Introduction to `cabinetry`

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Belle II pyhf workshop
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Intro: constructing and using statistical models

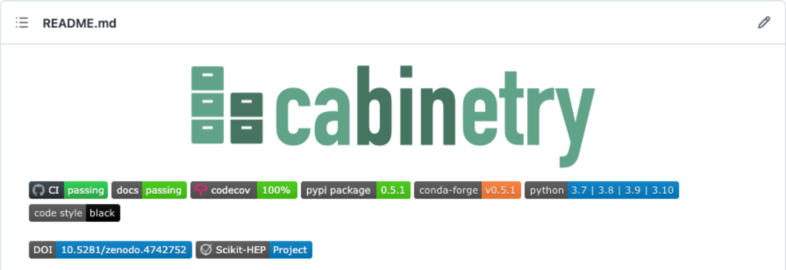
- **Disclaimer:** I am working with ATLAS and probably have a biased view! Curious to learn where things differ in Belle II.

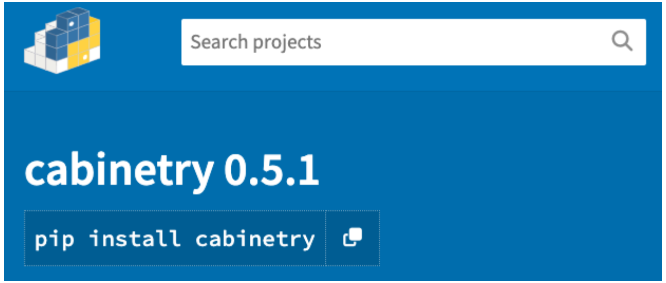
- **Binned template fits** are widely used for **statistical inference**

- **Statistical models** used in particle physics are often **rather complex**
  - lots of book-keeping to handle $O(10k)$ histograms for typical ATLAS applications
  - frequent model modifications needed for tests & debugging

- A set of **tools** emerged over time to aid with **model construction** and **inference**
  - In ATLAS: `HistFitter` and many more internal tools, `Combine` for CMS
    - interested to learn more about what is used elsewhere
  - (some of) these tools also provide utilities to visualize inference result & simplify debugging

The cabinetry library



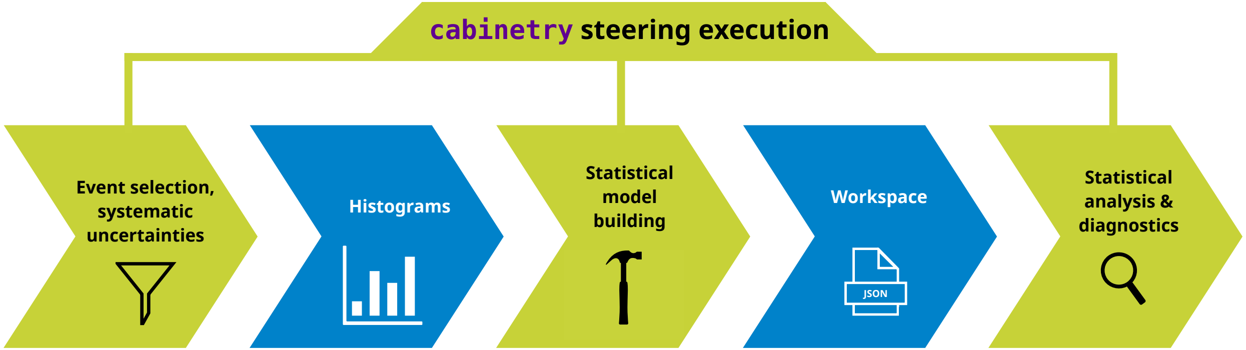


- **cabinetry** is a modern **Python library** for constructing and/or operating **HistFactory** models
    - ❯pip install cabinetry
    - uses pyhf, integrates seamlessly with the Python HEP ecosystem
    - modular design: use the pieces of cabinetry you need
    - part of the Scikit-HEP project

- **cabinetry** ↔ **pyhf** is roughly like **HistFitter** ↔ **ROOT (RooFit, HistFactory, RooStats)**

Working with cabinetry

- **cabinetry** is a **Python library** for creating and operating HistFactory models
  - **design** and **construct statistical models** (workspaces) from instructions in **declarative configuration**
    - analyzers specify selections for signal/control regions, (Monte Carlo) samples, systematic uncertainties
    - `cabinetry` steers creation or collects provided template histograms (region ⊗ sample ⊗ systematic)
    - `cabinetry` produces `HistFactory` workspaces (serialized fit model)
  - perform **statistical inference**
    - including diagnostics and visualization tools to study and disseminate results



Designing a statistical model

- **Declarative configuration** (JSON/YAML/dictionary) specifies everything needed to build a workspace
  - can concisely capture complex region ⊗ sample ⊗ systematic structure

general settings

list of phase space regions (channels)

list of samples (MC/data)

```yaml
General:
  Measurement: "Example"
  InputPath: "input/{SamplePaths}"
  HistogramFolder: "histograms/"
  POI: "Signal_norm"

Regions:
  - Name: "Signal_region"
    Filter: "nJets >= 8"
    Variable: "jet_pt"
    Binning: [200, 300, 400, 500]

Samples:
  - Name: "Data"
    SamplePaths: "data.root"
    Tree: "events"
    Data: True

  - Name: "Signal"
    SamplePaths: "signal.root"
    Tree: "events"
    Weight: "weight_nominal"

  - Name: "Background"
    SamplePaths: "background.root"
    Tree: "events"
    Weight: "weight_nominal"

Systematics:
  - Name: "Luminosity"
    Up:
      Normalization: 0.05
    Down:
      Normalization: -0.05
    Samples: ["Signal", "Background"]
    Type: "Normalization"

  - Name: "ModelingVariation"
    Up:
      Tree: "events_up"
      Weight: "weight_modeling"
    Down:
      Tree: "events_down"
      Weight: "weight_modeling"
    Smoothing:
      Algorithm: "353QH, twice"
    Samples: "Background"
    Type: "NormPlusShape"

NormFactors:
  - Name: "Signal_norm"
    Samples: "Signal"
    Nominal: 1
    Bounds: [0, 10]
```

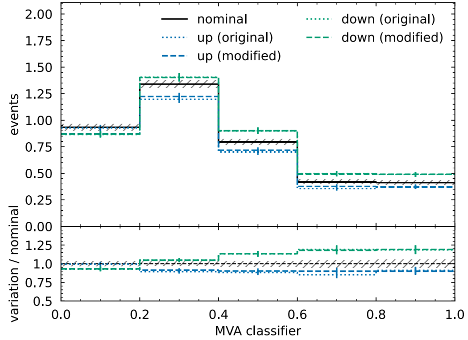
list of systematic uncertainties

list of normalization factors

Template histograms and workspace building

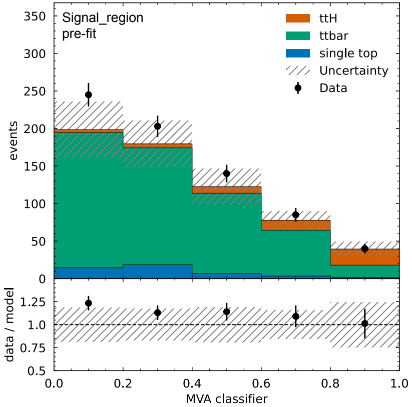
- **Workspaces construction** happens in three steps:
    1) create template histograms from columnar data following config instructions
        - backends execute instructions (default: `uproot`, experimental: coffea)
        - alternatively: collect existing user-provided histograms
    2) optional: apply post-processing to templates (e.g. smoothing)
    3) assemble templates into workspace (`JSON` file)

visualization of individual template histograms

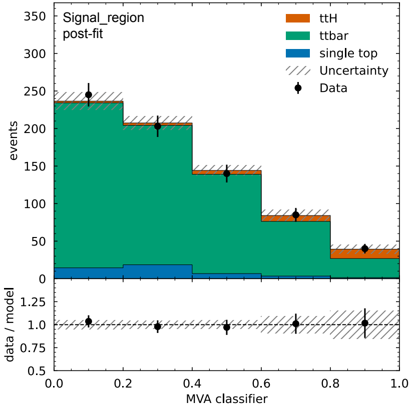


- Utilities provided to **visualize and debug** fit model

fit model visualization



fit to data



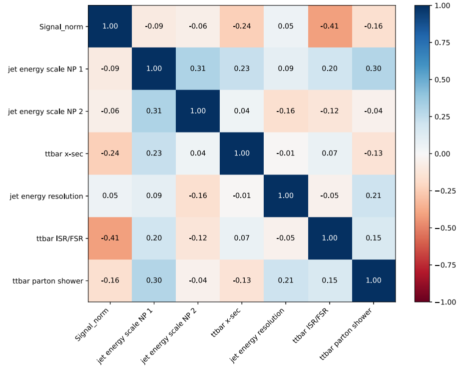
event yield table

sample	Control region	Signal region
single top	44.74	0.35
ttbar	635.98	13.28
z_ttH	30.90	1.80
total	711.61 ± 28.28	15.43 ± 2.69
data	713.00	14.00

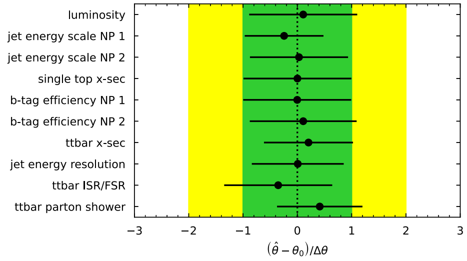
Statistical inference

- Implementations for **common inference tasks** exist
  - includes associated visualizations

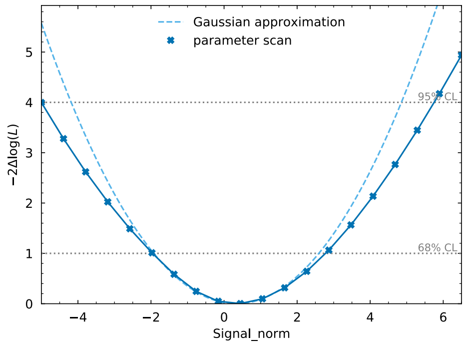
parameter correlations



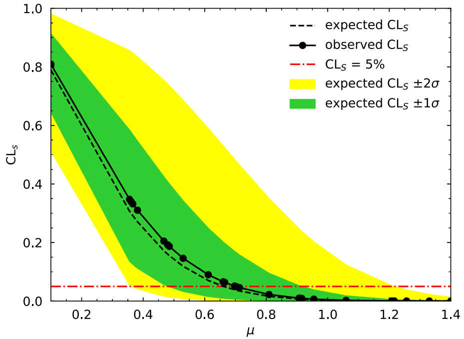
nuisance parameter pulls



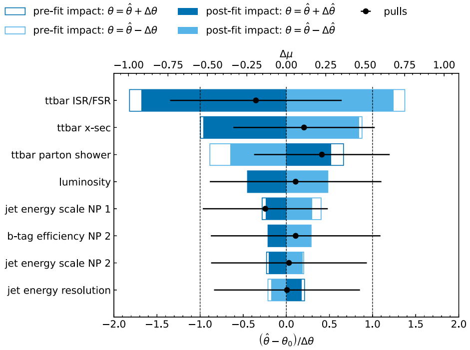
likelihood scans



upper parameter limits



nuisance parameter impacts



discovery significance

```
$ cabinetry significance workspaces/example_workspace.json
INFO - cabinetry.fit - calculating discovery significance
INFO - cabinetry.fit - observed p-value: 1.13053295%
INFO - cabinetry.fit - observed significance: 2.280
INFO - cabinetry.fit - expected p-value: 0.42110716%
INFO - cabinetry.fit - expected significance: 2.635
```

Working with an unknown workspace

- Pick a **workspace** from **HEPData**: 10.17182/hepdata.89408.v3 (analysis: JHEP 12 (2019) 060)
  - download workspace with `pyhf`
  - perform inference and visualize results with `cabinetry`
  - can use inference features regardless of how a workspace was built, functionality factorizes!

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

- See arXiv:2109.04981 and try it on Binder

```python
import json
import cabinetry
import pyhf
from cabinetry.model_utils import prediction
from pyhf.contrib.utils import download

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

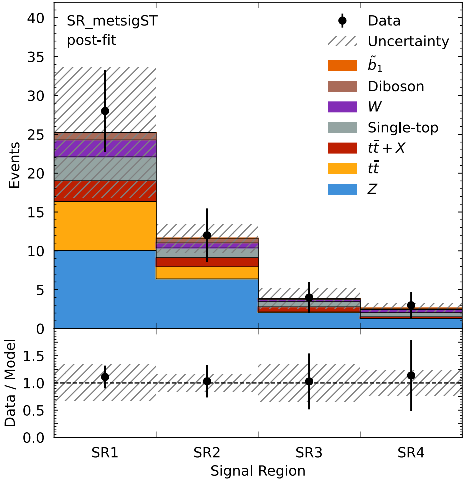
# construct a workspace from a background-only model and a signal hypothesis
bkg_only_workspace = pyhf.Workspace(json.load(open("bottom-squarks/RegionC/BkgOnly.json")))
patchset = pyhf.PatchSet(json.load(open("bottom-squarks/RegionC/patchset.json")))
workspace = patchset.apply(bkg_only_workspace, "sbottom_600_280_150")

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

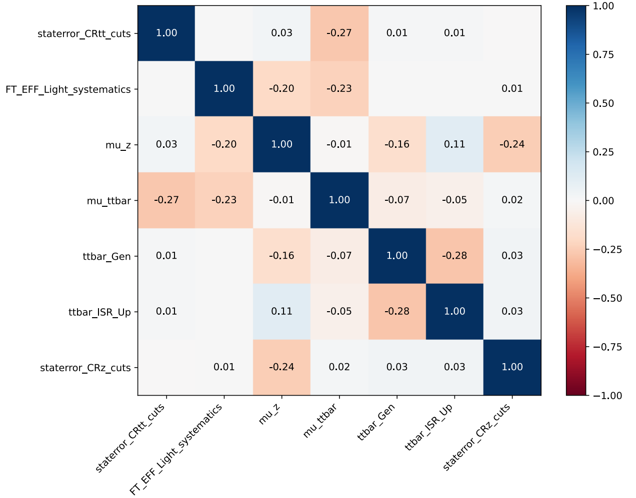
# produce visualizations of the pre-fit model and observed data
prefit_model = prediction(model)
cabinetry.visualize.data_mc(prefit_model, data)

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

# produce visualizations of the post-fit model and observed data
postfit_model = prediction(model, fit_results=fit_results)
cabinetry.visualize.data_mc(postfit_model, data)
```

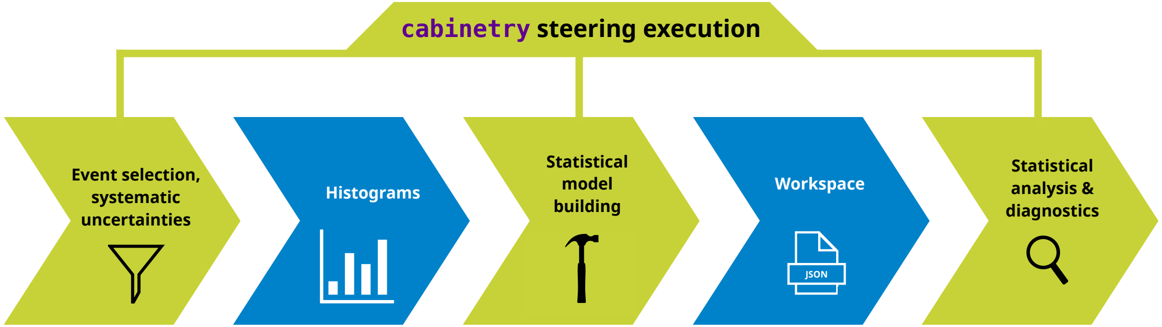


(workspace contains additional channels not shown here)



`cabinetry`: summary

- **`cabinetry`** is
  - a modular Python library to create and/or operate statistical models for inference with template fits
  - built upon the powerful and growing Python HEP ecosystem
  - using a slightly different design approach to other tools: more library, less framework
    - analyzers will generally need to write some code: hopefully less "black box" and more flexible, but more work



Backup

The `HistFactory` model

The `HistFactory` model: overview

- **`HistFactory`** is a statistical model for **binned template fits**
  - prescription for constructing probability density functions (pdfs) from small set of building blocks
  - covers wide range of use cases
  - models can be serialized to *workspaces*

unconstrained parameters, e.g. POI

prediction (summed over samples)

constraint term (e.g. Gaussian)

observed data

$$p(\vec{n}, \vec{a} \,|\, \vec{k}, \vec{\theta}) = \prod_i \mathrm{Pois}(n_i \,|\, \nu_i(\vec{k}, \vec{\theta})) \cdot \prod_j c_j(a_j \,|\, \theta_j)$$

auxiliary data, e.g. from calibration measurement

constrained nuisance parameters

product over all bins in all channels

Channels, samples, systematics

- The **`HistFactory`** model specifies how to construct the likelihood function from a set of building blocks
  - *Channels* (also called regions sometimes) are regions of phase space
  - Distributions of *samples* (MC and data) in channels are provided by template histograms
  - *Systematics* act on samples and are specified via the distribution at ±1σ shifts

unconstrained parameters, e.g. POI

prediction (summed over samples)

constraint term (e.g. Gaussian)

observed data

$$p(\vec{n},\vec{a}\,|\,\vec{k},\vec{\theta}) = \prod_i \mathrm{Pois}(n_i\,|\,\nu_i(\vec{k},\vec{\theta}))\cdot\prod_j c_j(a_j\,|\,\theta_j)$$

auxiliary data, e.g. from calibration measurement

constrained nuisance parameters

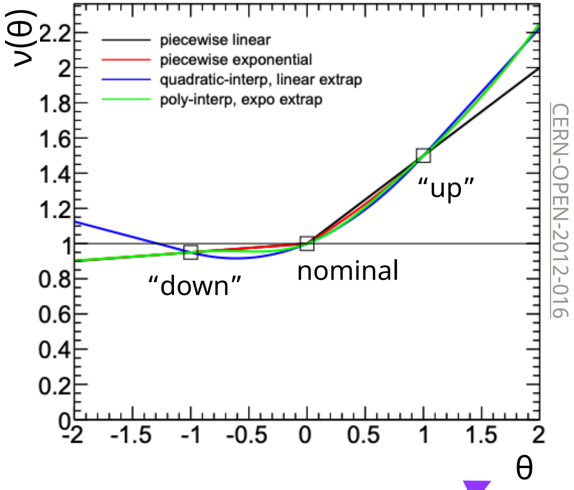
product over all bins in all channels

Systematic uncertainties with HistFactory

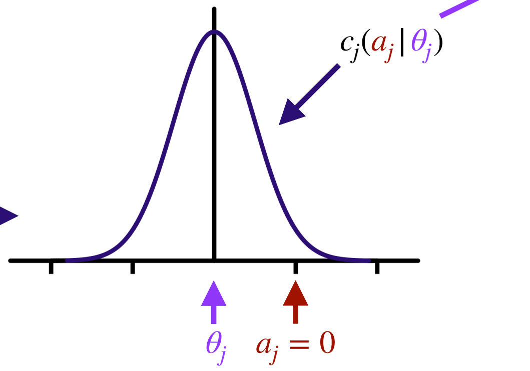
- Common **systematic uncertainties** specified with **two template histograms**
  - "up variation": model prediction for $\theta = +1$
  - "down variation": model prediction for $\theta = -1$
  - interpolation & extrapolation provides model predictions ν for *any* $\vec{\theta}$

- **Gaussian constraint terms** used to model auxiliary measurements (in most cases)
  - centered around nuisance parameter (NP) θ_j
  - normalized width ($\sigma = 1$) and mean (auxiliary data $a_j = 0$)
  - penalty for pulling NP away from best-fit auxiliary measurement value

prediction for one bin

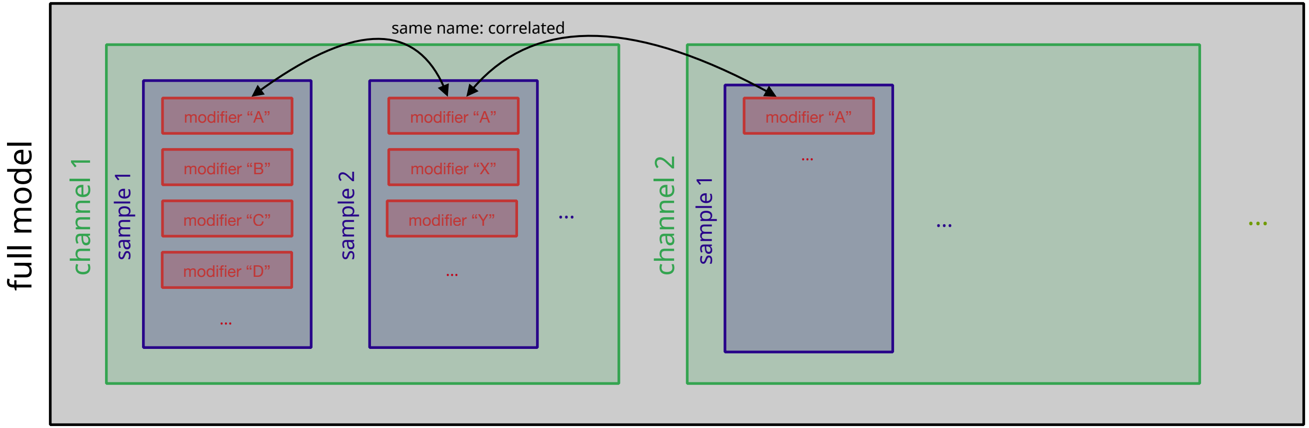


$$p(\vec{n}, \vec{a} \,|\, \vec{k}, \vec{\theta}) = \prod_i \mathrm{Pois}(n_i \,|\, \nu_i(\vec{k}, \vec{\theta})) \cdot \prod_j c_j(a_j \,|\, \theta_j)$$



The `HistFactory` model: structure

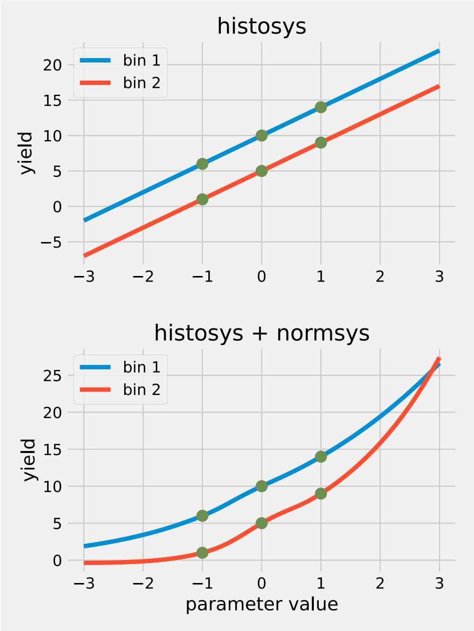
- **`HistFactory`** models follow a specific structure
  - a list of phase space regions: *channels* (defined by event selection, can have one or multiple bins)
  - each *channel* contains a list of *samples* (different type of physics processes)
  - each *sample* is affected by a list of *modifiers* (e.g. parameters of interest (POIs) or encoding systematic uncertainties)
    - *modifiers* with the same name are controlled by the same parameter and thus correlated
  - plus measurement configuration (e.g. “hold this parameter constant” and observations (e.g. real data))



Normalizing histosys modifiers

- Due to the use of **linear extrapolation**, **`histosys`** modifiers can cause **negative yield predictions**
  - example: Gist
  - (partial) solution: split overall channel normalization effect into correlated `normsys` [`OverallSys`]

exact match where templates are defined (green points) by design



pure `histosys`

```
"data": [10, 5],
"modifiers": [
    {
        "data": {"hi_data": [14, 9], "lo_data": [6, 1]},
        "name": "histosys_example",
        "type": "histosys",
    },
```

correlated `histosys` + `normsys`

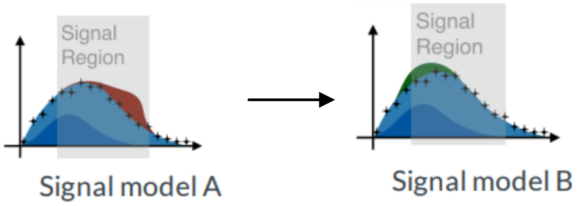
```
"data": [10, 5],
"modifiers": [
    {
        "data": {
            "hi_data": [9.1304347826, 5.8695652174],
            "lo_data": [12.8571428571, 2.1428571429],
        },
        "name": "histosys_and_normsys",
        "type": "histosys",
    },
    {
        "data": {"hi": 1.5333333333, "lo": 0.4666666667},
        "name": "histosys_and_normsys",
        "type": "normsys",
    },
```

More about `pyhf`

HistFactory: workspace formats

- **Until 2018**, the **HistFactory** model had only been implemented in **ROOT**
  - using RooFit, with RooStats available for statistical inference
  - workspaces can be serialized as
    - xml (model structure) + ROOT files (histograms) or single ROOT file (generic RooFit workspace)
    - experimental: JSON* (see Carsten Burgard's ROOT Users workshop contribution)

- **pyhf** introduced a new format: workspaces serialized to JSON
  - JSON format used by ATLAS to publish models on HEPData (list of public models)
    - JSON Patch to swap out workspace components (e.g. signal model)
    - versioned JSON schema describes the declarative model




```
# Using CLI
$ pyhf cls example.json | jq .CLs_obs
0.053994246621274014

$ cat new_signal.json
[{
    "op": "replace",
    "path": "/channels/0/samples/0/data",
    "value": [10.0, 6.0]
}]

$ pyhf cls example.json --patch new_signal.json | jq .CLs_obs
0.3536906623262466
```

*: more generic than the pyhf format, not HistFactory-specific

A HistFactory JSON workspace with pyhf

- JSON structure maps directly to workspace structure
  - highly human-readable!

single channel

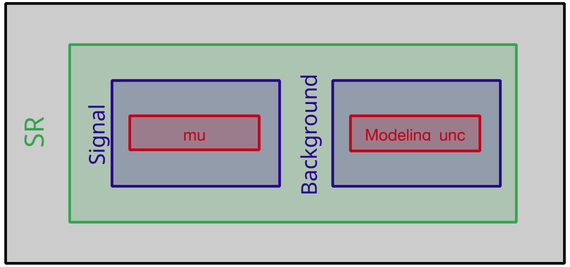
two samples

modifiers

```
{
    "channels": [
        {
            "name": "SR",
            "samples": [
                {
                    "data": [10.0, 15.0],
                    "modifiers": [
                        {"data": null, "name": "mu", "type": "normfactor"}
                    ],
                    "name": "Signal"
                },
                {
                    "data": [50.0, 45.0],
                    "modifiers": [
                        {"data": {"hi": 1.1, "lo": 0.9}, "name": "Modeling_unc", "type": "normsys"}
                    ],
                    "name": "Background"
                }
            ]
        }
    ],
    "measurements": [
        {
            "config": {"parameters": [], "poi": "mu"},
            "name": "minimal_example"
        }
    ],
    "observations": [{"data": [60.0, 60.0], "name": "SR"}],
    "version": "1.0.0"
}
```

measurement configuration

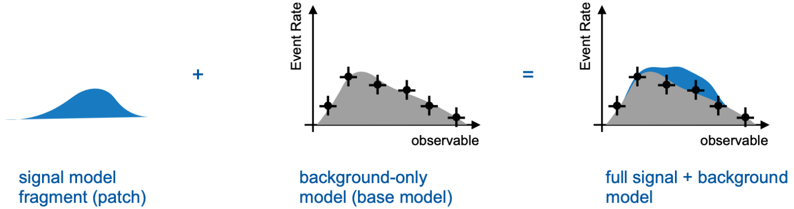
observed data



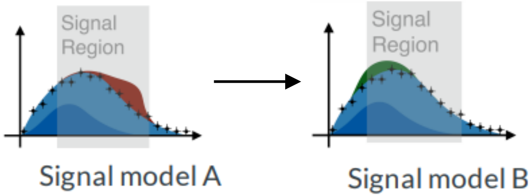
Model patching

- Especially in searches, it is common to use **many different models that slightly differ**
  - same background model but many different signal hypotheses (e.g. different resonance masses)

- It is possible to **edit and swap out pieces of a workspace** via [**JSON Patch**]
  - e.g. add a new component to your model



  - or replace your signal model

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[{
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    "value": [10.0, 6.0]
}]

$ pyhf cls example.json --patch new_signal.json | jq .CLs_obs
0.3536906623262466
```

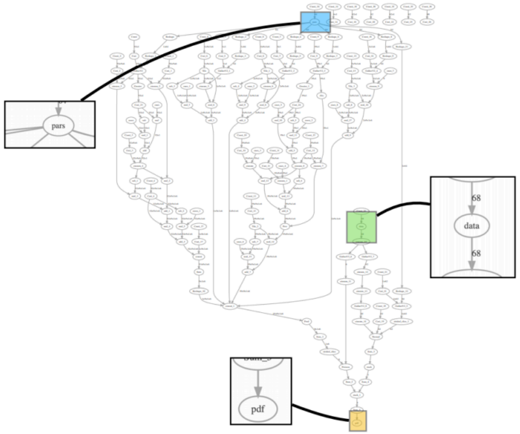
figure credit: Lukas Heinrich

HistFactory: implementations

- **Until 2018**, the **HistFactory** model had only been implemented in **ROOT**
  - using RooFit, with RooStats available for statistical inference

- **pyhf** implements the **HistFactory** model in **pure Python** (`pip install pyhf`)
  - leverages tensor backends: efficient vectorized calculations & hardware acceleration
    - can automatically differentiate through statistical model (computational graph)
      - exact gradients for minimizers
      - enables end-to-end analysis optimization: **neos**
    - backend-agnostic API (and CLI)

computational graph
for HistFactory

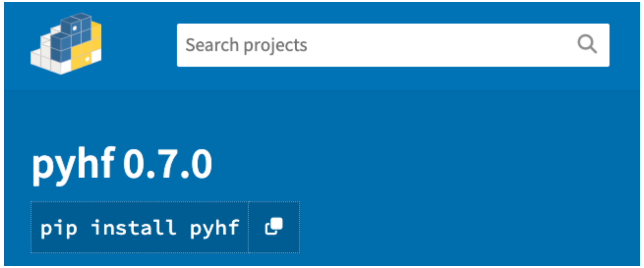


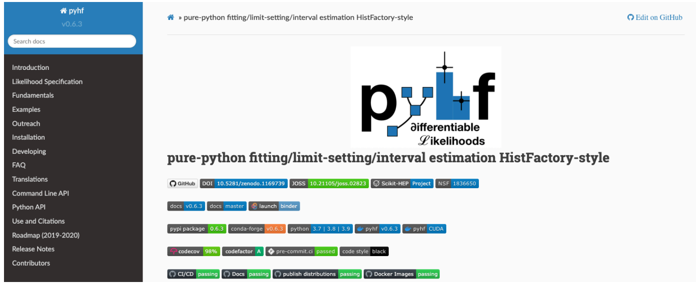
example: autodiff through model yield prediction (e.g. for uncertainty propagation)
it just works!

```python
from jax import jacfwd
import pyhf

pyhf.set_backend("jax")

model = pyhf.simplemodels.correlated_background(
    signal=[12.0, 11.0],
    bkg=[50.0, 52.0],
    bkg_up=[45.0, 53.0],
    bkg_down=[55.0, 51.0],
)

bin_yield = lambda val: model.expected_data([val, 0.0], include_auxdata=False)

par_val = 0.3
print("yield", bin_yield(par_val))
# derivative is -5, -1 which makes sense given the templates + linear interpolation
print("jacfwd", jacfwd(bin_yield)(par_val))
```

pyhf: where to find more

- **pyhf:**
  - can be installed via `$ pip install pyhf`
    - `pyhf[backends]` for all tensor backends
  - is open source and
    - developed on GitHub: scikit-hep/pyhf
    - published on PyPI
    - documented on Read the Docs
      - contains links to talks / paper as well
    - provides tutorials: pyhf.github.io/pyhf-tutorial

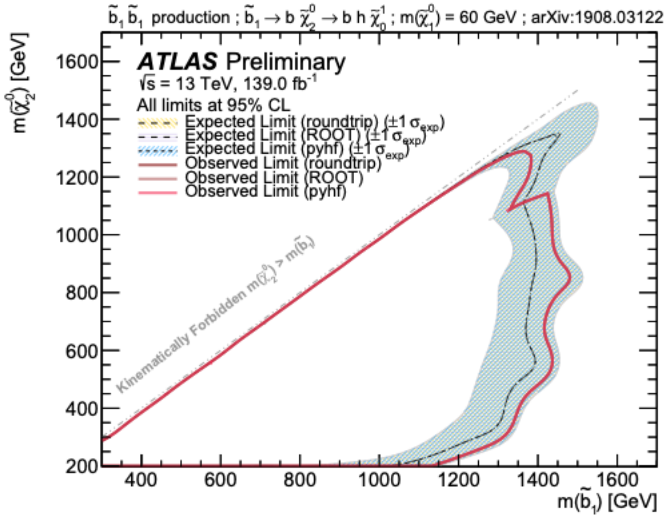


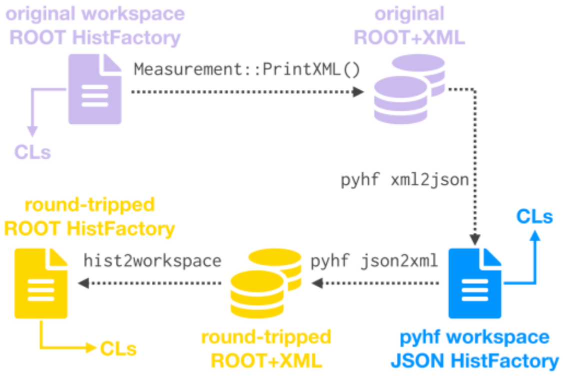


HistFactory: closure

- **Consistent results** of **ROOT** and **pyhf** implementations **demonstrated with many examples**

closure tests from ATL-PHYS-PUB-2019-029





pyhf: summary

- **pyhf** provides
  - a declarative JSON schema for workspaces, used for statistical model publication and reinterpretation
  - a HistFactory implementation in Python that leverages tensor backends

- **pyhf** is a **library** exposing an API providing relevant functionality also found in RooFit, HistFactory and RooStats
  - it does not provide high-level functionality which applications like HistFitter focus on
  - examples of things the pyhf API provides:
    - model yield prediction & NLL given parameters, details about model structure, MLE, workspace pruning
  - examples of things not in scope for pyhf:
    - post-fit model prediction plots, nuisance parameter ranking

Example: expected_data and MLE fits

- Example: **model predictions** and **maximum likelihood estimates**

```
{
    "channels": [
        {
            "name": "SR",
            "samples": [
                {
                    "data": [10.0, 15.0],
                    "modifiers": [
                        {"data": null, "name": "mu", "type": "normfactor"}
                    ],
                    "name": "Signal"
                },
                {
                    "data": [50.0, 45.0],
                    "modifiers": [
                        {"data": {"hi": 1.1, "lo": 0.9}, "name": "Modeling_unc", "type": "normsys"}
                    ],
                    "name": "Background"
                }
            ]
        }
    ],
    "measurements": [
        {
            "config": {"parameters": [], "poi": "mu"},
            "name": "minimal_example"
        }
    ],
    "observations": [{"data": [60.0, 60.0], "name": "SR"}],
    "version": "1.0.0"
}
```

two samples

modifiers

observed data

the model on the left

```
In [2]: import pyhf

        ws = pyhf.Workspace(spec)
        model = ws.model()      # the statistical model
        data = ws.data(model)   # observed data

        data  # includes auxiliary data! 0.0 here for the Modeling_unc NP
Out[2]: [60.0, 60.0, 0.0]

In [3]: # list the available model parameters:
        model.config.par_names()
Out[3]: ['mu', 'Modeling_unc']

In [4]: # nominal model prediction
        model.expected_data(model.config.suggested_init(), include_auxdata=False)
Out[4]: array([60., 60.])

In [5]: # model prediction with the Modeling_unc parameter set to 1.0 and mu=0
        model.expected_data([0.0, 1.0], include_auxdata=False)
Out[5]: array([55. , 49.5])
```

Why is the first bin `55`? Nominal background yield is `50` (no signal contribution since `mu=0`), scaled by `1.1` (`Modeling_unc = 1`).

```
In [6]: # perform a maximum likelihood fit of the model to data
        fit_results = pyhf.infer.mle.fit(data, model)
        for parname, result in zip(model.config.par_names(), fit_results):
            print(f"{parname} = {result}")

        mu = 1.0
        Modeling_unc = 0.0
```

Missing / incomplete features of interest for pyhf

- **Expression for normalization factors** pyhf#850 + pyhf#1627
  - to scale samples by (arbitrary) functions of normalization factors (instead of just linearly)
  - technically possible now, but requires boilerplate
- **Multi-POI support** pyhf#179
  - simple to work around, mostly used as metadata
  - requires schema change to support list of strings in workspace (`ROOT` uses single string, list is arguably better)
- **Configurable constraint terms** pyhf#1829 & constraint term removal pyhf#820
  - related bug in ROOT until recently for removing constrained terms with `HistoSys` root#9070
- **Staterror pruning** pyhf#662 + pyhf#760
  - cannot prune per-bin currently, pruning information not saved in `JSON`
- **Interpolation codes stored in workspace** (pyhf#1762 is related)
  - not currently stored in `ROOT` workspace with xml+root either, but arguably should be to fully specify model

Error propagation with pyhf

- **Code example** to give a better feeling for the `pyhf` API
  - this does both error propagation & bootstrapping
  - few lines each + boilerplate* to set everything up

- Comparison: cabinetry#221
  - choice of method can have a non-negligible impact

- `iminuit.util.propagate` (0.02 sec):

```
[[1.58724387, 5.67483153, 4.58648218, 2.45736349, 2.01580335, 1.08836720],
 [1.23555849, 2.11819107, 0.84599747]]
```

- **bootstrap** (12.7 sec for 50000 samples):

```
[[1.52698188 6.18734267 4.6615714  2.43653558 2.02972604 1.19337253],
 [1.18446726 2.30379686 0.92395196]]
```

- `model_utils.calculate_stdev` (~~1 sec~~ 0.03 sec after perf: vectorize yield uncertainty calculation #316, calculates additional things):

```
[[1.51192818, 5.84456980, 4.44760681, 2.37522912, 2.01413137, 1.15397110],
 [1.13756210, 2.11783607, 0.78566074]]
```

- `TRExFitter` **reference** (completely independent, including fit):

```
[[1.50978849, 5.85530619, 4.46335616, 2.37452751, 2.01563069, 1.14129006],
 [1.13406873, 2.11857512, 0.78459717]]
```

```python
import json
import pathlib

import jacobi
import numpy as np
import pyhf

# get statistcal model + data
fname = pathlib.Path("example_workspace.json")
spec = json.loads(fname.read_text())
ws = pyhf.Workspace(spec)
model = ws.model()
data = ws.data(model)

# fit with pyhf
pyhf.set_backend(pyhf.tensorlib, "minuit")
result, result_obj = pyhf.infer.mle.fit(data, model, return_result_obj=True)

# error propagation
y, ycov = jacobi.propagate(
    lambda p: model.expected_data(p, include_auxdata=False),
    result_obj.minuit.values,
    result_obj.minuit.covariance,
)
print(f"via error propagation:\nyield: {y}\nunc: {np.diag(ycov)** 0.5}\n")

# bootstrap sampling
rng = np.random.default_rng(1)
par_b = rng.multivariate_normal(
    result_obj.minuit.values, result_obj.minuit.covariance, size=50000
)
y_b = [model.expected_data(p, include_auxdata=False) for p in par_b]
yerr_boot = np.std(y_b, axis=0)
print(f"via bootstrapping:\nyield: {np.mean(y_b, axis=0)}\nunc: {yerr_boot}")
```

* can skip the remaining boilerplate code with `cabinetry`

Error propagation example: code

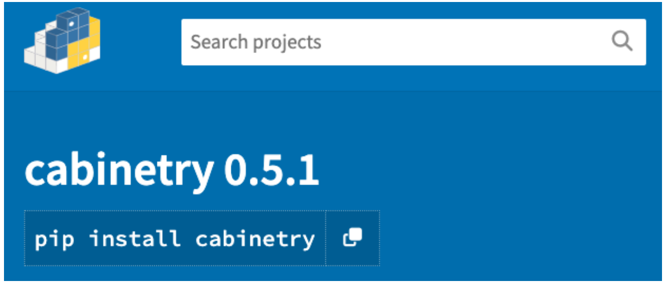
- Plain code for error propagation example

```
import json
import pathlib

import jacobi
import numpy as np
import pyhf

# get statistcal model + data
fname = pathlib.Path("example_workspace.json")
spec = json.loads(fname.read_text())
ws = pyhf.Workspace(spec)
model = ws.model()
data = ws.data(model)

# fit with pyhf
pyhf.set_backend(pyhf.tensorlib, "minuit")
result, result_obj = pyhf.infer.mle.fit(data, model, return_result_obj=True)

# error propagation
y, ycov = jacobi.propagate(
    lambda p: model.expected_data(p, include_auxdata=False),
    result_obj.minuit.values,
    result_obj.minuit.covariance,
)
print(f"via error propagation:\nyield: {y}\nunc: {np.diag(ycov)** 0.5}\n")

# bootstrap sampling
rng = np.random.default_rng(1)
par_b = rng.multivariate_normal(
    result_obj.minuit.values, result_obj.minuit.covariance, size=50000
)
y_b = [model.expected_data(p, include_auxdata=False) for p in par_b]
yerr_boot = np.std(y_b, axis=0)
print(f"via bootstrapping:\nyield: {np.mean(y_b, axis=0)}\nunc: {yerr_boot}")
```

More about `cabinetry`

Links to cabinetry

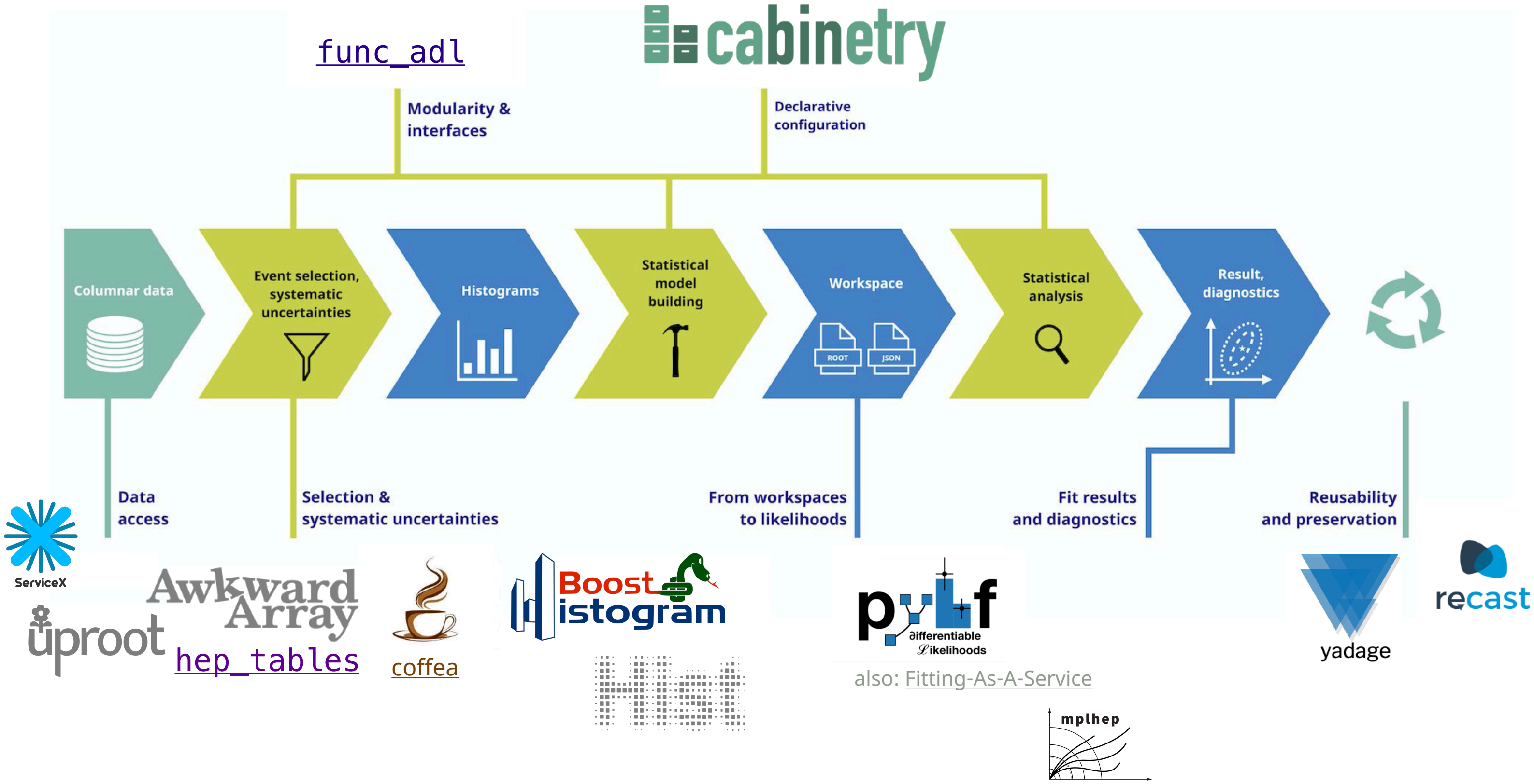
- **`cabinetry`:**
  - can be installed via `$ pip install cabinetry`
    - `cabinetry[contrib]` for extra features
  - is open source and
    - developed on GitHub: scikit-hep/cabinetry
    - published on PyPI
    - documented on Read the Docs
      - contains links to talks / paper as well
    - provides tutorials: cabinetry/cabinetry-tutorials



Future directions for `cabinetry`

- **Next steps and goals:**
  - nuisance parameter pruning (#311)
  - performance improvements for workspace construction from ntuple inputs
  - further improvements to plotting API (#265)
  - longer term: support end-to-end automatic differentiation (#233)
    - optimize analysis selection and design via gradient descent, see neos (PyHEP 2020 talk)
  - your ideas?
    - get involved: from feedback to development, your contributions are welcome!

pyhf and cabinetry within the broader ecosystem



Why `cabinetry`?

- **Why `cabinetry`?**
  - pure Python and no ROOT dependency, fills gap in Python ecosystem
  - modular approach: avoid lock-in
    - benefit from growing columnar analysis ecosystem (`coffea` etc.)
  - openly developed, fully available to broader community beyond a specific experiment
  - follow good practices with extensive automated testing (see coverage)
  - chance to take different design decisions informed by years of experience with existing tools
    - decouple fit model specification and implementation
    - declarative approach, but allow custom code injection at core steps in the workflow

- **Why the name?**
  - a workspace is like a cabinet: it organizes data into many bins (like drawers in a cabinet)
  - the building of these “workspace cabinets” is `cabinetry`