Introduction to `cabinetry`

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pyhf Users and Developers Workshop
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Intro: constructing and using statistical models

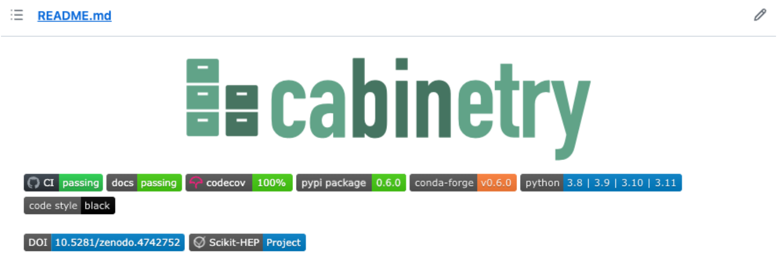
- **Disclaimer:** I am working with ATLAS and probably have a biased view! Curious to learn where things differ elsewhere.

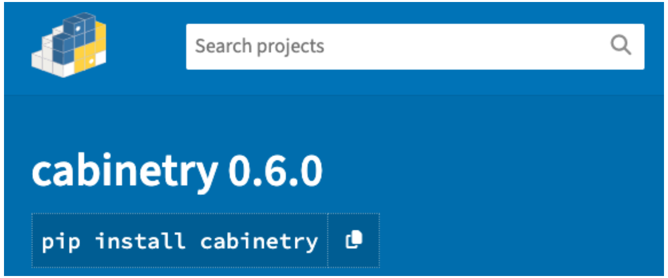
- **Binned template fits** are widely used for **statistical inference**

- **Statistical models** used in particle physics are often **rather complex**
  - lots of book-keeping to handle $O(10\text{k})$ 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
  - (some of) these tools also provide utilities to visualize inference result & simplify debugging

The cabinetry library

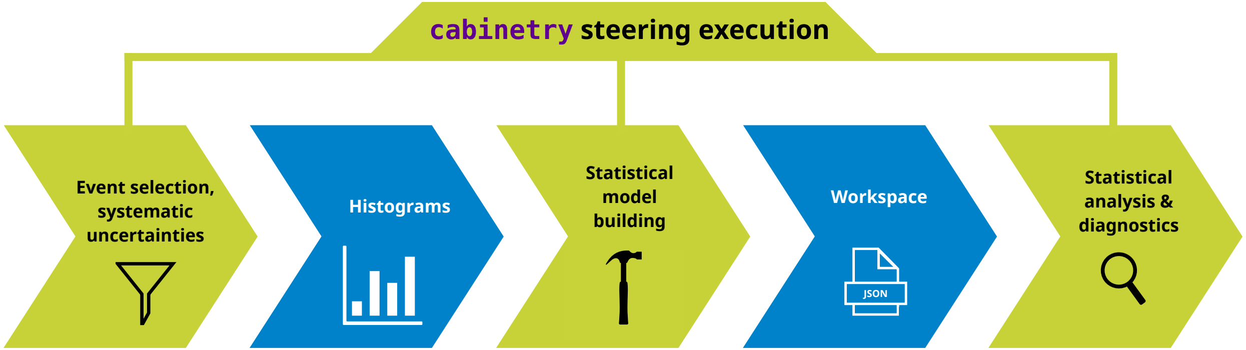




- **cabinetry** is a modern **Python library** for constructing and/or operating **HistFactory** models
  - ❯`pip install cabinetry`
  - uses pyhf, integrates seamlessly with the Python HEP ecosystem
  - modular design: use the pieces of cabinetry you need
  - part of the Scikit-HEP project
- **cabinetry**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

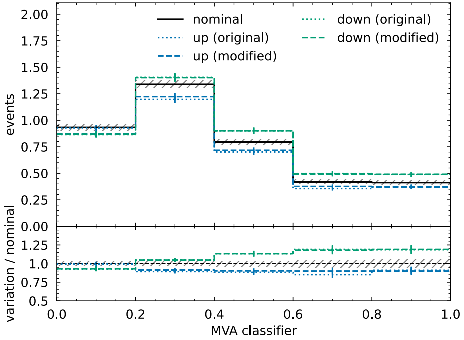
list of systematic uncertainties

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

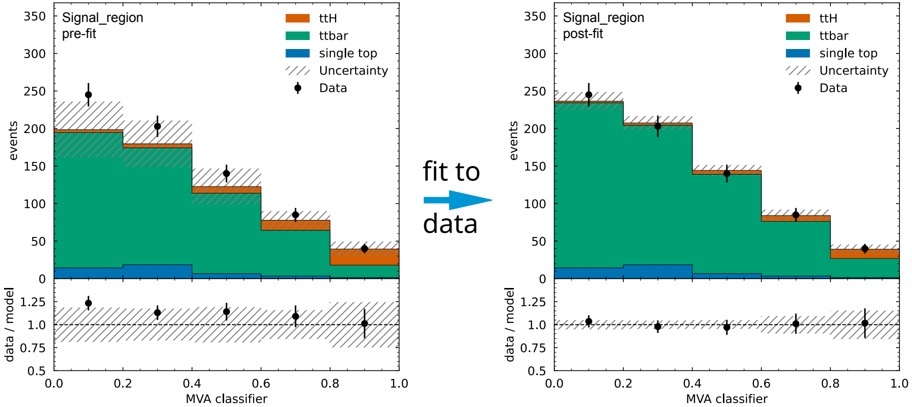


- Utilities provided to **visualize and debug** fit model

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

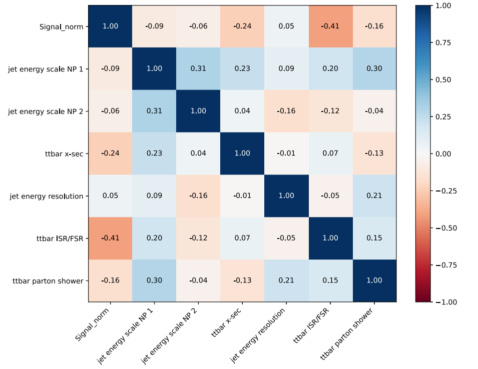
fit model visualization



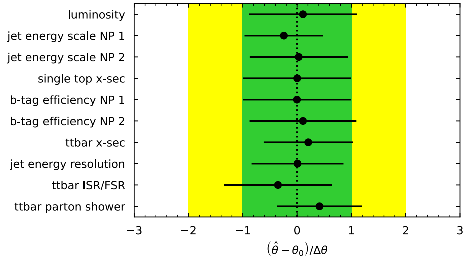
Statistical inference

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

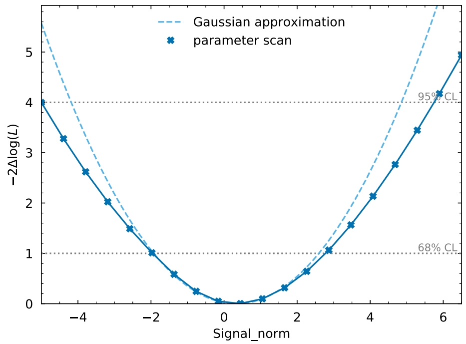
parameter correlations



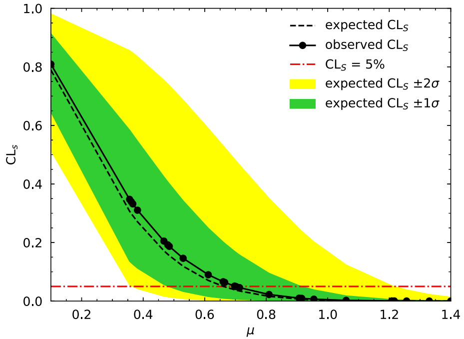
nuisance parameter pulls



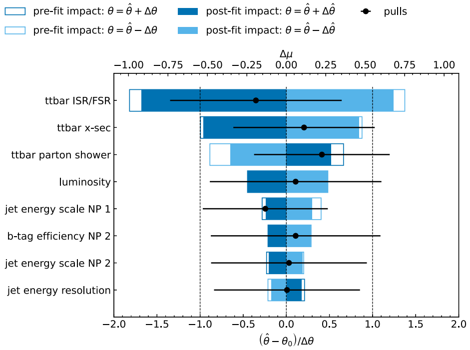
likelihood scans



upper parameter limits



nuisance parameter impacts



discovery significance

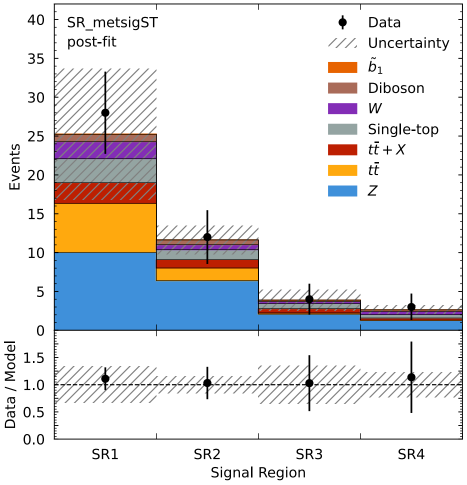
```
$ cabinetry significance workspaces/example_workspace.json
INFO - cabinetry.fit - calculating discovery significance
INFO - cabinetry.fit - observed p-value: 1.13053295%
INFO - cabinetry.fit - observed significance: 2.280
INFO - cabinetry.fit - expected p-value: 0.42110716%
INFO - cabinetry.fit -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

Working with an unknown workspace

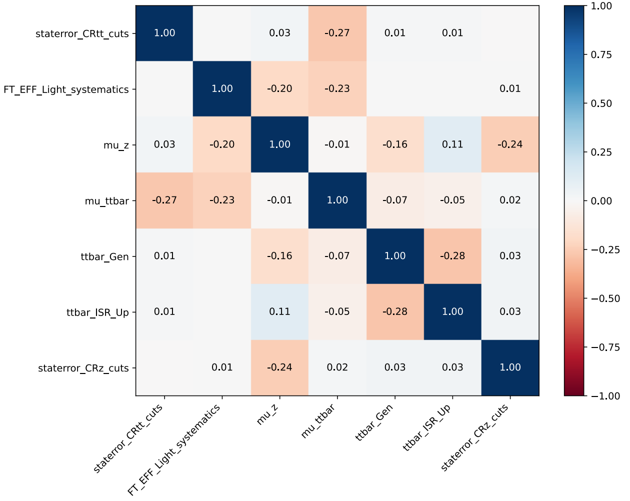
- Pick a **workspace** from **HEPData**: [10.17182/hepdata.89408.v3] (analysis: [JHEP 12 (2019) 060])
    - download workspace with `pyhf`
    - perform inference and visualize results with `cabinetry`
    - can use inference features regardless of how a workspace was built, functionality factorizes!
- See [arXiv:2109.04981] and try it [on Binder]

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

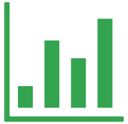
```python
import json
import cabinetry
import pyhf
from cabinetry.model_utils import prediction
from pyhf.contrib.utils import download

# 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)

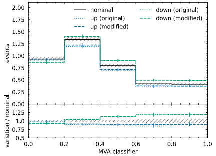


Full workflow example



generate histograms for all samples: nominal & variations

can read histograms or ntuples *with* `cabinetry`



workspace: serialized statistical model

built by `cabinetry`
or from *external source*

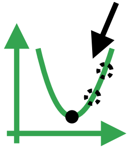

```json
{
    "channels": [
        {
            "name": "SR",
            "samples": [
                {
                    "data": [10.0, 15.0],
                    "modifiers": [
                        {"data": null, "name": "mu", "type": "normfactor"}
                    ],
                    "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"
}
```


$$L(\vec{k},\vec{\theta}) = p(\vec{n},\vec{a}\ \ \vec{k},\vec{\theta})$$

turn into likelihood function

a function, given
(observed + auxiliary)
data $\vec{n},\vec{a}$
done via `pyhf`

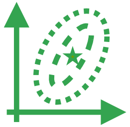
∂ifferentiable
ℒikelihoods



minimize NLL

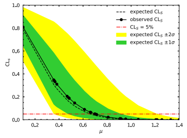
using function
minimizer, e.g. MINUIT
(MIGRAD algorithm)
via `iminuit`

can wrap these steps
with `cabinetry`



inference results

plots & tables
produced by `cabinetry`



Future directions for `cabinetry`

- **Short term** goal: address **backlog of open PRs** (especially user-contributed ones!)
  - (breaking) improvements to filter / weight specification for model building (#310)
  - plotting improvements (#342, #387)
  - histogram re-binning (#418)
  - API for histogram creation parallelization (#421) →
  - more modifier flexibility (#434)

```python
from dask.distributed import Client, LocalCluster, wait

def produce_single_template(template):
    cabinetry.templates.build(config, template_list=[template])

template_list = cabinetry.route.required_templates(config)

with LocalCluster(n_workers=2) as cluster:
    client = Client(cluster)
    wait(client.map(produce_single_template, template_list))
```

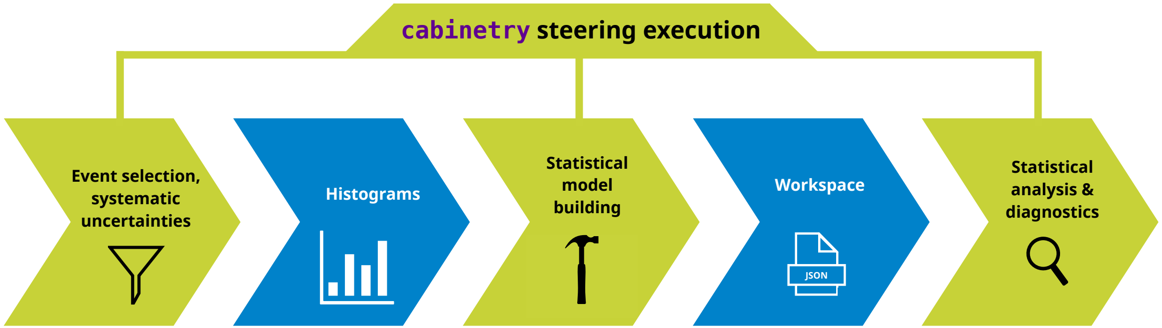
- **Longer term goals**
  - lots of feature ideas (see relevant issues): feedback for helping with prioritization is welcome!
  - support end-to-end automatic differentiation (#233)
    - optimize analysis selection and design via gradient descent, see neos (PyHEP 2020 talk)
  - your ideas: from feedback to development, your contributions are welcome!

What about features that are not in `cabinetry`?

- Some features are **not available yet** or likely **out of scope**
  - `cabinetry` attempts to strike a balance between useful and maintainable
- Overall idea: users **writing a few lines of Python** can be **good**, *especially* if it makes **assumption explicit**
  - no blackbox function "fit control region, extrapolate to signal region, get realistic sensitivity estimate"
  - instead: APIs to help with common needs (e.g. `model_utils.match_fit_results`)
- Started collecting **examples for "how do I do xyz"** in dedicated GitHub discussion
  - see cabinetry/discussions/443
- Always **happy to discuss requests**, scope is not set in stone

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

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

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

observed data

prediction (summed over samples)

constraint term (e.g. Gaussian)

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

auxiliary data, e.g. from calibration measurement

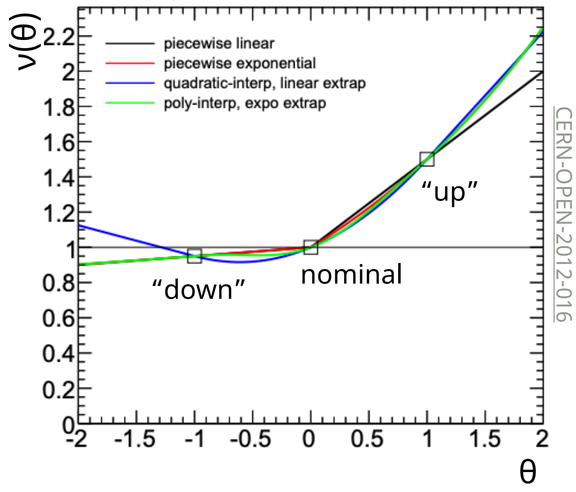
constrained nuisance parameters

product over all bins in all channels

Systematic uncertainties with HistFactory

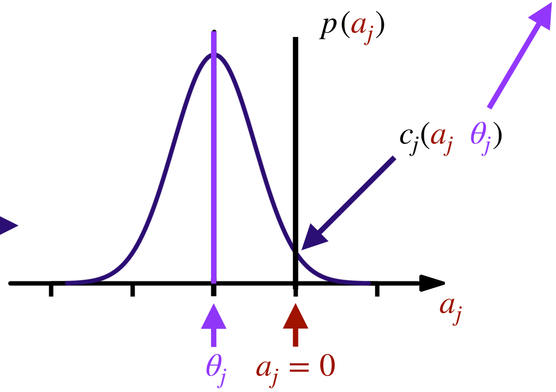
- Common **systematic uncertainties** specified with **two template histograms**
  - "up variation": model prediction for $\theta = +1$
  - "down variation": model prediction for $\theta = -1$
  - interpolation & extrapolation provides model predictions ν for *any* $\vec{\theta}$

prediction for one bin



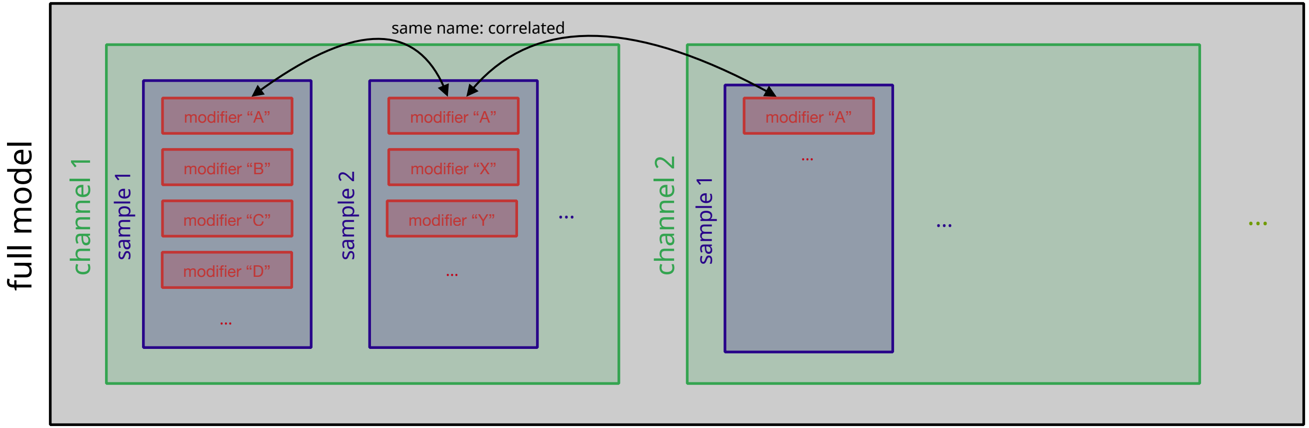
- **Gaussian constraint terms** used to model auxiliary measurements (in most cases)
  - centered around nuisance parameter (NP) θ_j
  - normalized width ($\sigma = 1$) and mean (auxiliary data $a_j = 0$)
  - penalty for pulling NP away from best-fit auxiliary measurement value

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



The `HistFactory` model: structure

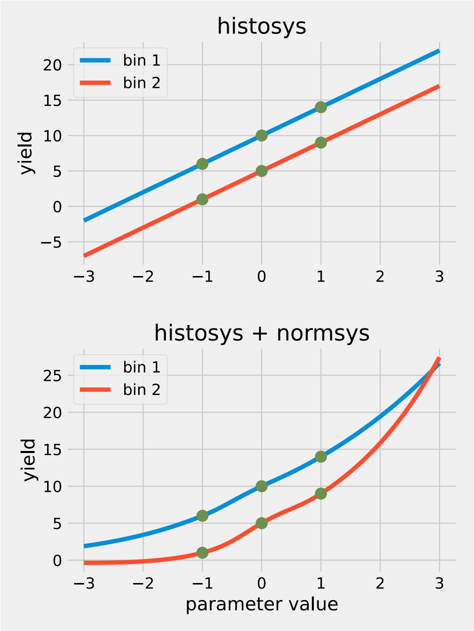
- **`HistFactory`** models follow a specific structure
  - a list of phase space regions: *channels* (defined by event selection, can have one or multiple bins)
  - each *channel* contains a list of *samples* (different type of physics processes)
  - each *sample* is affected by a list of *modifiers* (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`

A HistFactory JSON workspace with pyhf

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

```
{
    "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"
}
```

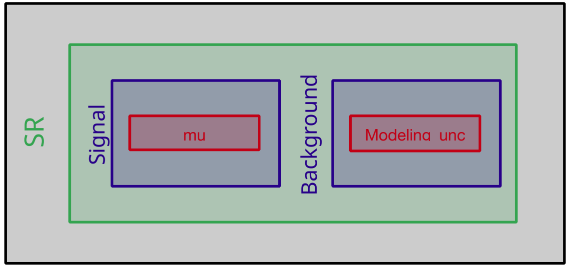
single channel

two samples

modifiers

measurement configuration

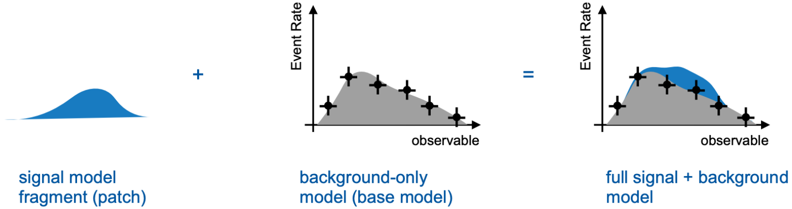
observed data



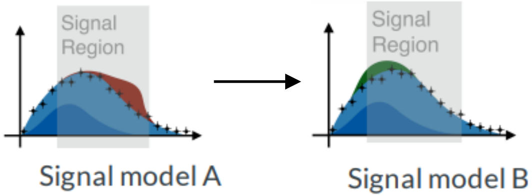
Model patching

- 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




```
# 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
```

figure credit: Lukas Heinrich

Example: expected_data and MLE fits

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

two samples

```
{
    "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"
}
```

modifiers

observed data

the model on the left

In [2]:
```python
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]:
```python
# list the available model parameters:
model.config.par_names()
```

Out[3]: `['mu', 'Modeling_unc']`

In [4]:
```python
# nominal model prediction
model.expected_data(model.config.suggested_init(), include_auxdata=False)
```

Out[4]: `array([60., 60.])`

In [5]:
```python
# 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]:
```python
# 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`

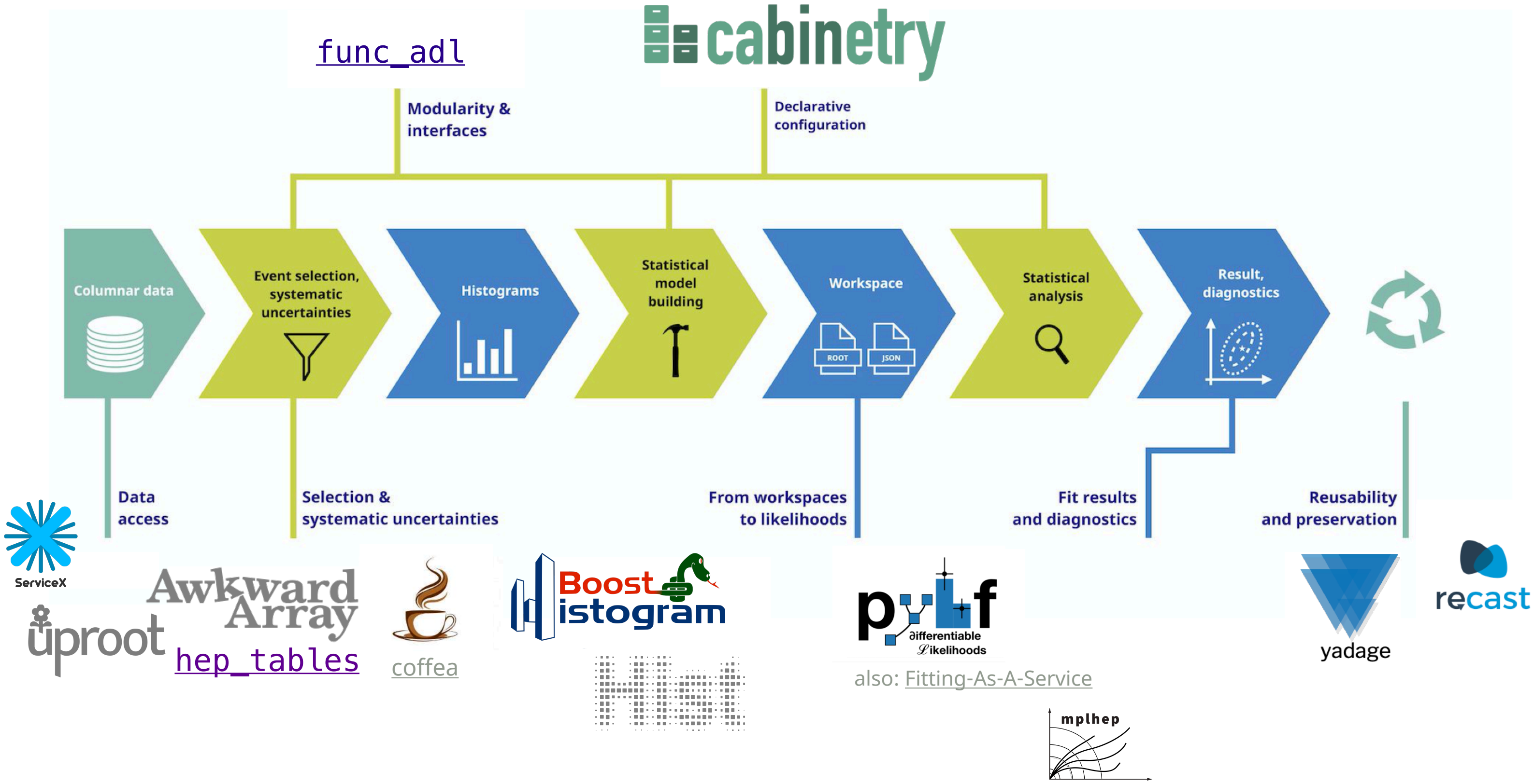
Error propagation example: code

- 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

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`