, CLs
(array(0.03), array(0.37), array(0.08108108))
```

Parameters

- **teststat** (tensor) – The test statistic.
- **sig_plus_bkg_distribution** (EmpiricalDistribution) – The distribution for the signal + background hypothesis.
- **bkg_only_distribution** (EmpiricalDistribution) – The distribution for the background-only hypothesis.

Returns The p-values for the test statistic corresponding to the CL_{s+b}, CL_b, and CL_s.

Return type Tuple (tensor)

teststatistic(*poi_test*)

Compute the test statistic for the observed data under the studied model.

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> toy_calculator = pyhf.infer.calculators.ToyCalculator(
...     data, model, ntoys=100, track_progress=False
... )
>>> toy_calculator.teststatistic(mu_test)
array(3.93824492)
```

Parameters **poi_test** (float or tensor) – The value for the parameter of interest.

Returns The value of the test statistic.

Return type Tensor

pyhf.infer.utils.create_calculator

pyhf.infer.utils.**create_calculator**(*calctype*, **args*, ***kwargs*)

Creates a calculator object of the specified *calctype*.

See *AsymptoticCalculator* and *ToyCalculator* on additional arguments to be specified.

Example

```
>>> import pyhf
>>> import numpy.random as random
>>> random.seed(0)
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0],
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> mu_test = 1.0
>>> toy_calculator = pyhf.infer.utils.create_calculator(
...     "toybased", data, model, ntoys=100, test_stat="qtilde", track_progress=False
... )
>>> qmu_sig, qmu_bkg = toy_calculator.distributions(mu_test)
>>> qmu_sig.pvalue(mu_test), qmu_bkg.pvalue(mu_test)
(array(0.14), array(0.79))
```

Parameters

- **calctype** (str) – The calculator to create. Choose either

- **'toybased'.** (*'asymptotics' or*) –

Returns A calculator.

Return type calculator (object)

13.8.3 Fits and Tests

mle.twice_nll	Two times the negative log-likelihood of the model parameters, $(\mu, \boldsymbol{\theta})$, given the observed data.
mle.fit	Run a maximum likelihood fit.
mle.fixed_poi_fit	Run a maximum likelihood fit with the POI value fixed.
hypotest	Compute p-values and test statistics for a single value of the parameter of interest.
intervals.upperlimit	Calculate an upper limit interval `(0, poi_up)` for a single Parameter of Interest (POI) using a fixed scan through POI-space.
utils.all_pois_floating	Check whether all POI(s) are floating (i.e.

pyhf.infer.mle.twice_nll

pyhf.infer.mle.**twice_nll**(*pars*, *data*, *pdf*)

Two times the negative log-likelihood of the model parameters, $(\mu, \boldsymbol{\theta})$, given the observed data. It is used in the calculation of the test statistic, t_μ, as defined in Equation (8) in [1007.1727]

$$t_\mu = -2 \ln \lambda (\mu)$$

where $\lambda (\mu)$ is the profile likelihood ratio as defined in Equation (7)

$$\lambda (\mu) = \frac{L \left(\mu, \hat{\hat{\boldsymbol{\theta}}}\right)}{L \left(\hat{\mu}, \hat{\boldsymbol{\theta}}\right)} .$$

It serves as the objective function to minimize in *fit()* and *fixed_poi_fit()*.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> parameters = model.config.suggested_init()  # nominal parameters
>>> twice_nll = pyhf.infer.mle.twice_nll(parameters, data, model)
>>> twice_nll
array([30.77525435])
>>> -2 * model.logpdf(parameters, data) == twice_nll
array([ True])
```

Parameters

- **pars** (tensor) – The parameters of the HistFactory model
- **data** (tensor) – The data to be considered
- **pdf** (Model) – The statistical model adhering to the schema model.json

Returns Two times the negative log-likelihood, $-2\ln L\left(\mu,\boldsymbol{\theta}\right)$

Return type Tensor

pyhf.infer.mle.fit

pyhf.infer.mle.**fit**(*data*, *pdf*, *init_pars=None*, *par_bounds=None*, *fixed_params=None*, ***kwargs*)

Run a maximum likelihood fit. This is done by minimizing the objective function *twice_nll()* of the model parameters given the observed data. This is used to produce the maximal likelihood $L\left(\hat{\mu},\hat{\boldsymbol{\theta}}\right)$ in the profile likelihood ratio in Equation (7) in [1007.1727]

$$\lambda\left(\mu\right) = \frac{L\left(\mu,\hat{\hat{\boldsymbol{\theta}}}\right)}{L\left(\hat{\mu},\hat{\boldsymbol{\theta}}\right)}$$

Note: *twice_nll()* is the objective function given to the optimizer and is returned evaluated at the best fit model parameters when the optional kwarg `return_fitted_val` is `True`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> bestfit_pars, twice_nll = pyhf.infer.mle.fit(data, model, return_fitted_
↪val=True)
>>> bestfit_pars
array([0.        , 1.0030512 , 0.96266961])
>>> twice_nll
array(24.98393521)
>>> -2 * model.logpdf(bestfit_pars, data) == twice_nll
array([ True])
```

Parameters

- **data** (tensor) – The data
- **pdf** (Model) – The statistical model adhering to the schema model.json
- **init_pars** (list of float) – The starting values of the model parameters for minimization.
- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.

- **fixed_params** (list of bool) – The flag to set a parameter constant to its starting value during minimization.
- **kwargs** – Keyword arguments passed through to the optimizer API

Returns See optimizer API

pyhf.infer.mle.fixed_poi_fit

pyhf.infer.mle.**fixed_poi_fit**(*poi_val*, *data*, *pdf*, *init_pars=None*, *par_bounds=None*, *fixed_params=None*, ***kwargs*)

Run a maximum likelihood fit with the POI value fixed. This is done by minimizing the objective function of *twice_nll()* of the model parameters given the observed data, for a given fixed value of μ. This is used to produce the constrained maximal likelihood for the given μ, $L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}\right)$, in the profile likelihood ratio in Equation (7) in [1007.1727]

$$\lambda\left(\mu\right) = \frac{L\left(\mu, \hat{\hat{\boldsymbol{\theta}}}\right)}{L\left(\hat{\mu}, \hat{\boldsymbol{\theta}}\right)}$$

Note: *twice_nll()* is the objective function given to the optimizer and is returned evaluated at the best fit model parameters when the optional kwarg `return_fitted_val` is `True`.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> test_poi = 1.0
>>> bestfit_pars, twice_nll = pyhf.infer.mle.fixed_poi_fit(
...     test_poi, data, model, return_fitted_val=True
... )
>>> bestfit_pars
array([1.        , 0.97224597, 0.87553894])
>>> twice_nll
array(28.92218013)
>>> -2 * model.logpdf(bestfit_pars, data) == twice_nll
array([ True])
```

Parameters

- **data** – The data
- **pdf** (Model) – The statistical model adhering to the schema model.json
- **init_pars** (list of float) – The starting values of the model parameters for minimization.
- **par_bounds** (list of list/tuple) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.

- **fixed_params** (list of bool) – The flag to set a parameter constant to its starting value during minimization.
- **kwargs** – Keyword arguments passed through to the optimizer API

Returns See optimizer API

pyhf.infer.hypotest

pyhf.infer.**hypotest**(*poi_test*, *data*, *pdf*, *init_pars=None*, *par_bounds=None*, *fixed_params=None*, *calctype='asymptotics'*, *return_tail_probs=False*, *return_expected=False*, *return_expected_set=False*, *return_calculator=False*, ***kwargs*)

Compute p-values and test statistics for a single value of the parameter of interest.

See *AsymptoticCalculator* and *ToyCalculator* on additional keyword arguments to be specified.

Example

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> mu_test = 1.0
>>> CLs_obs, CLs_exp_band = pyhf.infer.hypotest(
...     mu_test, data, model, return_expected_set=True, test_stat="qtilde"
... )
>>> CLs_obs
array(0.05251497)
>>> CLs_exp_band
[array(0.00260626), array(0.01382005), array(0.06445321), array(0.23525644),␣
↪array(0.57303621)]
```

Parameters

- **poi_test** (*Number or Tensor*) – The value of the parameter of interest (POI)
- **data** (*Number or Tensor*) – The data considered
- **pdf** (Model) – The statistical model adhering to the schema `model.json`
- **init_pars** (tensor of float) – The starting values of the model parameters for minimization.
- **par_bounds** (tensor) – The extrema of values the model parameters are allowed to reach in the fit. The shape should be `(n, 2)` for `n` model parameters.
- **fixed_params** (tensor of bool) – The flag to set a parameter constant to its starting value during minimization.
- **calctype** (str) – The calculator to create. Choose either 'asymptotics' (default) or 'toy-based'.
- **return_tail_probs** (bool) – Bool for returning CL_{s+b} and CL_{b}
- **return_expected** (bool) – Bool for returning $\mathrm{CL}_{\mathrm{exp}}$

- **return_expected_set** (bool) – Bool for returning the $(-2,-1,0,1,2)\sigma$ $\mathrm{CL}_{\mathrm{exp}}$ — the "Brazil band"
- **return_calculator** (bool) – Bool for returning calculator.

Returns

Tuple of Floats and lists of Floats and a *AsymptoticCalculator* or *ToyCalculator* instance:

- CL_s: The modified p-value compared to the given threshold α, typically taken to be 0.05, defined in [1007.1727] as

$$\mathrm{CL}_s = \frac{\mathrm{CL}_{s+b}}{\mathrm{CL}_b} = \frac{p_{s+b}}{1-p_b}$$

to protect against excluding signal models in which there is little sensitivity. In the case that $\mathrm{CL}_s \leq \alpha$ the given signal model is excluded.

- $[\mathrm{CL}_{s+b}, \mathrm{CL}_b]$: The signal + background model hypothesis p-value

$$\mathrm{CL}_{s+b} = p_{s+b} = p\left(q \geq q_{\mathrm{obs}} | s+b\right) = \int_{q_{\mathrm{obs}}}^{\infty} f\left(q\,|s+b\right)\,dq = 1 - F\left(q_{\mathrm{obs}}(\mu)\,|\mu'\right)$$

and 1 minus the background only model hypothesis p-value

$$\mathrm{CL}_b = 1 - p_b = p\left(q \geq q_{\mathrm{obs}} | b\right) = 1 - \int_{-\infty}^{q_{\mathrm{obs}}} f\left(q\,|b\right)\,dq = 1 - F\left(q_{\mathrm{obs}}(\mu)\,|0\right)$$

for signal strength μ and model hypothesis signal strength μ', where the cumulative density functions $F\left(q(\mu)\,|\mu'\right)$ are given by Equations (57) and (65) of [1007.1727] for upper-limit-like test statistic $q \in \{q_\mu, \tilde{q}_\mu\}$. Only returned when `return_tail_probs` is `True`.

Note: The definitions of the CL_{s+b} and CL_b used are based on profile likelihood ratio test statistics. This procedure is common in the LHC-era, but differs from procedures used in the LEP and Tevatron eras, as briefly discussed in § 3.8 of [1007.1727].

- $\mathrm{CL}_{s,\mathrm{exp}}$: The expected CL_s value corresponding to the test statistic under the background only hypothesis ($\mu = 0$). Only returned when `return_expected` is `True`.
- $\mathrm{CL}_{s,\mathrm{exp}}$ band: The set of expected CL_s values corresponding to the median significance of variations of the signal strength from the background only hypothesis ($\mu = 0$) at $(-2,-1,0,1,2)\sigma$. That is, the p-values that satisfy Equation (89) of [1007.1727]

$$\mathrm{band}_{N\sigma} = \mu' + \sigma\,\Phi^{-1}\left(1-\alpha\right) \pm N\sigma$$

for $\mu' = 0$ and $N \in \{-2,-1,0,1,2\}$. These values define the boundaries of an uncertainty band sometimes referred to as the "Brazil band". Only returned when `return_expected_set` is `True`.

- a calculator: The calculator instance used in the computation of the p-values. Either an instance of *AsymptoticCalculator* or *ToyCalculator*, depending on the value of `calctype`. Only returned when `return_calculator` is `True`.

pyhf.infer.intervals.upperlimit

pyhf.infer.intervals.**upperlimit**(*data*, *model*, *scan*, *level=0.05*, *return_results=False*, ***hypotest_kwargs*)
Calculate an upper limit interval `(0, poi_up)` for a single Parameter of Interest (POI) using a fixed scan through POI-space.

Example

```
>>> import numpy as np
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = pyhf.tensorlib.astensor(observations + model.config.auxdata)
>>> scan = np.linspace(0, 5, 21)
>>> obs_limit, exp_limits, (scan, results) = pyhf.infer.intervals.upperlimit(
...     data, model, scan, return_results=True
... )
>>> obs_limit
array(1.01764089)
>>> exp_limits
[array(0.59576921), array(0.76169166), array(1.08504773), array(1.50170482),␣
↪array(2.06654952)]
```

Parameters

- **data** (tensor) – The observed data.
- **model** (Model) – The statistical model adhering to the schema `model.json`.
- **scan** (iterable) – Iterable of POI values.
- **level** (float) – The threshold value to evaluate the interpolated results at.
- **return_results** (bool) – Whether to return the per-point results.
- **hypotest_kwargs** (string) – Kwargs for the calls to *hypotest* to configure the fits.

Returns

- Tensor: The observed upper limit on the POI.
- Tensor: The expected upper limits on the POI.
- Tuple of Tensors: The given `scan` along with the *hypotest* results at each test POI. Only returned when `return_results` is `True`.

Return type Tuple of Tensors

pyhf.infer.utils.all_pois_floating

pyhf.infer.utils.**all_pois_floating**(*pdf*, *fixed_params*)
Check whether all POI(s) are floating (i.e. not within the fixed set).

Parameters

- **pdf** (Model) – The statistical model adhering to the schema model.json.
- **fixed_params** (list or *tensor* of bool) – Array of bool indicating if model parameters are fixed.

Returns The result whether all POIs are floating.

Return type bool

13.9 Exceptions

Various exceptions, apart from standard python exceptions, that are raised from using the pyhf API.

InvalidMeasurement	InvalidMeasurement is raised when a specified measurement is invalid given the specification.
InvalidNameReuse	
InvalidSpecification	InvalidSpecification is raised when a specification does not validate against the given schema.
InvalidPatchSet	InvalidPatchSet is raised when a given patchset object does not have the right configuration, even though it validates correctly against the schema.
InvalidPatchLookup	InvalidPatchLookup is raised when the patch lookup from a patchset object has failed
PatchSetVerificationError	PatchSetVerificationError is raised when the workspace digest does not match the patchset digests as part of the verification procedure
InvalidWorkspaceOperation	InvalidWorkspaceOperation is raised when an operation on a workspace fails.
InvalidModel	InvalidModel is raised when a given model does not have the right configuration, even though it validates correctly against the schema.
InvalidModifier	InvalidModifier is raised when an invalid modifier is requested.
InvalidInterpCode	InvalidInterpCode is raised when an invalid/unimplemented interpolation code is requested.
ImportBackendError	MissingLibraries is raised when something is imported by sustained an import error due to missing additional, non-default libraries.
InvalidBackend	InvalidBackend is raised when trying to set a backend that does not exist.
InvalidOptimizer	InvalidOptimizer is raised when trying to set an optimizer that does not exist.
InvalidPdfParameters	InvalidPdfParameters is raised when trying to evaluate a pdf with invalid parameters.

continues on next page

Table 26 – continued from previous page

InvalidPdfData	InvalidPdfData is raised when trying to evaluate a pdf with invalid data.

13.9.1 pyhf.exceptions.InvalidMeasurement

exception pyhf.exceptions.**InvalidMeasurement**
InvalidMeasurement is raised when a specified measurement is invalid given the specification.

13.9.2 pyhf.exceptions.InvalidNameReuse

exception pyhf.exceptions.**InvalidNameReuse**

13.9.3 pyhf.exceptions.InvalidSpecification

exception pyhf.exceptions.**InvalidSpecification**(*ValidationError*, *schema=None*)
InvalidSpecification is raised when a specification does not validate against the given schema.

13.9.4 pyhf.exceptions.InvalidPatchSet

exception pyhf.exceptions.**InvalidPatchSet**
InvalidPatchSet is raised when a given patchset object does not have the right configuration, even though it validates correctly against the schema.

13.9.5 pyhf.exceptions.InvalidPatchLookup

exception pyhf.exceptions.**InvalidPatchLookup**
InvalidPatchLookup is raised when the patch lookup from a patchset object has failed

13.9.6 pyhf.exceptions.PatchSetVerificationError

exception pyhf.exceptions.**PatchSetVerificationError**
PatchSetVerificationError is raised when the workspace digest does not match the patchset digests as part of the verification procedure

13.9.7 pyhf.exceptions.InvalidWorkspaceOperation

exception pyhf.exceptions.**InvalidWorkspaceOperation**
InvalidWorkspaceOperation is raised when an operation on a workspace fails.

13.9.8 pyhf.exceptions.InvalidModel

exception pyhf.exceptions.**InvalidModel**
InvalidModel is raised when a given model does not have the right configuration, even though it validates correctly against the schema.

This can occur, for example, when the provided parameter of interest to fit against does not get declared in the specification provided.

13.9.9 pyhf.exceptions.InvalidModifier

exception pyhf.exceptions.**InvalidModifier**
InvalidModifier is raised when an invalid modifier is requested. This includes:

- creating a custom modifier with the wrong structure
- initializing a modifier that does not exist, or has not been loaded

13.9.10 pyhf.exceptions.InvalidInterpCode

exception pyhf.exceptions.**InvalidInterpCode**
InvalidInterpCode is raised when an invalid/unimplemented interpolation code is requested.

13.9.11 pyhf.exceptions.ImportBackendError

exception pyhf.exceptions.**ImportBackendError**
MissingLibraries is raised when something is imported by sustained an import error due to missing additional, non-default libraries.

13.9.12 pyhf.exceptions.InvalidBackend

exception pyhf.exceptions.**InvalidBackend**
InvalidBackend is raised when trying to set a backend that does not exist.

13.9.13 pyhf.exceptions.InvalidOptimizer

exception pyhf.exceptions.**InvalidOptimizer**
InvalidOptimizer is raised when trying to set an optimizer that does not exist.

13.9.14 pyhf.exceptions.InvalidPdfParameters

exception pyhf.exceptions.**InvalidPdfParameters**
InvalidPdfParameters is raised when trying to evaluate a pdf with invalid parameters.

13.9.15 pyhf.exceptions.InvalidPdfData

exception pyhf.exceptions.**InvalidPdfData**
InvalidPdfData is raised when trying to evaluate a pdf with invalid data.

13.10 Utilities

load_schema
validate
options_from_eqdelimstring

digest	Get the digest for the provided object.
citation	Get the bibtex citation for pyhf

13.10.1 pyhf.utils.load_schema

pyhf.utils.**load_schema**(*schema_id*, *version=None*)

13.10.2 pyhf.utils.validate

pyhf.utils.**validate**(*spec*, *schema_name*, *version=None*)

13.10.3 pyhf.utils.options_from_eqdelimstring

pyhf.utils.**options_from_eqdelimstring**(*opts*)

13.10.4 pyhf.utils.digest

pyhf.utils.**digest**(*obj*, *algorithm='sha256'*)
Get the digest for the provided object. Note: object must be JSON-serializable.

The hashing algorithms supported are in hashlib, part of Python's Standard Libraries.

Example

```
>>> import pyhf
>>> obj = {'a': 2.0, 'b': 3.0, 'c': 1.0}
>>> pyhf.utils.digest(obj)
'a38f6093800189b79bc22ef677baf90c75705af2cfc7ff594159eca54eaa7928'
>>> pyhf.utils.digest(obj, algorithm='md5')
'2c0633f242928eb55c3672fed5ba8612'
>>> pyhf.utils.digest(obj, algorithm='sha1')
'49a27f499e763766c9545b294880df277be6f545'
```

Raises `ValueError` – If the object is not JSON-serializable or if the algorithm is not supported.

Parameters

- **obj** (`jsonable`) – A JSON-serializable object to compute the digest of. Usually a *Workspace* object.
- **algorithm** (`str`) – The hashing algorithm to use.

Returns The digest for the JSON-serialized object provided and hash algorithm specified.

Return type digest (`str`)

13.10.5 pyhf.utils.citation

pyhf.utils.**citation**(*oneline=False*)
Get the bibtex citation for pyhf

Example

```
>>> import pyhf
>>> pyhf.utils.citation(oneline=True)
'@software{pyhf, author = {Lukas Heinrich and Matthew Feickert and Giordon Stark},␣
↪ title = "{pyhf: v0.6.3}", version = {0.6.3}, doi = {10.5281/zenodo.1169739}, ␣
↪url = {https://doi.org/10.5281/zenodo.1169739}, note = {https://github.com/
↪scikit-hep/pyhf/releases/tag/v0.6.3}}@article{pyhf_joss, doi = {10.21105/joss.
↪02823}, url = {https://doi.org/10.21105/joss.02823}, year = {2021}, publisher␣
↪= {The Open Journal}, volume = {6}, number = {58}, pages = {2823}, author =
↪{Lukas Heinrich and Matthew Feickert and Giordon Stark and Kyle Cranmer}, title␣
↪= {pyhf: pure-Python implementation of HistFactory statistical models}, journal␣
↪= {Journal of Open Source Software}}'
```

Keyword Arguments **oneline** (`bool`) – Whether to provide citation with new lines (default) or as a one-liner.

Returns The citation for this software

Return type citation (`str`)

13.11 Contrib

viz.brazil	Brazil Band Plots.
utils.download	Download the patchset archive from the remote URL and extract it in a directory at the path given.

13.11.1 pyhf.contrib.viz.brazil

Description

Brazil Band Plots.

Classes

BrazilBandCollection(cls_obs, cls_exp, ...)	`collections.namedtuple` containing the `matplotlib.artist.Artist` objects of the "Brazil Band" and the observed CL_{s+b} and CL_b --- the components of the CL_s ratio.

BrazilBandCollection

class pyhf.contrib.viz.brazil.**BrazilBandCollection**(*cls_obs*, *cls_exp*, *one_sigma_band*, *two_sigma_band*, *test_size*, *clsb*, *clb*, *axes*)

Bases: *pyhf.contrib.viz.brazil.BrazilBandCollection*

`collections.namedtuple` containing the `matplotlib.artist.Artist` objects of the "Brazil Band" and the observed CL_{s+b} and CL_b — the components of the CL_s ratio. Returned by *plot_results()*.

Parameters

- **cls_obs** – The `matplotlib.lines.Line2D` of the $\mathrm{CL}_{s,\mathrm{obs}}$ line.
- **cls_exp** – The `list` of `matplotlib.lines.Line2D` of the $\mathrm{CL}_{s,\mathrm{exp}}$ lines.
- **one_sigma_band** – The `matplotlib.collections.PolyCollection` of the $\mathrm{CL}_{s,\mathrm{exp}}$ $\pm 1\sigma$ band.
- **two_sigma_band** – The `matplotlib.collections.PolyCollection` of the $\mathrm{CL}_{s,\mathrm{exp}}$ $\pm 2\sigma$ band.
- **test_size** – The `matplotlib.lines.Line2D` of the test size line.
- **clsb** – The `matplotlib.lines.Line2D` of the observed CL_{s+b} line.
- **clb** – The `matplotlib.lines.Line2D` of the observed CL_b line.
- **axes** – The `matplotlib.axes.Axes` the artists are plotted on.

__init__()

Attributes

axes
Alias for field number 7

clb
Alias for field number 6

cls_exp
Alias for field number 1

cls_obs
Alias for field number 0

clsb
Alias for field number 5

one_sigma_band
Alias for field number 2

test_size
Alias for field number 4

two_sigma_band
Alias for field number 3

Methods

Functions

plot_brazil_band(test_pois, cls_obs, ...)	Plot the values of $\mathrm{CL}_{s,\mathrm{obs}}$ and the $\mathrm{CL}_{s,\mathrm{exp}}$ band (the "Brazil band") for a series of hypothesis tests for various POI values.
plot_cls_components(test_pois, tail_probs, ...)	Plot the values of CL_{s+b} and CL_{b} --- the components of the CL_{s} ratio --- for a series of hypothesis tests for various POI values.
plot_results(test_pois, tests[, test_size, ax])	Plot a series of hypothesis tests for various POI values.

pyhf.contrib.viz.brazil.plot_brazil_band

pyhf.contrib.viz.brazil.**plot_brazil_band**(*test_pois*, *cls_obs*, *cls_exp*, *test_size*, *ax*, ***kwargs*)
Plot the values of $\mathrm{CL}_{s,\mathrm{obs}}$ and the $\mathrm{CL}_{s,\mathrm{exp}}$ band (the "Brazil band") for a series of hypothesis tests for various POI values.

Example

plot_brazil_band() is generally meant to be used inside *plot_results()* but can be used by itself.

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> import pyhf
>>> import pyhf.contrib.viz.brazil
>>> pyhf.set_backend("numpy")
>>> model  = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> test_pois = np.linspace(0, 5, 41)
>>> results = [
...     pyhf.infer.hypotest(test_poi, data, model, return_expected_set=True)
...     for test_poi in test_pois
... ]
>>> cls_obs = np.array([test[0] for test in results]).flatten()
>>> cls_exp = [
...     np.array([test[1][sigma_idx] for test in results]).flatten()
```

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```
...     for sigma_idx in range(5)
... ]
>>> test_size = 0.05
>>> fig, ax = plt.subplots()
>>> artists = pyhf.contrib.viz.brazil.plot_brazil_band(
...     test_pois, cls_obs, cls_exp, test_size, ax
... )
```

Parameters

- **test_pois** (list or array) – The values of the POI where the hypothesis tests were performed.
- **cls_obs** (list or array) – The values of $\mathrm{CL}_{s,\mathrm{obs}}$ for the POIs tested in test_pois.
- **cls_exp** (list or array) – The values of the $\mathrm{CL}_{s,\mathrm{exp}}$ band for the POIs tested in test_pois.
- **test_size** (float) – The size, α, of the test.
- **ax** (matplotlib.axes.Axes) – The matplotlib axis object to plot on.

Returns The matplotlib.aritst objects drawn.

Return type tuple

pyhf.contrib.viz.brazil.plot_cls_components

pyhf.contrib.viz.brazil.**plot_cls_components**(*test_pois*, *tail_probs*, *ax*, ***kwargs*)

Plot the values of CL_{s+b} and CL_b — the components of the CL_s ratio — for a series of hypothesis tests for various POI values.

Example

plot_cls_components() is generally meant to be used inside *plot_results()* but can be used by itself.

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> import pyhf
>>> import pyhf.contrib.viz.brazil
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> test_pois = np.linspace(0, 5, 41)
>>> results = [
...     pyhf.infer.hypotest(
...         test_poi, data, model, return_expected_set=True, return_tail_probs=True
...     )
...     for test_poi in test_pois
... ]
>>> tail_probs = np.array([test[1] for test in results])
```

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(continued from previous page)

```
>>> fig, ax = plt.subplots()
>>> artists = pyhf.contrib.viz.brazil.plot_cls_components(test_pois, tail_probs, ax)
```

Parameters

- **test_pois** (list or array) – The values of the POI where the hypothesis tests were performed.
- **tail_probs** (list or array) – The values of CL_{s+b} and CL_{b} for the POIs tested in test_pois.
- **ax** (matplotlib.axes.Axes) – The matplotlib axis object to plot on.
- **Keywords** –
  - no_clb (bool): Bool for not plotting the CL_{b} component.
  - no_clsb (bool): Bool for not plotting the CL_{s+b} component.

Returns The matplotlib.lines.Line2D artists drawn.

Return type tuple

pyhf.contrib.viz.brazil.plot_results

pyhf.contrib.viz.brazil.**plot_results**(*test_pois*, *tests*, *test_size=0.05*, *ax=None*, ***kwargs*)

Plot a series of hypothesis tests for various POI values. For more detail on use of keywords see *plot_brazil_band()* and *plot_cls_components()*.

Example

A Brazil band plot.

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> import pyhf
>>> import pyhf.contrib.viz.brazil
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> test_pois = np.linspace(0, 5, 41)
>>> results = [
...     pyhf.infer.hypotest(test_poi, data, model, return_expected_set=True)
...     for test_poi in test_pois
... ]
>>> fig, ax = plt.subplots()
>>> artists = pyhf.contrib.viz.brazil.plot_results(test_pois, results, ax=ax)
```

A Brazil band plot with the components of the CL_{s} ratio drawn on top.

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> import pyhf
>>> import pyhf.contrib.viz.brazil
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> observations = [51, 48]
>>> data = observations + model.config.auxdata
>>> test_pois = np.linspace(0, 5, 41)
>>> results = [
...     pyhf.infer.hypotest(
...         test_poi, data, model, return_expected_set=True, return_tail_probs=True
...     )
...     for test_poi in test_pois
... ]
>>> fig, ax = plt.subplots()
>>> artists = pyhf.contrib.viz.brazil.plot_results(
...     test_pois, results, ax=ax, components=True
... )
```

Parameters

- **test_pois** (list or array) – The values of the POI where the hypothesis tests were performed.
- **tests** (list or array) – The collection of p-value-like values (CL_s values or tail probabilities) from the hypothesis tests. If the components keyword argument is True, tests is required to have the same structure as *pyhf.infer.hypotest()*'s return when using return_expected_set=True and return_tail_probs=True: a tuple of CL_s, $[\mathrm{CL}_{s+b}, \mathrm{CL}_b]$, $\mathrm{CL}_{s,\mathrm{exp}}$ band.
- **test_size** (float) – The size, α, of the test.
- **ax** (matplotlib.axes.Axes) – The matplotlib axis object to plot on.

Returns Artist containing the matplotlib.artist objects drawn.

Return type *BrazilBandCollection*

13.11.2 pyhf.contrib.utils.download

pyhf.contrib.utils.**download**(*archive_url*, *output_directory*, *force=False*, *compress=False*)

Download the patchset archive from the remote URL and extract it in a directory at the path given.

Example

```
>>> from pyhf.contrib.utils import download
>>> download("https://doi.org/10.17182/hepdata.90607.v3/r3", "1Lbb-likelihoods")
>>> import os
>>> sorted(os.listdir("1Lbb-likelihoods"))
['BkgOnly.json', 'README.md', 'patchset.json']
>>> download("https://doi.org/10.17182/hepdata.90607.v3/r3", "1Lbb-likelihoods.tar.
↪gz", compress=True)
>>> import glob
>>> glob.glob("1Lbb-likelihoods.tar.gz")
['1Lbb-likelihoods.tar.gz']
```

Parameters

- **archive_url** (str) – The URL of the *PatchSet* archive to download.
- **output_directory** (str) – Name of the directory to unpack the archive into.
- **force** (bool) – Force download from non-approved host. Default is False.
- **compress** (bool) – Keep the archive in a compressed tar.gz form. Default is False.

Raises **InvalidArchiveHost** – if the provided archive host name is not known to be valid

CHAPTER

FOURTEEN

USE AND CITATIONS

14.1 Citation

The preferred BibTeX entry for citation of `pyhf` includes both the Zenodo archive and the JOSS paper:

```
@software{pyhf,
  author = {Lukas Heinrich and Matthew Feickert and Giordon Stark},
  title = "{pyhf: v0.6.3}",
  version = {0.6.3},
  doi = {10.5281/zenodo.1169739},
  url = {https://doi.org/10.5281/zenodo.1169739},
  note = {https://github.com/scikit-hep/pyhf/releases/tag/v0.6.3}
}

@article{pyhf_joss,
  doi = {10.21105/joss.02823},
  url = {https://doi.org/10.21105/joss.02823},
  year = {2021},
  publisher = {The Open Journal},
  volume = {6},
  number = {58},
  pages = {2823},
  author = {Lukas Heinrich and Matthew Feickert and Giordon Stark and Kyle Cranmer},
  title = {pyhf: pure-Python implementation of HistFactory statistical models},
  journal = {Journal of Open Source Software}
}
```

14.2 Use in Publications

The following is an updating list of citations and use cases of `pyhf`. There is an incomplete but automatically updated list of citations on INSPIRE as well.

14.2.1 Use Citations

1. ATLAS Collaboration. Implementation of simplified likelihoods in HistFactory for searches for supersymmetry. Geneva, Sep 2021. URL: https://cds.cern.ch/record/2782654.
2. Michael J. Baker, Darius A. Faroughy, and Sokratis Trifinopoulos. Collider Signatures of Coannihilating Dark Matter in Light of the B-Physics Anomalies. 9 2021. arXiv:2109.08689.
3. Kyle Cranmer and others. Publishing statistical models: Getting the most out of particle physics experiments. 9 2021. arXiv:2109.04981.
4. Kyle Cranmer and Alexander Held. Building and steering binned template fits with cabinetry. *EPJ Web Conf.*, 251:03067, 2021. doi:10.1051/epjconf/202125103067.
5. ATLAS Collaboration. Search for chargino–neutralino pair production in final states with three leptons and missing transverse momentum in $\sqrt s = 13$ TeV pp collisions with the ATLAS detector. 6 2021. arXiv:2106.01676.
6. Belle II Collaboration. Search for $B^+ \to K^+ \nu \bar \nu $ decays with an inclusive tagging method at the Belle II experiment. In *55th Rencontres de Moriond on Electroweak Interactions and Unified Theories*. 5 2021. arXiv:2105.05754.
7. Belle II Collaboration. Search for $B^+\to K^+\nu \bar \nu $ decays using an inclusive tagging method at Belle II. 4 2021. arXiv:2104.12624.
8. Andrei Angelescu, Damir Bečirević, Darius A. Faroughy, Florentin Jaffredo, and Olcyr Sumensari. On the single leptoquark solutions to the B-physics anomalies. 3 2021. arXiv:2103.12504.
9. Matthew Feickert, Lukas Heinrich, Giordon Stark, and Ben Galewsky. Distributed statistical inference with pyhf enabled through funcX. *EPJ Web Conf.*, 251:02070, 2021. arXiv:2103.02182, doi:10.1051/epjconf/202125102070.
10. Rodolfo Capdevilla, Federico Meloni, Rosa Simoniello, and Jose Zurita. Hunting wino and higgsino dark matter at the muon collider with disappearing tracks. 2 2021. arXiv:2102.11292.
11. Vincenzo Cirigliano, Kaori Fuyuto, Christopher Lee, Emanuele Mereghetti, and Bin Yan. Charged Lepton Flavor Violation at the EIC. *JHEP*, 03:256, 2021. arXiv:2102.06176, doi:10.1007/JHEP03(2021)256.
12. Jack Y. Araz and others. Proceedings of the second MadAnalysis 5 workshop on LHC recasting in Korea. *Mod. Phys. Lett. A*, 36(01):2102001, 2021. arXiv:2101.02245, doi:10.1142/S0217732321020016.
13. Wolfgang Waltenberger, André Lessa, and Sabine Kraml. Artificial Proto-Modelling: Building Precursors of a Next Standard Model from Simplified Model Results. 12 2020. arXiv:2012.12246.
14. Simone Amoroso, Deepak Kar, and Matthias Schott. How to discover QCD Instantons at the LHC. *Eur. Phys. J. C*, 81(7):624, 2021. arXiv:2012.09120, doi:10.1140/epjc/s10052-021-09412-1.
15. Gaël Alguero, Jan Heisig, Charanjit K. Khosa, Sabine Kraml, Suchita Kulkarni, Andre Lessa, Philipp Neuhuber, Humberto Reyes-González, Wolfgang Waltenberger, and Alicia Wongel. New developments in SModelS. In *Tools for High Energy Physics and Cosmology*. 12 2020. arXiv:2012.08192.
16. Matthew Feickert, Lukas Heinrich, and Giordon Stark. Likelihood preservation and statistical reproduction of searches for new physics. *EPJ Web Conf.*, 2020. doi:10.1051/epjconf/202024506017.

17. Gaël Alguero, Sabine Kraml, and Wolfgang Waltenberger. A SModelS interface for pyhf likelihoods. Sep 2020. arXiv:2009.01809.

18. ATLAS Collaboration. Search for new phenomena in events with two opposite-charge leptons, jets and missing transverse momentum in pp collisions at $\sqrt s = 13$ TeV with the ATLAS detector. 2 2021. arXiv:2102.01444.

19. Charanjit K. Khosa, Sabine Kraml, Andre Lessa, Philipp Neuhuber, and Wolfgang Waltenberger. SModelS database update v1.2.3. *LHEP*, 158:2020, 5 2020. arXiv:2005.00555, doi:10.31526/lhep.2020.158.

20. G. Brooijmans and others. Les Houches 2019 Physics at TeV Colliders: New Physics Working Group Report. In 2020. arXiv:2002.12220.

21. Andrei Angelescu, Darius A. Faroughy, and Olcyr Sumensari. Lepton Flavor Violation and Dilepton Tails at the LHC. *Eur. Phys. J. C*, 80(7):641, 2020. arXiv:2002.05684, doi:10.1140/epjc/s10052-020-8210-5.

22. B.C. Allanach, Tyler Corbett, and Maeve Madigan. Sensitivity of Future Hadron Colliders to Leptoquark Pair Production in the Di-Muon Di-Jets Channel. *Eur. Phys. J. C*, 80(2):170, 2020. arXiv:1911.04455, doi:10.1140/epjc/s10052-020-7722-3.

23. ATLAS Collaboration. Reproducing searches for new physics with the ATLAS experiment through publication of full statistical likelihoods. Geneva, Aug 2019. URL: https://cds.cern.ch/record/2684863.

24. Lukas Heinrich, Holger Schulz, Jessica Turner, and Ye-Ling Zhou. Constraining A_4 Leptonic Flavour Model Parameters at Colliders and Beyond. 2018. arXiv:1810.05648.

14.2.2 General Citations

1. Jean-Loup Tastet, Oleg Ruchayskiy, and Inar Timiryasov. Reinterpreting the ATLAS bounds on heavy neutral leptons in a realistic neutrino oscillation model. 7 2021. arXiv:2107.12980.

2. Jeffrey Krupa and others. GPU coprocessors as a service for deep learning inference in high energy physics. 7 2020. arXiv:2007.10359.

3. Waleed Abdallah and others. Reinterpretation of LHC Results for New Physics: Status and Recommendations after Run 2. *SciPost Phys.*, 9(2):022, 2020. arXiv:2003.07868, doi:10.21468/SciPostPhys.9.2.022.

4. J. Alison and others. Higgs boson potential at colliders: Status and perspectives. *Rev. Phys.*, 5:100045, 2020. arXiv:1910.00012, doi:10.1016/j.revip.2020.100045.

5. Johann Brehmer, Felix Kling, Irina Espejo, and Kyle Cranmer. MadMiner: Machine learning-based inference for particle physics. *Comput. Softw. Big Sci.*, 4(1):3, 2020. arXiv:1907.10621, doi:10.1007/s41781-020-0035-2.

14.3 Published Statistical Models

Updating list of HEPData entries for publications using `HistFactory` JSON statistical models:

1. Search for charginos and neutralinos in final states with two boosted hadronically decaying bosons and missing transverse momentum in pp collisions at $\sqrt s=13$ TeV with the ATLAS detector. 2021. URL: https://doi.org/10.17182/hepdata.104458, doi:10.17182/hepdata.104458.

2. Search for R-parity violating supersymmetry in a final state containing leptons and many jets with the ATLAS experiment using $\sqrt s = 13$ TeV proton-proton collision data. 2021. URL: https://doi.org/10.17182/hepdata.104860, doi:10.17182/hepdata.104860.

3. Search for chargino–neutralino pair production in final states with three leptons and missing transverse momentum in $\sqrt s = 13$ TeV pp collisions with the ATLAS detector. 2021. URL: https://doi.org/10.17182/hepdata.95751, doi:10.17182/hepdata.95751.

4. Search for squarks and gluinos in final states with one isolated lepton, jets, and missing transverse momentum at $\sqrt s=13$ with the ATLAS detector. 2021. URL: https://doi.org/10.17182/hepdata.97041, doi:10.17182/hepdata.97041.

5. Search for trilepton resonances from chargino and neutralino pair production in $\sqrt s$ = 13 TeV pp collisions with the ATLAS detector. 2020. URL: https://doi.org/10.17182/hepdata.99806, doi:10.17182/hepdata.99806.

6. Search for displaced leptons in $\sqrt s = 13$ TeV pp collisions with the ATLAS detector. 2020. URL: https://doi.org/10.17182/hepdata.98796, doi:10.17182/hepdata.98796.

7. Search for squarks and gluinos in final states with jets and missing transverse momentum using 139 fb$^-1$ of $\sqrt s$ =13 TeV pp collision data with the ATLAS detector. 2021. URL: https://doi.org/10.17182/hepdata.95664, doi:10.17182/hepdata.95664.

8. Search for long-lived, massive particles in events with a displaced vertex and a muon with large impact parameter in pp collisions at $\sqrt s = 13$ TeV with the ATLAS detector. 2020. URL: https://doi.org/10.17182/hepdata.91760, doi:10.17182/hepdata.91760.

9. Search for chargino-neutralino production with mass splittings near the electroweak scale in three-lepton final states in $\sqrt s$ = 13 TeV pp collisions with the ATLAS detector. 2019. URL: https://doi.org/10.17182/hepdata.91127, doi:10.17182/hepdata.91127.

10. Searches for electroweak production of supersymmetric particles with compressed mass spectra in $\sqrt s=$ 13 TeV pp collisions with the ATLAS detector. 2020. URL: https://doi.org/10.17182/hepdata.91374, doi:10.17182/hepdata.91374.

11. Search for direct stau production in events with two hadronic -leptons in $\sqrt s = 13$ TeV pp collisions with the ATLAS detector. 2019. URL: https://doi.org/10.17182/hepdata.92006, doi:10.17182/hepdata.92006.

12. Search for direct production of electroweakinos in final states with one lepton, missing transverse momentum and a Higgs boson decaying into two b-jets in (pp) collisions at $\sqrt s=13$ TeV with the ATLAS detector. 2020. URL: https://doi.org/10.17182/hepdata.90607.v2, doi:10.17182/hepdata.90607.v2.

13. Search for squarks and gluinos in final states with same-sign leptons and jets using 139 fb$^-1$ of data collected with the ATLAS detector. 2020. URL: https://doi.org/10.17182/hepdata.91214.v3, doi:10.17182/hepdata.91214.v3.

14. Search for bottom-squark pair production with the ATLAS detector in final states containing Higgs bosons, b-jets and missing transverse momentum. 2019. URL: https://doi.org/10.17182/hepdata.89408, doi:10.17182/hepdata.89408.

Note: ATLAS maintains a public list of all published statistical models for supersymmetry searches.

CHAPTER

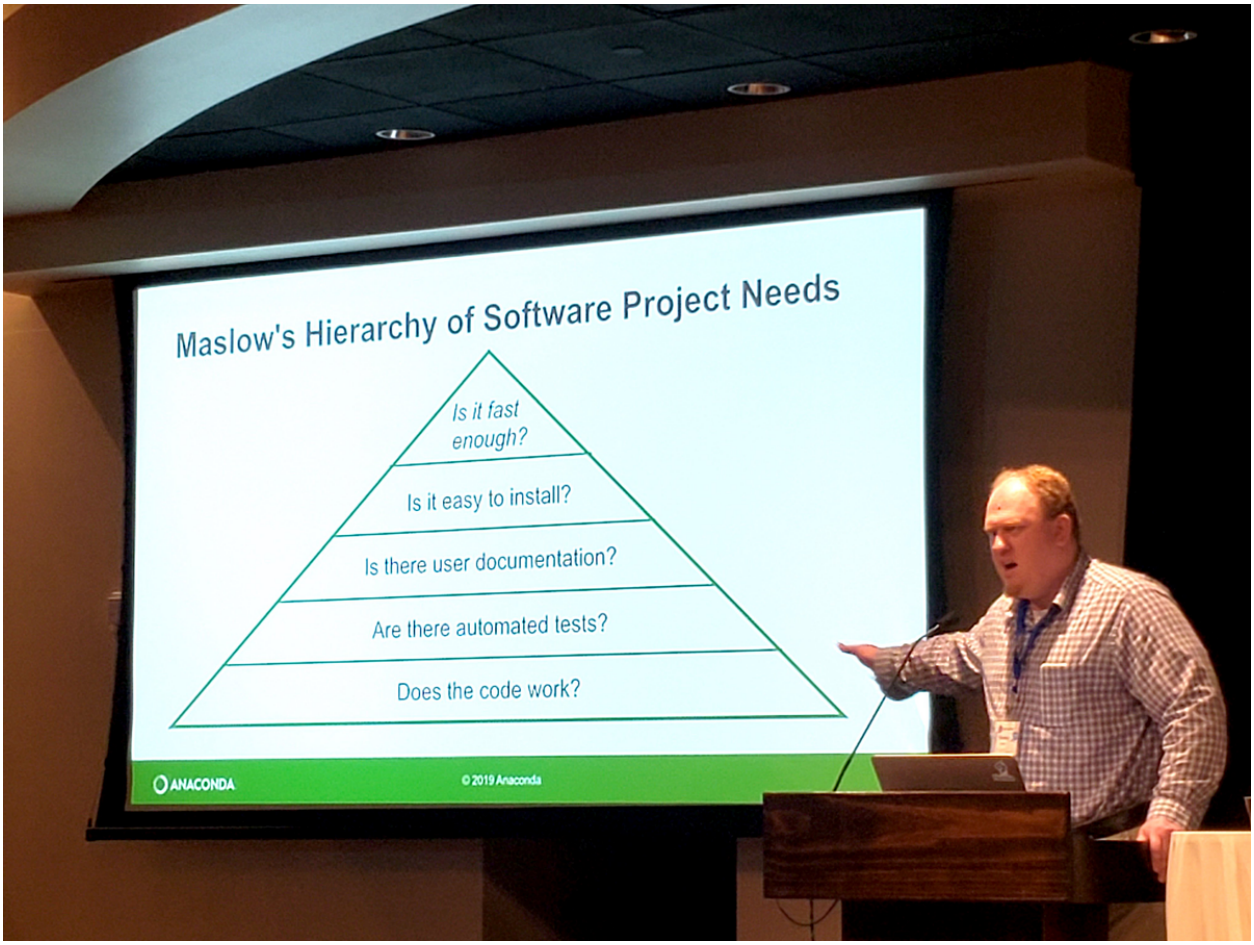
FIFTEEN

ROADMAP (2019-2020)

This is the pyhf 2019 into 2020 Roadmap (Issue #561).

15.1 Overview and Goals

We will follow loosely Seibert's Heirarchy of Needs



(Stan Seibert, SciPy 2019)

As a general overview that will include:

- Improvements to docs

  - Add lots of examples
  - Add at least 5 well documented case studies
- Issue cleanup
- Adding core feature support
- "pyhf evolution": integration with columnar data analysis systems
- GPU support and testing
- Publications
  - Submit pyhf to JOSS
  - Submit pyhf to pyOpenSci
  - Start pyhf paper in 2020
- Align with IRIS-HEP Analysis Systems NSF milestones

15.2 Time scale

The roadmap will be executed over mostly Quarter 3 of 2019 through Quarter 1 of 2020, with some projects continuing into Quarter 2 of 2020

- 2019-Q3
- 2019-Q4
- 2020-Q1
- (2020-Q2)

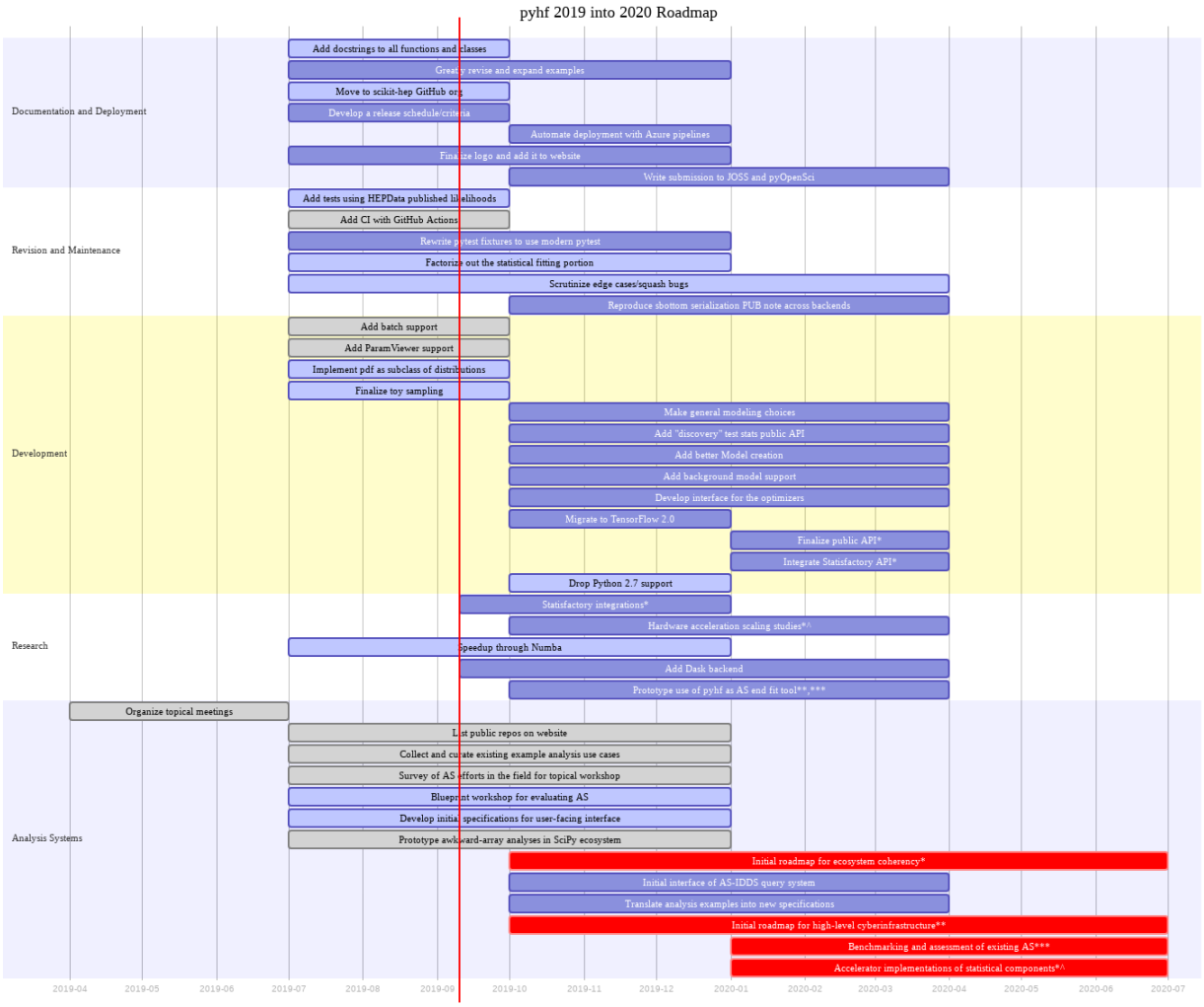
15.3 Roadmap

1. **Documentation and Deployment**
   - Add docstrings to all functions and classes (Issues #38, #349) [2019-Q3]
   - Greatly revise and expand examples (Issues #168, #202, #212, #325, #342, #349, #367) [2019-Q3 → 2019-Q4]
     - Add small case studies with published sbottom likelihood from HEPData
   - Move to scikit-hep GitHub organization [2019-Q3]
   - Develop a release schedule/criteria [2019-Q4]
   - Automate deployment with [STRIKEOUT:Azure pipeline (talk with Henry Schreiner) (Issue #517)] GitHub Actions (Issue #508) [2019-Q3]
   - Finalize logo and add it to website (Issue #453) [2019-Q3 → 2019-Q4]
   - Write submission to JOSS (Issue #502) and write submission to pyOpenSci [2019-Q4 → 2020-Q2]
   - Contribute to IRIS-HEP Analysis Systems Milestones "Initial roadmap for ecosystem coherency" and "Initial roadmap for high-level cyberinfrastructure components of analysis system" [2019-Q4 → 2020-Q2]
2. **Revision and Maintenance**
   - Add tests using HEPData published sbottom likelihoods (Issue #518) [2019-Q3]

- Add CI with GitHub Actions and Azure Pipelines (PR #527, Issue #517) [2019-Q3]
- Investigate rewrite of pytest fixtures to use modern pytest (Issue #370) [2019-Q3 → 2019-Q4]
- Factorize out the statistical fitting portion into `pyhf.infer` (PR #531) [2019-Q3 → 2019-Q4]
- Bug squashing at large [2019-Q3 → 2020-Q2]
  - Unexpected use cases (Issues #324, #325, #529)
  - Computational edge cases (Issues #332, #445)
- Make sure that all backends reproduce sbottom results [2019-Q4 → 2020-Q2]

3. **Development**
   - Batch support (PR #503) [2019-Q3]
   - Add ParamViewer support (PR #519) [2019-Q3]
   - Add setting of NPs constant/fixed (PR #653) [2019-Q3]
   - Implement pdf as subclass of distributions (PR #551) [2019-Q3]
   - Add sampling with toys (PR #558) [2019-Q3]
   - Make general modeling choices (e.g., Issue #293) [2019-Q4 → 2020-Q1]
   - Add "discovery" test stats (p0) (PR #520) [2019-Q4 → 2020-Q1]
   - Add better Model creation [2019-Q4 → 2020-Q1]
   - Add background model support (Issues #514, #946) [2019-Q4 → 2020-Q1]
   - Develop interface for the optimizers similar to tensor/backend (Issue #754, PR #951) [2019-Q4 → 2020-Q1]
   - Migrate to TensorFlow v2.0 (PR #541) [2019-Q4]
   - Drop Python 2.7 support at end of 2019 (Issue #469) [2019-Q4 (last week of December 2019)]
   - Finalize public API [2020-Q1]
   - Integrate pyfitcore/Statisfactory API [2020-Q1]
4. **Research**
   - Add pyfitcore/Statisfactory integrations (Issue #344, zfit Issue 120) [2019-Q4]
   - Hardware acceleration scaling studies (Issues #93, #301) [2019-Q4 → 2020-Q1]
   - Speedup through Numba (Issue #364) [2019-Q3 → 2019-Q4]
   - Dask backend (Issue #259) [2019-Q3 → 2020-Q1]
   - Attempt to use pyhf as fitting tool for full Analysis Systems pipeline test in early 2020 [2019-Q4 → 2020-Q1]
   - pyhf should satisfy IRIS-HEP Analysis Systems Milestone "GPU/accelerator-based implementation of statistical and other appropriate components" [2020-Q1 → 2020-Q2] and contributes to "Benchmarking and assessment of prototype analysis system components" [2020-Q3 → 2020-Q4]

15.3.1 Roadmap as Gantt Chart



15.4 Presentations During Roadmap Timeline

- Talk at IRIS-HEP Institute Retreat (September 12-13th, 2019)
- Talk at PyHEP 2019 (October 16-18th, 2019)
- Talk at CHEP 2019 (November 4-8th, 2019)
- Poster at CHEP 2019 (November 4-8th, 2019)

CHAPTER

SIXTEEN

RELEASE NOTES

16.1 v0.6.3

This is a patch release from `v0.6.2` → `v0.6.3`.

16.1.1 Important Notes

- With the addition of writing ROOT files in `uproot` `v4.1.0` the `xmlio` extra no longer requires `uproot3` and all dependencies on `uproot3` and `uproot3-methods` have been dropped. (PR #1567) `uproot4` additionally brings large speedups to writing, which results in an order of magnitude faster conversion time for most workspace conversions from JSON back to XML + ROOT with `pyhf json2xml`.
- All backends are now fully compatible and tested with Python 3.9. (PR #1574)
- The TensorFlow backend now supports compatibility with TensorFlow `v2.2.1` and later and TensorFlow Probability `v0.10.1` and later. (PR #1001)
- The *pyhf.workspace.Workspace.data()* `with_aux` keyword arg has been renamed to `include_auxdata` to improve API consistency. (PR #1562)

16.1.2 Fixes

- The weakref bug with Click `v8.0`+ was resolved. `pyhf` is now fully compatible with Click `v7` and `v8` releases. (PR #1530)

16.1.3 Features

Python API

- Model parameter names are now propagated to optimizers through addition of the *pyhf.pdf._ModelConfig.par_names()* API. *pyhf.pdf._ModelConfig.par_names()* also handles non-scalar modifiers with 1 parameter. (PRs #1536, #1560)

```
>>> import pyhf
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> model.config.parameters
['mu', 'uncorr_bkguncrt']
```

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```
>>> model.config.npars
3
>>> model.config.par_names()
['mu', 'uncorr_bkguncrt[0]', 'uncorr_bkguncrt[1]']
```

- The *pyhf.pdf._ModelConfig* `channel_nbins` dict is now sorted by keys to match the order of the `channels` list. (PR #1546)
- The *pyhf.workspace.Workspace.data()* `with_aux` keyword arg has been renamed to `include_auxdata` to improve API consistency. (PR #1562)

16.2 v0.6.2

This is a patch release from `v0.6.1` → `v0.6.2`.

16.2.1 Important Notes

- The `pyhf.simplemodels.hepdata_like()` API has been deprecated in favor of *pyhf.simplemodels.uncorrelated_background()*. The `pyhf.simplemodels.hepdata_like()` API will be removed in `pyhf v0.7.0`. (PR #1438)
- There is a small breaking API change for *pyhf.contrib.viz.brazil.plot_results()*. See the Python API changes section for more information.
- The *pyhf.patchset.PatchSet* schema now allows string types for patch values in patchsets. (PR #1488)
- Only lower bounds on core dependencies are now set. This allows for greater developer freedom and reduces the risk of breaking user's applications by unnecessarily constraining libraries. This also means that users will be responsible for ensuring that their installed dependencies do not conflict with or break `pyhf`. c.f. Hynek Schlawack's blog post Semantic Versioning Will Not Save You for more in-depth coverage on this topic. For most users nothing should change. This mainly affects developers of other libraries in which `pyhf` is a dependency. (PR #1382)
- Calling `dir()` on any `pyhf` module or trying to tab complete an API will now provide a more helpfully restricted view of the available APIs. This should help provide better exploration of the `pyhf` API. (PR #1403)
- Docker images of releases are now published to both Docker Hub and to the GitHub Container Registry. (PR #1444)
- CUDA enabled Docker images are now available for release `v0.6.1` and later on Docker Hub and the GitHub Container Registry. Visit github.com/pyhf/cuda-images for more information.

16.2.2 Fixes

- Allow for precision to be properly set for the tensorlib `ones` and `zeros` methods through a `dtype` argument. This allows for precision to be properly set through the *pyhf.set_backend()* `precision` argument. (PR #1369)
- The default precision for all backends is now `64b`. (PR #1400)
- Add check to ensure that POIs are not fixed during a fit. (PR #1409)
- Parameter name strings are now normalized to remove trailing spaces. (PR #1436)
- The logging level is now not automatically set in `pyhf.contrib.utils`. (PR #1460)

16.2.3 Features

Python API

- The `pyhf.simplemodels.hepdata_like()` API has been deprecated in favor of *pyhf.simplemodels.uncorrelated_background()*. The `pyhf.simplemodels.hepdata_like()` API will be removed in `pyhf v0.7.0`. (PR #1438)
- The *pyhf.simplemodels.correlated_background()* API has been added to provide an example model with a single channel with a correlated background uncertainty. (PR #1435)
- Add CLs component plotting kwargs to *pyhf.contrib.viz.brazil.plot_results()*. This allows CLs+b and CLb components of the CLs ratio to be plotted as well. To be more consistent with the `matplotlib` API, *pyhf.contrib.viz.brazil.plot_results()* now returns a lists of the artists drawn on the axis and moves the `ax` arguments to the to the last argument. (PR #1377)
- The `pyhf.compat` module has been added to aid in translating to and from ROOT names. (PR #1439)

CLI API

- The CLI API now supports a `patchset inspect` API to list the individual patches in a `PatchSet`. (PR #1412)

```
pyhf patchset inspect [OPTIONS] [PATCHSET]
```

16.2.4 Contributors

`v0.6.2` benefited from contributions from:

- Alexander Held

16.3 v0.6.1

This is a patch release from `v0.6.0` → `v0.6.1`.

16.3.1 Important Notes

- As a result of changes to the default behavior of `torch.distributions` in PyTorch `v1.8.0`, accommodating changes have been made in the underlying implementations for *pyhf.tensor.pytorch_backend.pytorch_backend()*. These changes require a new lower bound of `torch v1.8.0` for use of the PyTorch backend.

16.3.2 Fixes

- In the PyTorch backend the `validate_args` kwarg is used with `torch.distributions` to ensure a continuous approximation of the Poisson distribution in `torch v1.8.0`+.

16.3.3 Features

Python API

- The `solver_options` kwarg can be passed to the *pyhf.optimize.opt_scipy.scipy_optimizer()* optimizer for additional configuration of the minimization. See `scipy.optimize.show_options()` for additional options of optimization solvers.
- The `torch` API is now used to provide the implementations of the `ravel`, `tile`, and `outer` tensorlib methods for the PyTorch backend.

16.4 v0.6.0

This is a minor release from `v0.5.4` → `v0.6.0`.

16.4.1 Important Notes

- Please note this release has **API breaking changes** and carefully read these notes while updating your code to the `v0.6.0` API. Perhaps most relevant is the changes to the *pyhf.infer.hypotest()* API, which now uses a `calctype` argument to differentiate between using an asymptotic calculator or a toy calculator, and a `test_stat` kwarg to specify which test statistic the calculator should use, with `'qtilde'`, corresponding to *pyhf.infer.test_statistics.qmu_tilde()*, now the default option. It also relies more heavily on using kwargs to pass options through to the optimizer.
- Following the recommendations of NEP 29 — Recommend Python and NumPy version support as a community policy standard `pyhf v0.6.0` drops support for Python 3.6. PEP 494 – Python 3.6 Release Schedule also notes that Python 3.6 will be end of life in December 2021, so `pyhf` is moving forward with a minimum required runtime of Python 3.7.
- Support for the discovery test statistic, q_0, has now been added through the *pyhf.infer.test_statistics.q0()* API.
- Support for pseudoexperiments (toys) has been added through the *pyhf.infer.calculators.ToyCalculator()* API. Please see the corresponding example notebook for more detailed exploration of the API.
- The `minuit` extra, `python -m pip install pyhf[minuit]`, now uses and requires the `iminuit v2.X` release series and API. Note that `iminuit v2.X` can result in slight differences in minimization results from `iminuit v1.X`.
- The documentation will now be versioned with releases on ReadTheDocs. Please use pyhf.readthedocs.io to access the documentation for the latest stable release of `pyhf`.
- `pyhf` is transtioning away from Stack Overflow to GitHub Discussions for resolving user questions not covered in the documentation. Please check the GitHub Discussions page to search for discussions addressing your questions and to open up a new discussion if your question is not covered.
- `pyhf` has published a paper in the Journal of Open Source Software. Please make sure to include the paper reference in all citations of `pyhf`, as documented in the Use and Citations section of the documentation.

16.4.2 Fixes

- Fix bug where all extras triggered warning for installation of the `contrib` extra.
- `float`-like values are used in division for *pyhf.writexml()*.
- `Model.spec` now supports building new models from existing models.
- p-values are now reported based on their quantiles, instead of interpolating test statistics and converting to p-values.
- Namespace collisions between `uproot3` and `uproot`/`uproot4` have been fixed for the `xmlio` extra.
- The `normsys` modifier now uses the *pyhf.interpolators.code4* interpolation method by default.
- The `histosys` modifier now uses the *pyhf.interpolators.code4p* interpolation method by default.

16.4.3 Features

Python API

- The `tensorlib` API now supports a `tensorlib.to_numpy` and `tensorlib.ravel` API.
- The *pyhf.infer.calculators.ToyCalculator()* API has been added to support pseudoexperiments (toys).
- The empirical test statistic distribution API has been added to help support the `ToyCalculator` API.
- Add a `tolerance` kwarg to the optimizer API to set a `float` value as a tolerance for termination of the fit.
- The *pyhf.optimize.opt_minuit.minuit_optimizer()* optimizer now can return correlations of the fitted parameters through use of the `return_correlation` Boolean kwarg.
- Add the `pyhf.utils.citation` API to get a `str` of the preferred BibTeX entry for citation of the version of `pyhf` installed. See the example for the CLI API for more information.
- The *pyhf.infer.hypotest()* API now uses a `calctype` argument to differentiate between using an asymptotic calculator or a toy calculator, and a `test_stat` kwarg to specify which test statistic to use. It also relies more heavily on using kwargs to pass options through to the optimizer.
- The default `test_stat` kwarg for *pyhf.infer.hypotest()* and the calculator APIs is `'qtilde'`, which corresponds to the alternative test statistic *pyhf.infer.test_statistics.qmu_tilde()*.
- The return type of p-value like functions is now a 0-dimensional `tensor` (with shape `()`) instead of a `float`. This is required to support end-to-end automatic differentiation in future releases.

CLI API

- The CLI API now supports a `--citation` or `--cite` option to print the preferred BibTeX entry for citation of the version of `pyhf` installed.

```
$ pyhf --citation
@software{pyhf,
  author = {Lukas Heinrich and Matthew Feickert and Giordon Stark},
  title = "{pyhf: v0.6.0}",
  version = {0.6.0},
  doi = {10.5281/zenodo.1169739},
  url = {https://doi.org/10.5281/zenodo.1169739},
  note = {https://github.com/scikit-hep/pyhf/releases/tag/v0.6.0}
}
```

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```
@article{pyhf_joss,
  doi = {10.21105/joss.02823},
  url = {https://doi.org/10.21105/joss.02823},
  year = {2021},
  publisher = {The Open Journal},
  volume = {6},
  number = {58},
  pages = {2823},
  author = {Lukas Heinrich and Matthew Feickert and Giordon Stark and Kyle Cranmer},
  title = {pyhf: pure-Python implementation of HistFactory statistical models},
  journal = {Journal of Open Source Software}
}
```

16.4.4 Contributors

`v0.6.0` benefited from contributions from:

- Alexander Held
- Marco Gorelli
- Pradyumna Rahul K
- Eric Schanet
- Henry Schreiner

16.5 v0.5.4

This is a patch release from `v0.5.3` → `v0.5.4`.

16.5.1 Fixes

- Require `uproot3` instead of `uproot` `v3.X` releases to avoid conflicts when `uproot4` is installed in an environment with `uproot` `v3.X` installed and namespace conflicts with `uproot-methods`. Adoption of `uproot3` in `v0.5.4` will ensure `v0.5.4` works far into the future if XML and ROOT I/O through uproot is required.

Example:

Without the `v0.5.4` patch release there is a regression in using `uproot` `v3.X` and `uproot4` in the same environment (which was swiftly identified and patched by the fantastic `uproot` team)

```
$ python -m pip install "pyhf[xmlio]<0.5.4"
$ python -m pip list | grep "pyhf\|uproot"
pyhf           0.5.3
uproot         3.13.1
uproot-methods 0.8.0
$ python -m pip install uproot4
$ python -m pip list | grep "pyhf\|uproot"
pyhf           0.5.3
uproot         4.0.0
```

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```
uproot-methods 0.8.0
uproot4        4.0.0
```

this is resolved in `v0.5.4` with the requirement of `uproot3`

```
$ python -m pip install "pyhf[xmlio]>=0.5.4"
$ python -m pip list | grep "pyhf\|uproot"
pyhf             0.5.4
uproot3          3.14.1
uproot3-methods 0.10.0
$ python -m pip install uproot4 # or uproot
$ python -m pip list | grep "pyhf\|uproot"
pyhf             0.5.4
uproot           4.0.0
uproot3          3.14.1
uproot3-methods 0.10.0
uproot4          4.0.0
```

16.6 v0.5.3

This is a patch release from `v0.5.2` → `v0.5.3`.

16.6.1 Fixes

- Workspaces are now immutable
- ShapeFactor support added to XML reading and writing
- An error is raised if a fit initialization parameter is outside of its bounds (preventing hypotest with POI outside of bounds)

16.6.2 Features

Python API

- Inverting hypothesis tests to get upper limits now has an API with `pyhf.infer.intervals.upperlimit`
- Building workspaces from a model and data added with `pyhf.workspace.build`

CLI API

- Added CLI API for `pyhf.infer.fit`: `pyhf fit`
- pyhf combine now allows for merging channels: `pyhf combine --merge-channels --join <join option>`
- Added utility to download archived pyhf pallets (workspaces + patchsets) to contrib module: `pyhf contrib download`

16.6.3 Contributors

`v0.5.3` benefited from contributions from:

- Karthikeyan Singaravelan

CHAPTER

SEVENTEEN

CONTRIBUTORS

`pyhf` is openly developed and benefits from the contributions and feedback from its users. The `pyhf` dev team would like to thank all contributors to the project for their support and help. Thank you!

Contributors include:

- Jessica Forde
- Ruggero Turra
- Tadej Novak
- Frank Sauerburger
- Lars Nielsen
- Kanishk Kalra
- Nikolai Hartmann
- Alexander Held
- Karthikeyan Singaravelan
- Marco Gorelli
- Pradyumna Rahul K
- Eric Schanet
- Henry Schreiner
- Saransh Chopra
- Sviatoslav Sydorenko
- Mason Proffitt
- Lars Henkelmann
- Aryan Roy


pyhf
∂ifferentiable
ℒikelihoods

CHAPTER

EIGHTEEN

PURE-PYTHON FITTING/LIMIT-SETTING/INTERVAL ESTIMATION HISTFACTORY-STYLE

The HistFactory p.d.f. template [CERN-OPEN-2012-016] is per-se independent of its implementation in ROOT and sometimes, it's useful to be able to run statistical analysis outside of ROOT, RooFit, RooStats framework.

This repo is a pure-python implementation of that statistical model for multi-bin histogram-based analysis and its interval estimation is based on the asymptotic formulas of "Asymptotic formulae for likelihood-based tests of new physics" [arXiv:1007.1727]. The aim is also to support modern computational graph libraries such as PyTorch and TensorFlow in order to make use of features such as autodifferentiation and GPU acceleration.

18.1 Hello World

This is how you use the `pyhf` Python API to build a statistical model and run basic inference:

```
>>> import pyhf
>>> pyhf.set_backend("numpy")
>>> model = pyhf.simplemodels.uncorrelated_background(
...     signal=[12.0, 11.0], bkg=[50.0, 52.0], bkg_uncertainty=[3.0, 7.0]
... )
>>> data = [51, 48] + model.config.auxdata
>>> test_mu = 1.0
>>> CLs_obs, CLs_exp = pyhf.infer.hypotest(
...     test_mu, data, model, test_stat="qtilde", return_expected=True
... )
>>> print(f"Observed: {CLs_obs:.9f}, Expected: {CLs_exp:.9f}")
Observed: 0.052514974, Expected: 0.064453205
```

Alternatively the statistical model and observational data can be read from its serialized JSON representation (see next section).

```
>>> import pyhf
>>> import requests
```

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```
>>> pyhf.set_backend("numpy")
>>> wspace = pyhf.Workspace(requests.get("https://git.io/JJYDE").json())
>>> model = wspace.model()
>>> data = wspace.data(model)
>>> test_mu = 1.0
>>> CLs_obs, CLs_exp = pyhf.infer.hypotest(
...     test_mu, data, model, test_stat="qtilde", return_expected=True
... )
>>> print(f"Observed: {CLs_obs:.9f}, Expected: {CLs_exp:.9f}")
Observed: 0.359984092, Expected: 0.359984092
```

Finally, you can also use the command line interface that `pyhf` provides

```
$ cat << EOF  | tee likelihood.json | pyhf cls
{
    "channels": [
        { "name": "singlechannel",
          "samples": [
            { "name": "signal",
              "data": [12.0, 11.0],
              "modifiers": [ { "name": "mu", "type": "normfactor", "data": null} ]
            },
            { "name": "background",
              "data": [50.0, 52.0],
              "modifiers": [ {"name": "uncorr_bkguncrt", "type": "shapesys", "data": [3.
↪0, 7.0]} ]
            }
          ]
        }
    ],
    "observations": [
        { "name": "singlechannel", "data": [51.0, 48.0] }
    ],
    "measurements": [
        { "name": "Measurement", "config": {"poi": "mu", "parameters": []} }
    ],
    "version": "1.0.0"
}
EOF
```

which should produce the following JSON output:

```
{
   "CLs_exp": [
      0.0026062609501074576,
      0.01382005356161206,
      0.06445320535890459,
      0.23525643861460702,
      0.573036205919389
   ],
   "CLs_obs": 0.05251497423736956
}
```

18.2 What does it support

Implemented variations:

- HistoSys
- OverallSys
- ShapeSys
- NormFactor
- Multiple Channels
- Import from XML + ROOT via uproot
- ShapeFactor
- StatError
- Lumi Uncertainty
- Non-asymptotic calculators

Computational Backends:

- NumPy
- PyTorch
- TensorFlow
- JAX

Optimizers:

- SciPy (`scipy.optimize`)
- MINUIT (`iminuit`)

All backends can be used in combination with all optimizers. Custom user backends and optimizers can be used as well.

18.3 Todo

- StatConfig

results obtained from this package are validated against output computed from HistFactory workspaces

18.4 A one bin example

```
import pyhf
import numpy as np
import matplotlib.pyplot as plt
from pyhf.contrib.viz import brazil

pyhf.set_backend("numpy")
model = pyhf.simplemodels.uncorrelated_background(
    signal=[10.0], bkg=[50.0], bkg_uncertainty=[7.0]
```

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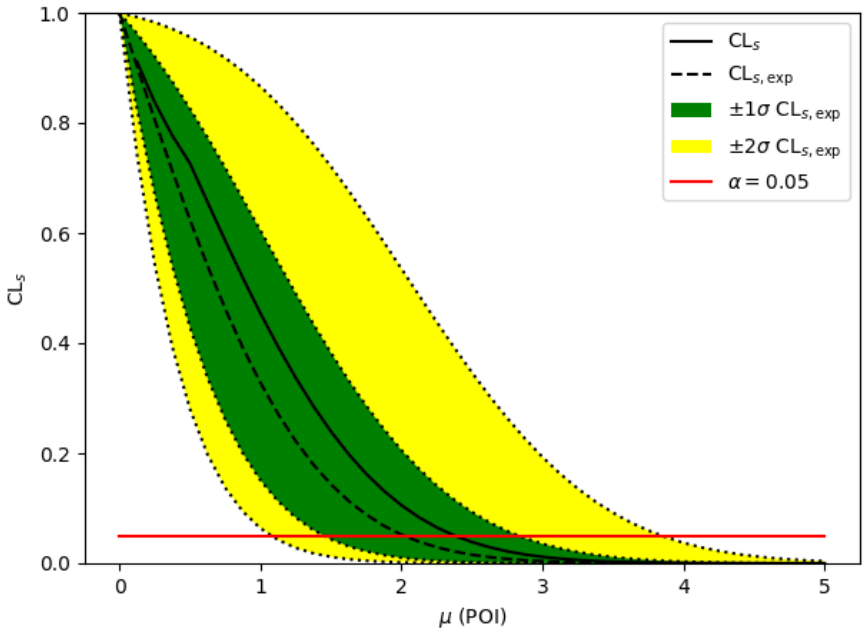
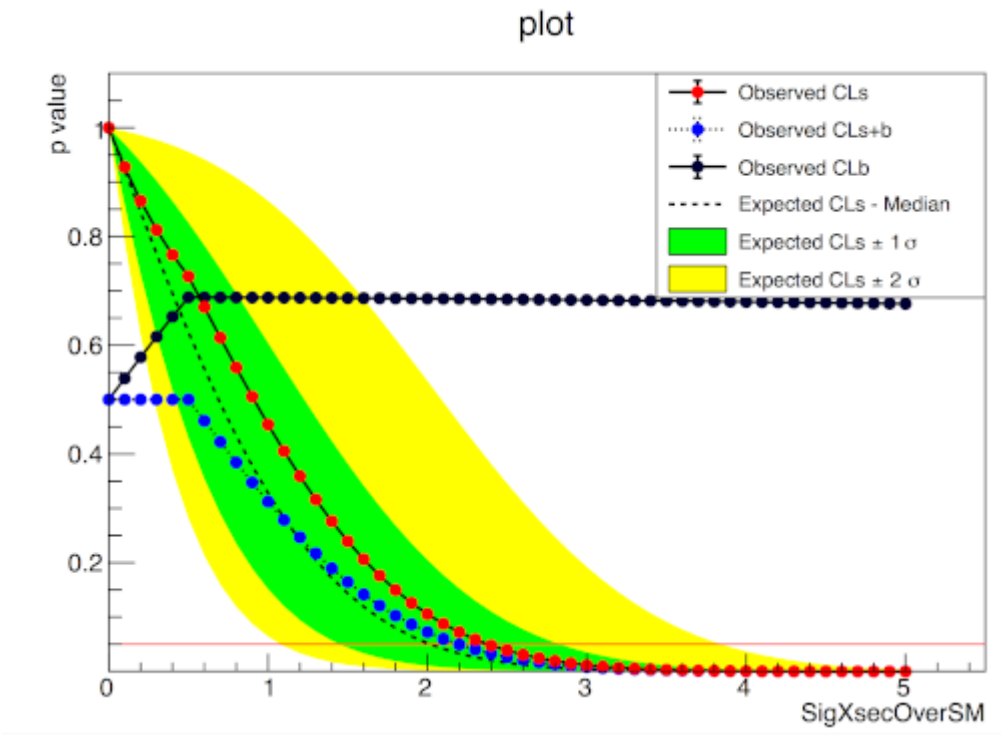
```
)
data = [55.0] + model.config.auxdata

poi_vals = np.linspace(0, 5, 41)
results = [
    pyhf.infer.hypotest(
        test_poi, data, model, test_stat="qtilde", return_expected_set=True
    )
    for test_poi in poi_vals
]

fig, ax = plt.subplots()
fig.set_size_inches(7, 5)
brazil.plot_results(poi_vals, results, ax=ax)
fig.show()
```

pyhf



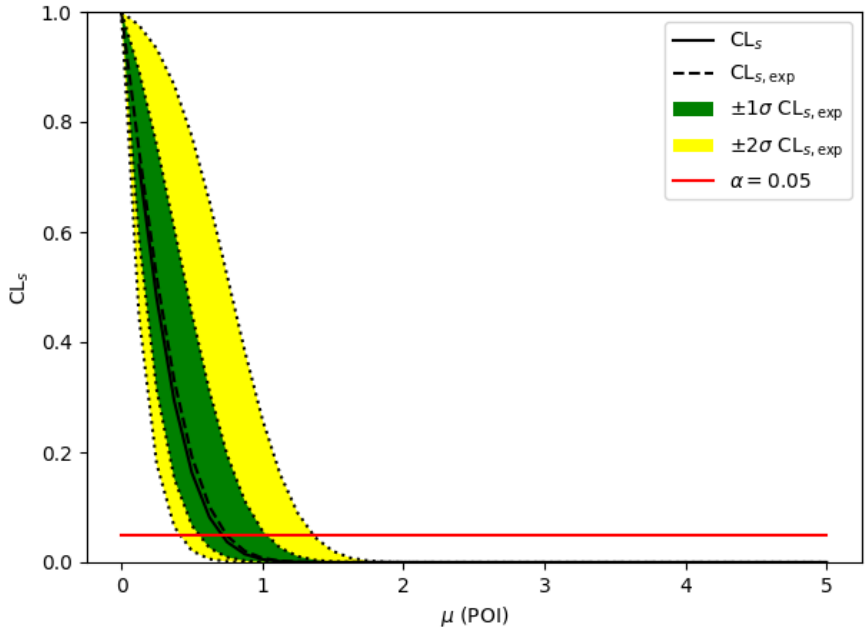
ROOT



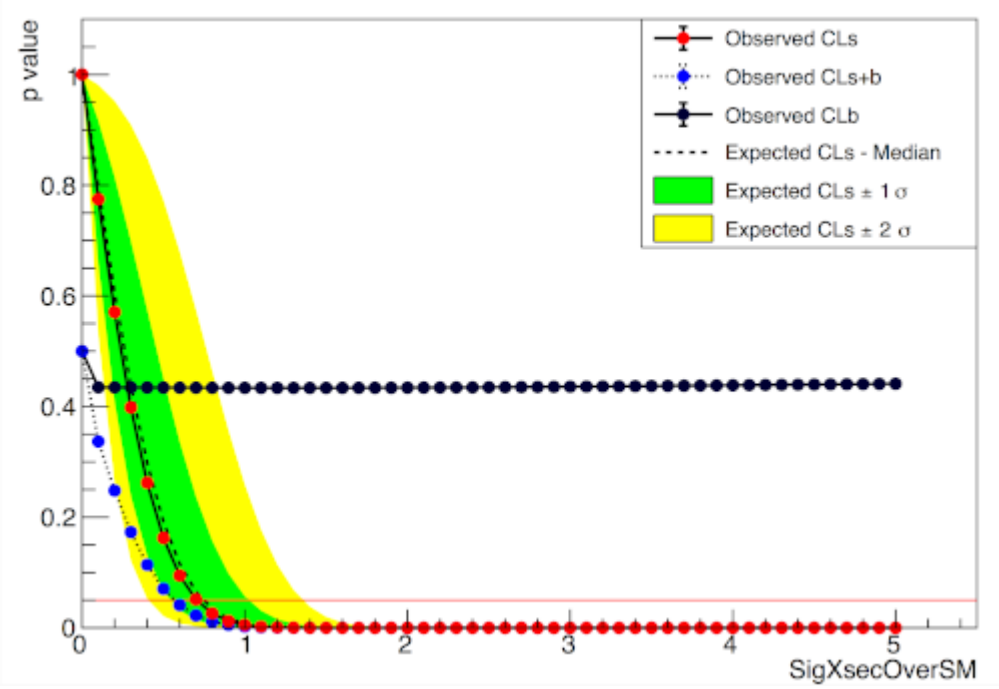
18.5 A two bin example

```
import pyhf
import numpy as np
import matplotlib.pyplot as plt
from pyhf.contrib.viz import brazil

pyhf.set_backend("numpy")
model = pyhf.simplemodels.uncorrelated_background(
    signal=[30.0, 45.0], bkg=[100.0, 150.0], bkg_uncertainty=[15.0, 20.0]
)
data = [100.0, 145.0] + model.config.auxdata

poi_vals = np.linspace(0, 5, 41)
results = [
    pyhf.infer.hypotest(
        test_poi, data, model, test_stat="qtilde", return_expected_set=True
    )
    for test_poi in poi_vals
]

fig, ax = plt.subplots()
fig.set_size_inches(7, 5)
brazil.plot_results(poi_vals, results, ax=ax)
fig.show()
```

pyhf


1.0
0.8
0.6
0.4
0.2
0.0
CL_s
0
1
2
3
4
5
μ (POI)
CL_s
$CL_{s,\,exp}$
$\pm 1\sigma$ $CL_{s,\,exp}$
$\pm 2\sigma$ $CL_{s,\,exp}$
$\alpha = 0.05$

ROOT


p value
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4
5
SigXsecOverSM
Observed CLs
Observed CLs+b
Observed CLb
Expected CLs - Median
Expected CLs ± 1 σ
Expected CLs ± 2 σ

18.6 Installation

To install `pyhf` from PyPI with the NumPy backend run

```
python -m pip install pyhf
```

and to install `pyhf` with all additional backends run

```
python -m pip install pyhf[backends]
```

or a subset of the options.

To uninstall run

```
python -m pip uninstall pyhf
```

18.7 Questions

If you have a question about the use of `pyhf` not covered in the documentation, please ask a question on the GitHub Discussions.

If you believe you have found a bug in `pyhf`, please report it in the GitHub Issues. If you're interested in getting updates from the `pyhf` dev team and release announcements you can join the `pyhf-announcements` mailing list.

18.8 Citation

As noted in Use and Citations, the preferred BibTeX entry for citation of `pyhf` includes both the Zenodo archive and the JOSS paper:

```
@software{pyhf,
  author = {Lukas Heinrich and Matthew Feickert and Giordon Stark},
  title = "{pyhf: v0.6.3}",
  version = {0.6.3},
  doi = {10.5281/zenodo.1169739},
  url = {https://doi.org/10.5281/zenodo.1169739},
  note = {https://github.com/scikit-hep/pyhf/releases/tag/v0.6.3}
}

@article{pyhf_joss,
  doi = {10.21105/joss.02823},
  url = {https://doi.org/10.21105/joss.02823},
  year = {2021},
  publisher = {The Open Journal},
  volume = {6},
  number = {58},
  pages = {2823},
  author = {Lukas Heinrich and Matthew Feickert and Giordon Stark and Kyle Cranmer},
  title = {pyhf: pure-Python implementation of HistFactory statistical models},
  journal = {Journal of Open Source Software}
}
```

18.9 Authors

pyhf is openly developed by Lukas Heinrich, Matthew Feickert, and Giordon Stark.

Please check the contribution statistics for a list of contributors.

18.10 Milestones

- 2020-07-28: 1000 GitHub issues and pull requests. (See PR #1000)

18.11 Acknowledgements

Matthew Feickert has received support to work on pyhf provided by NSF cooperative agreement OAC-1836650 (IRIS-HEP) and grant OAC-1450377 (DIANA/HEP).

CHAPTER

NINETEEN

INDICES AND TABLES

- genindex
- modindex
- search

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[intro-2] Kyle Cranmer, George Lewis, Lorenzo Moneta, Akira Shibata, and Wouter Verkerke. HistFactory: A tool for creating statistical models for use with RooFit and RooStats. Technical Report CERN-OPEN-2012-016, New York U., New York, Jan 2012. URL: https://cds.cern.ch/record/1456844.

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[faq-2] Lukas Heinrich, Holger Schulz, Jessica Turner, and Ye-Ling Zhou. Constraining A_4 Leptonic Flavour Model Parameters at Colliders and Beyond. 2018. arXiv:1810.05648.

PYTHON MODULE INDEX

p

INDEX

Symbols

A

B

C

D

E

F

G

H

I

J

L

M

N

O

P

Q

R

U

V

W

Z