scalable pythonic fitting

# Model fitting in Python with zfit and Scikit-HEP

**Jonas Eschle**
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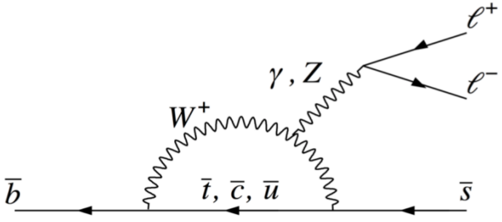
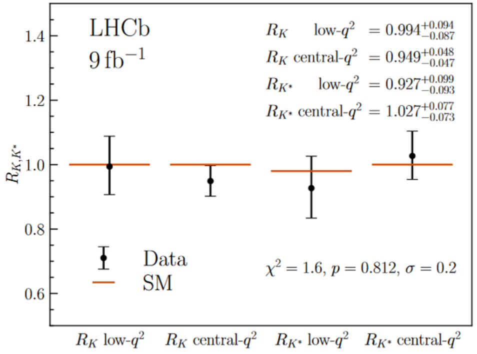
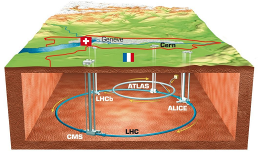
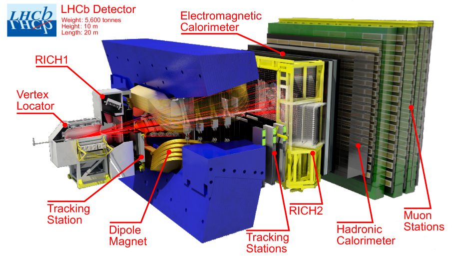
Syracuse University

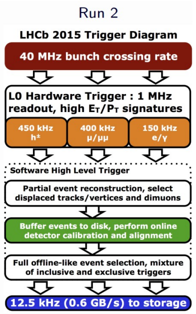
# HEP Analysis

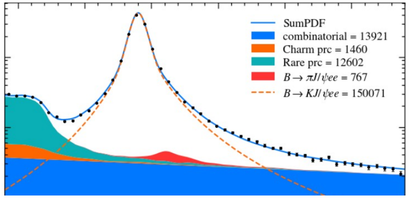


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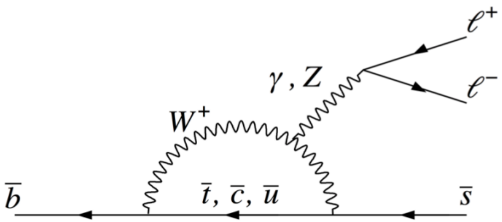
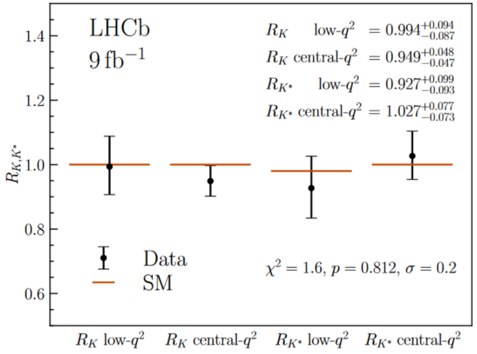
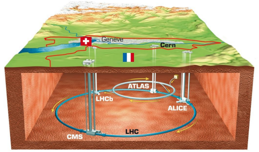
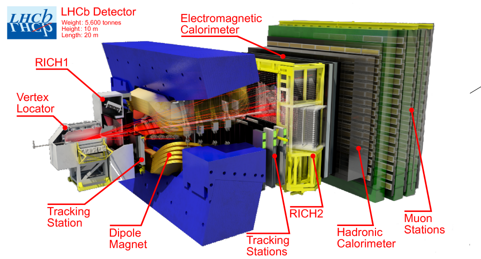



Lots of code

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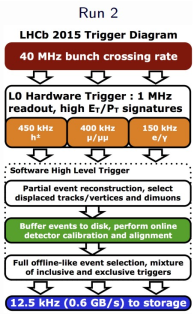


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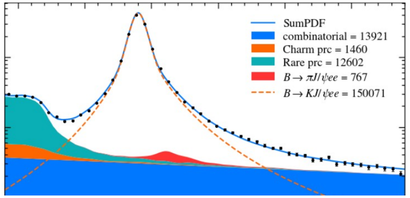


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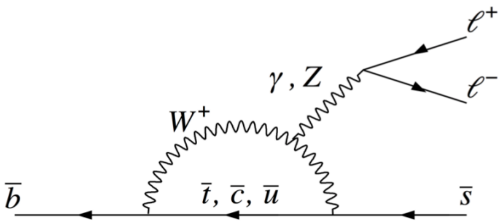


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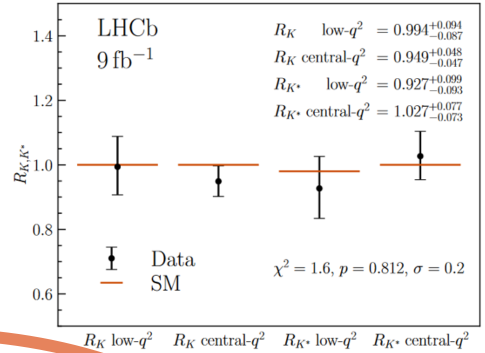


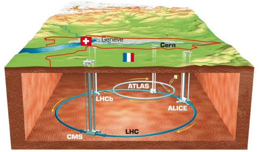


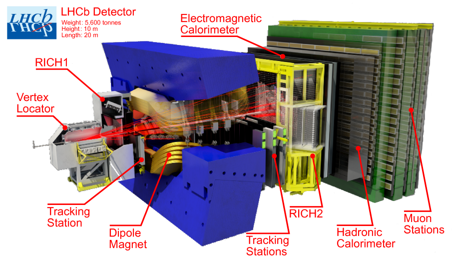


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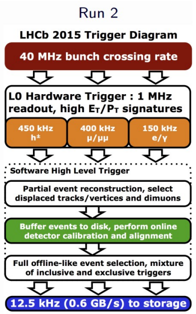


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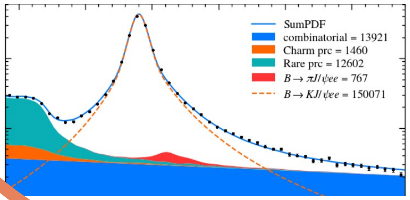



Lots of code

**End-user analysis**

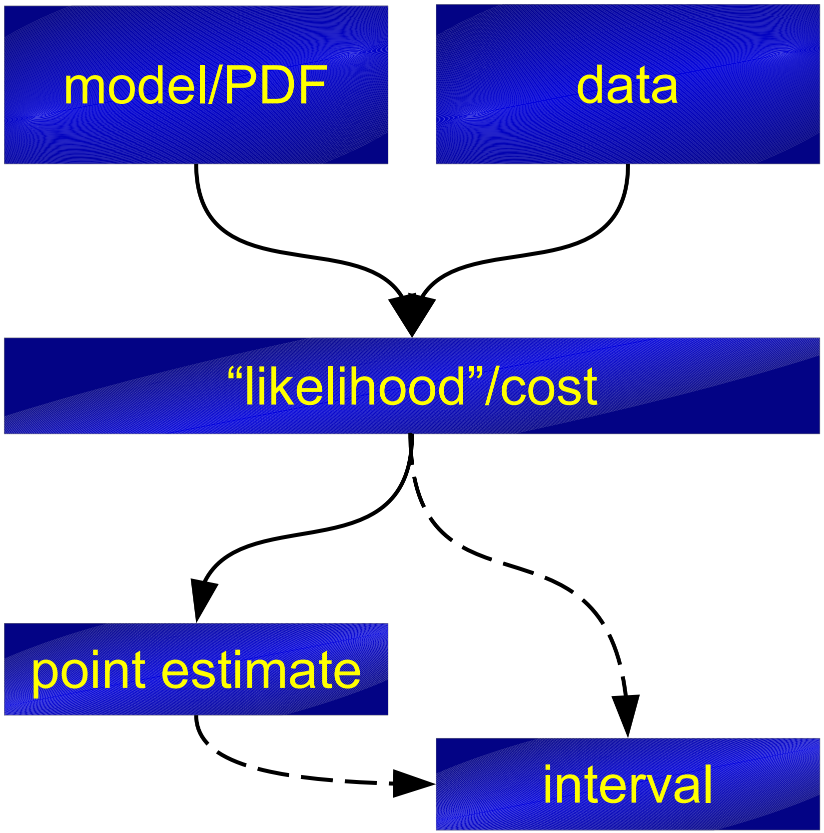
**Focus on «fitting»**

# «Fitting»

«statistical inference»

Variety of possibilities

Focus on likelihood based
(as is very common in HEP)



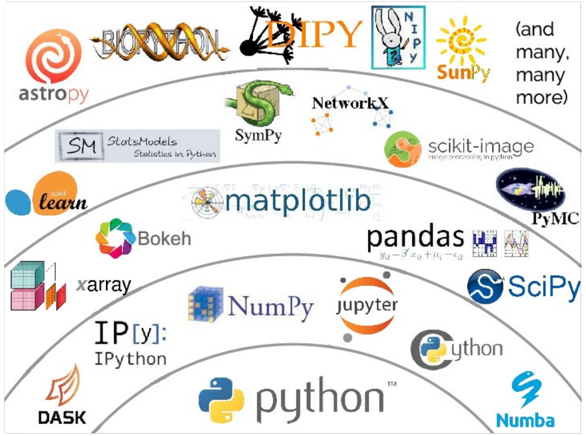
# Historic landscape

<u>Analyses transition from C++ to Python</u>

Many, non-monolithic packages

Talk by Eduardo

Philosophy: extend/build on existing ecosystem





2018

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2018

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## Why even move to Python?

2018

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FILE COPY

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

CERN – DD /89/ 18

May 16, 1989

**The Comparison and Selection of Programming Languages for High Energy Physics Applications**

Bebo White

Data Handling Division, CERN
and
SLAC Computing Services

10.1016/0010-4655(89)90283-X

Zanella [32] has said " If HEP wishes to keep to its level of achievement, credibility and excellence, then it needs an injection of bright young computer-wise scientists and engineers." This means that HEP cannot become "an island." HEP applications must be able to utilize "state of the art" facilities in all areas of applicability including data processing. HEP must be able to take advantage of the technological advancements in other arenas of science and engineering. Many of these advancements are occurring in fields which are presently *not software compatible* with HEP. Much of the work being done in embedded systems with Ada or telecommuni-

2018

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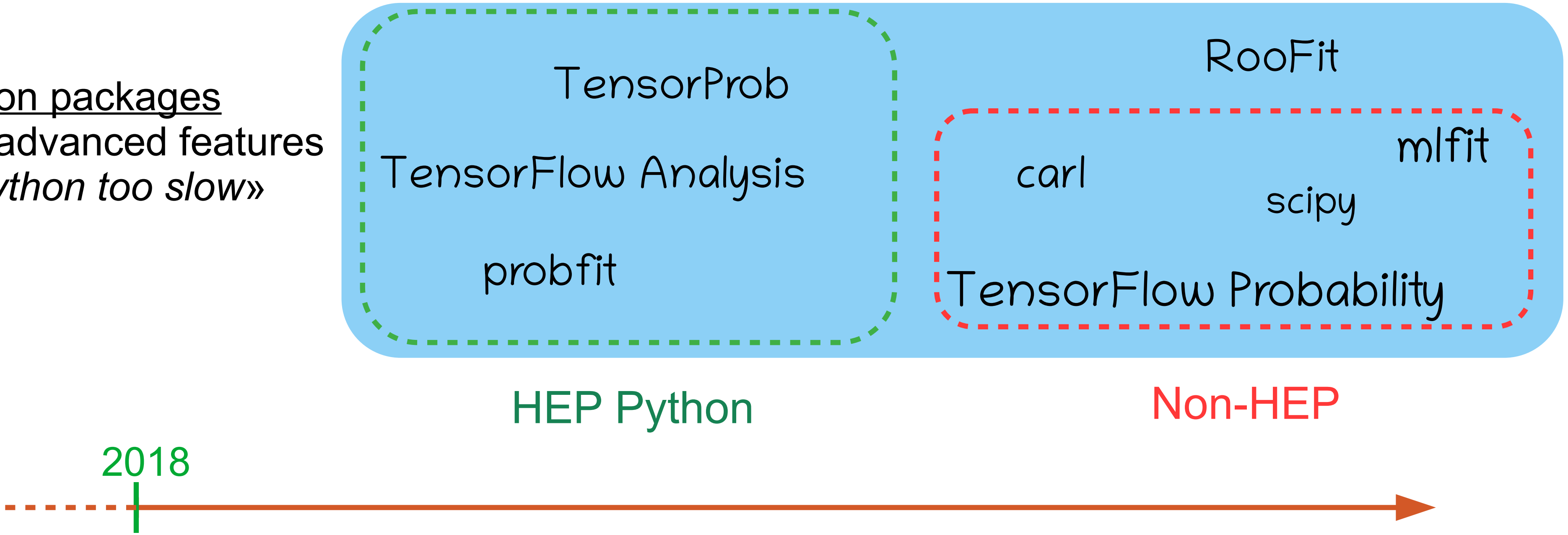
<u>Python packages</u>
- no advanced features
- «*Python too slow*»



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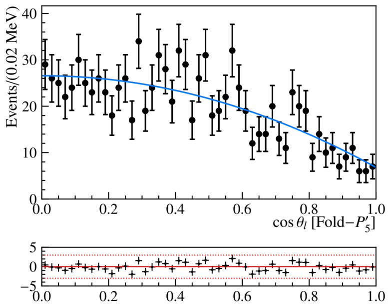
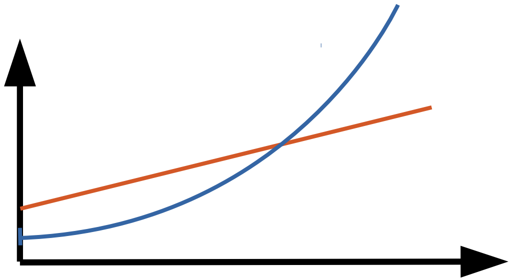



**HEP**

advanced features, simply extendable



**Scalable**

large data, complex models

**Pythonic**

integrate into ecosystem, stable API

# History

5 years ago

first presentation HSF/WLCG Workshop

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5 years ago

first presentation
HSF/WLCG
Workshop

## Summary

zfit

scalable pythonic fitting

- Beta stage, usable! (already used in LHCb analyses)
  - Not feature complete, but API stabilizing
- Contributions in form of *feedback and criticism* very welcome
  - API, use-cases, bugs,…
  - Any crazy idea!

**It's about a reliable library**

not about

«we need to get it working fast»

# Different kind of fits

- Binned (*vs histfactory*) vs unbinned
  - Refers to data, cost/loss/likelihood and PDF
  - Unbinned data: product of probabilities
  - Binned data: «counting experiments»

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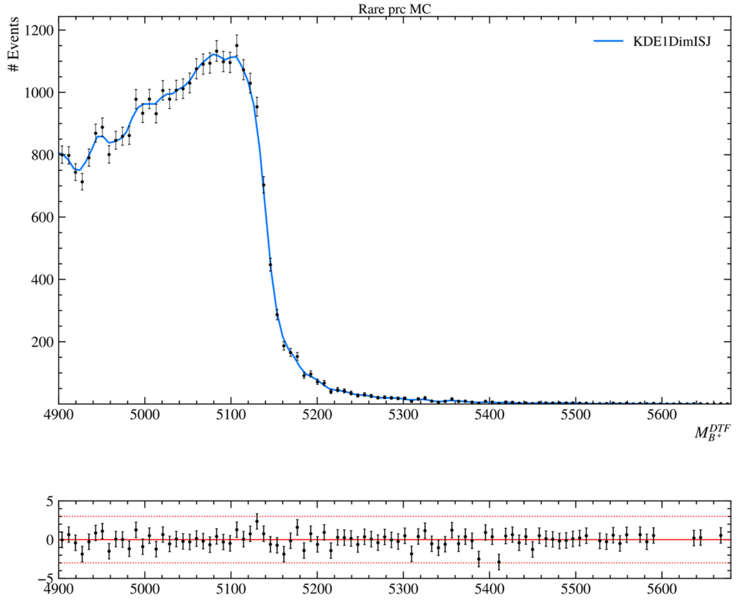


**KDE**

Gaussian kernel → analytic norm

ISJ → numeric norm

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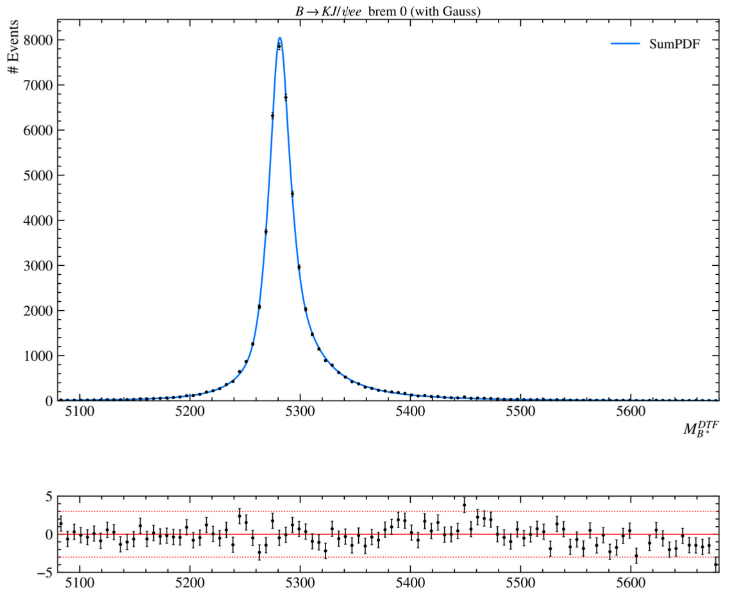


**Double Crystalball**

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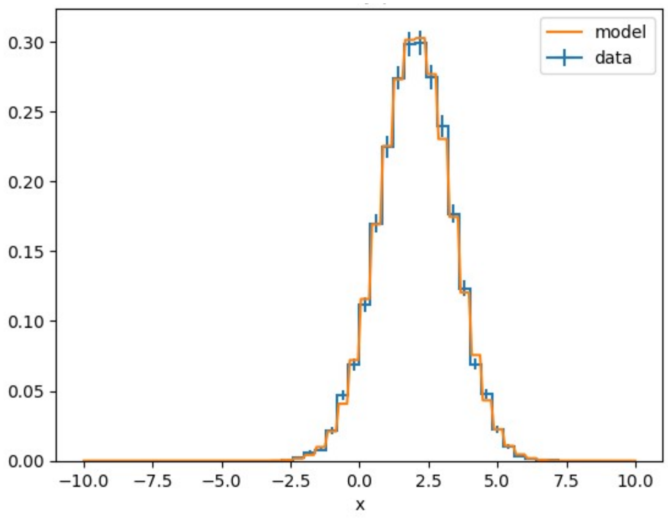


**(binned) Gaussian fit to histogram**

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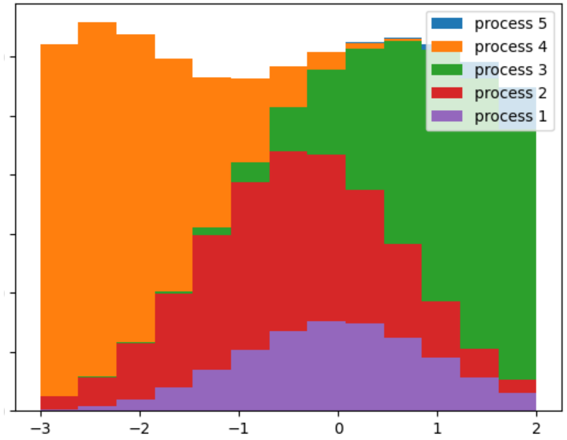


**Stacked histograms PDFs**

# pyhf-like models

- One extreme: HistFactory model (pyhf)
  - Template, binned, analytic normalization
  - Assumption: Bins «free-standing», not next to each other

- «Closed-world» fitter
  - Limited scope, specialized on 80%+ use-case in CMS/ATLAS
  - extremely powerful/tested, serializable

# Different kind of fits

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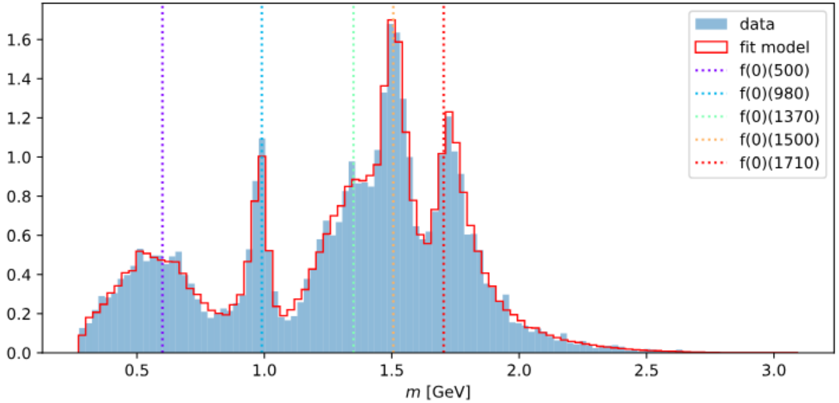



**Amplitude (partial wave) analysis**
**Angular analysis**

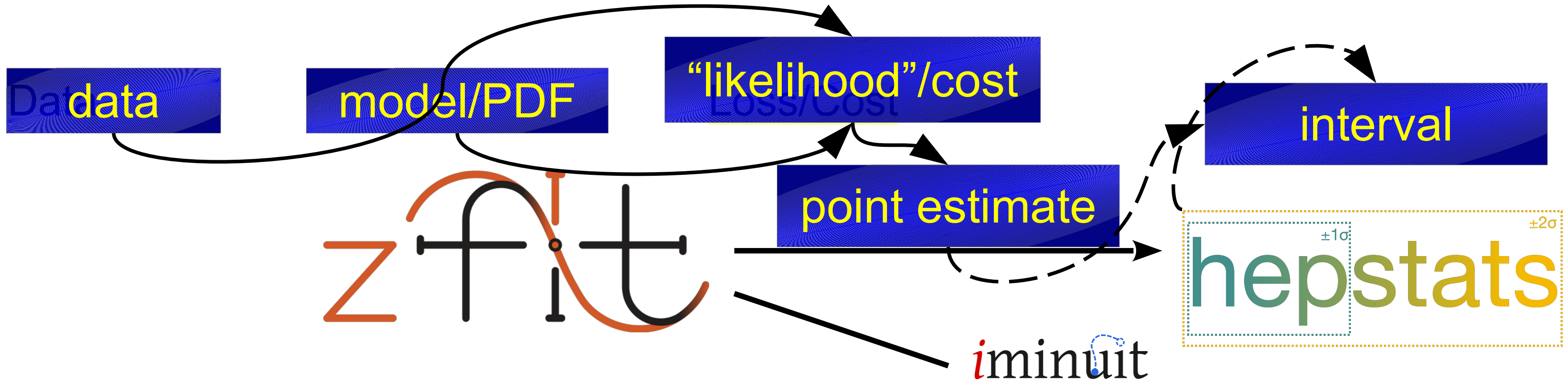
# Partial wave analysis

- The other extreme: amplitude analysis (ComPWA, …)
  - Unbinned, analytic, numerical normalisation
  - Description of observable based on amplitude, can be 1k + lines
- Fitting is also hard
  - Fitting time (~100 parameters): hours/days, up to weeks (one fit)
  - Bottleneck: evaluation of PDF

# Statistical inference landscape

Closed-world
HistFactory-like

Open-world
Binned,
unbinned,
mixed



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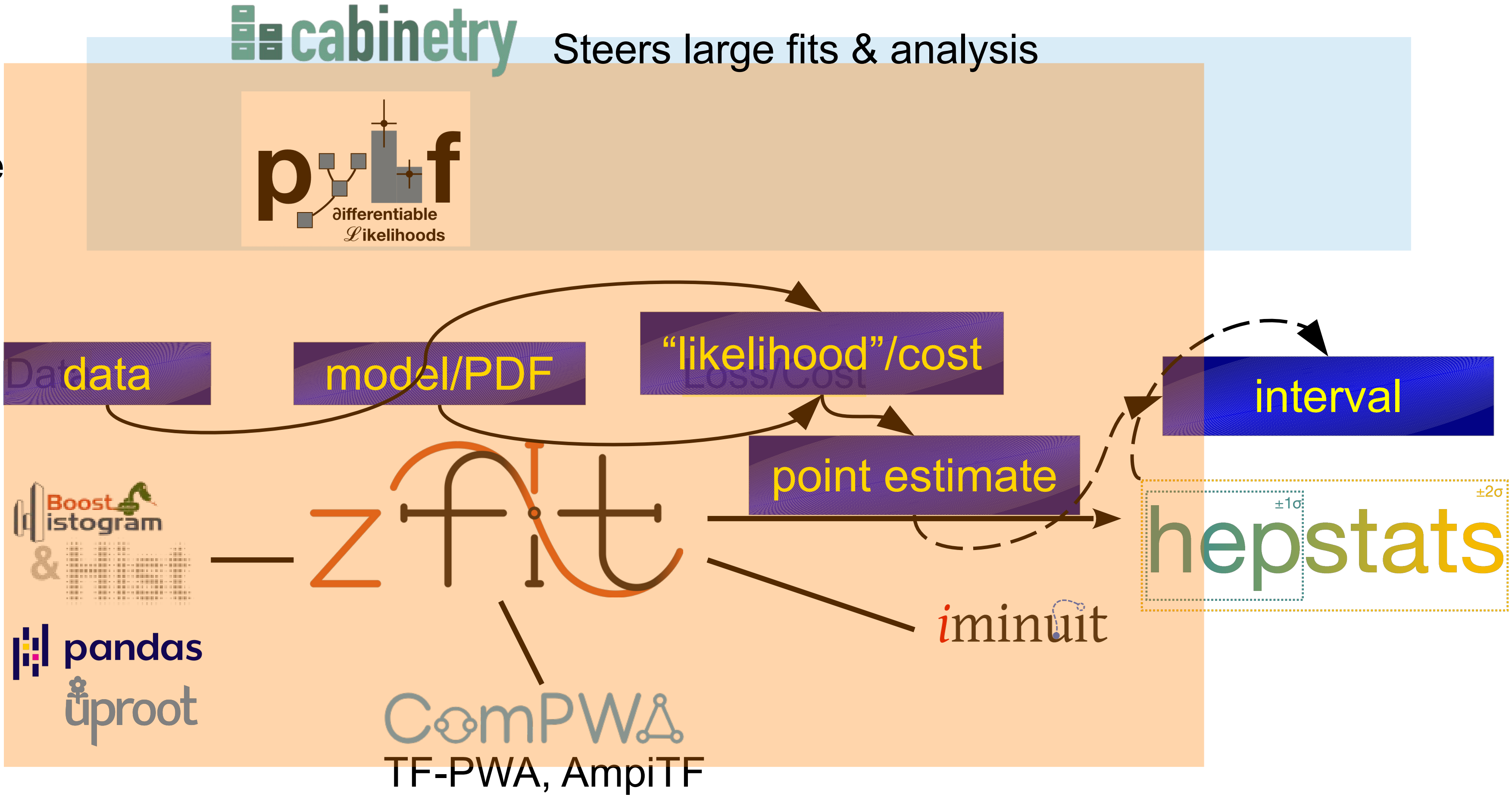

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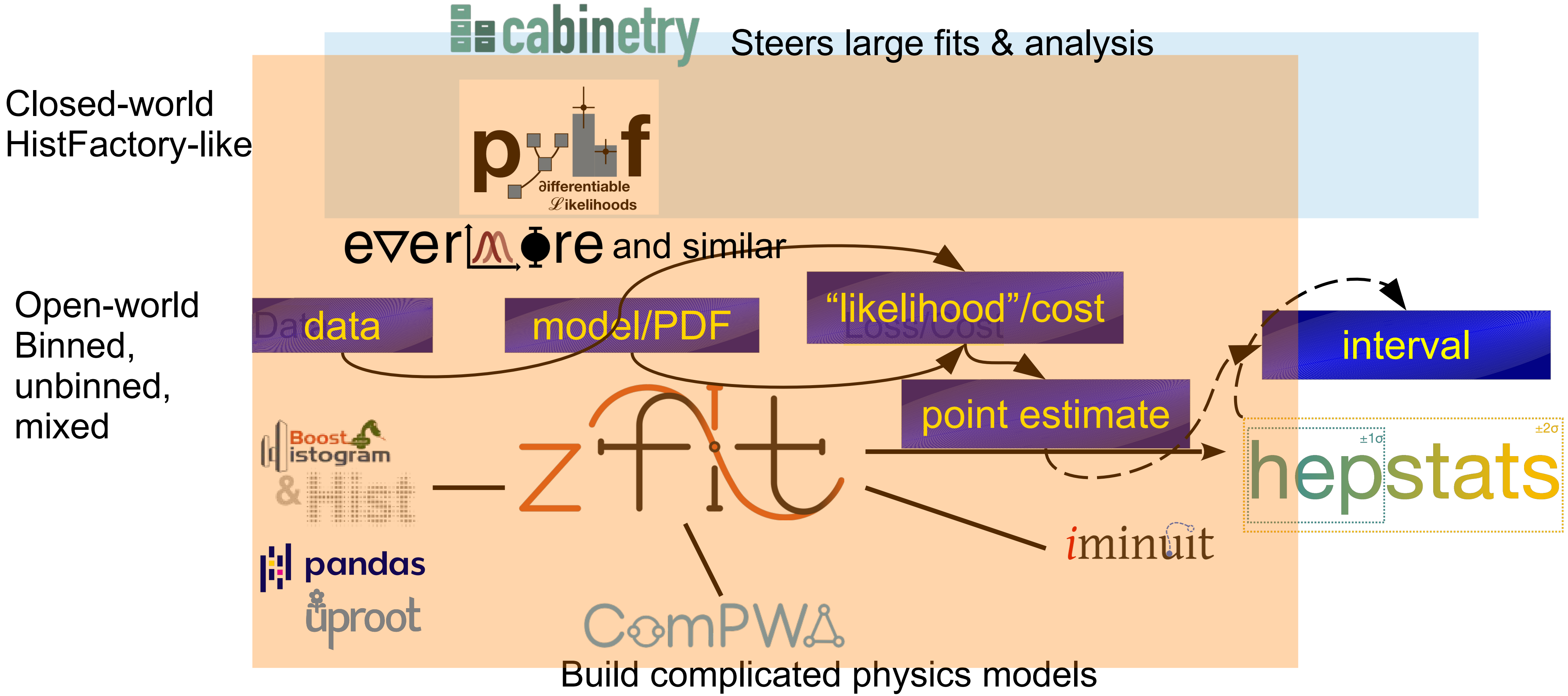

# Statistical inference landscape

Steers large fits & analysis

Closed-world
HistFactory-like

Open-world
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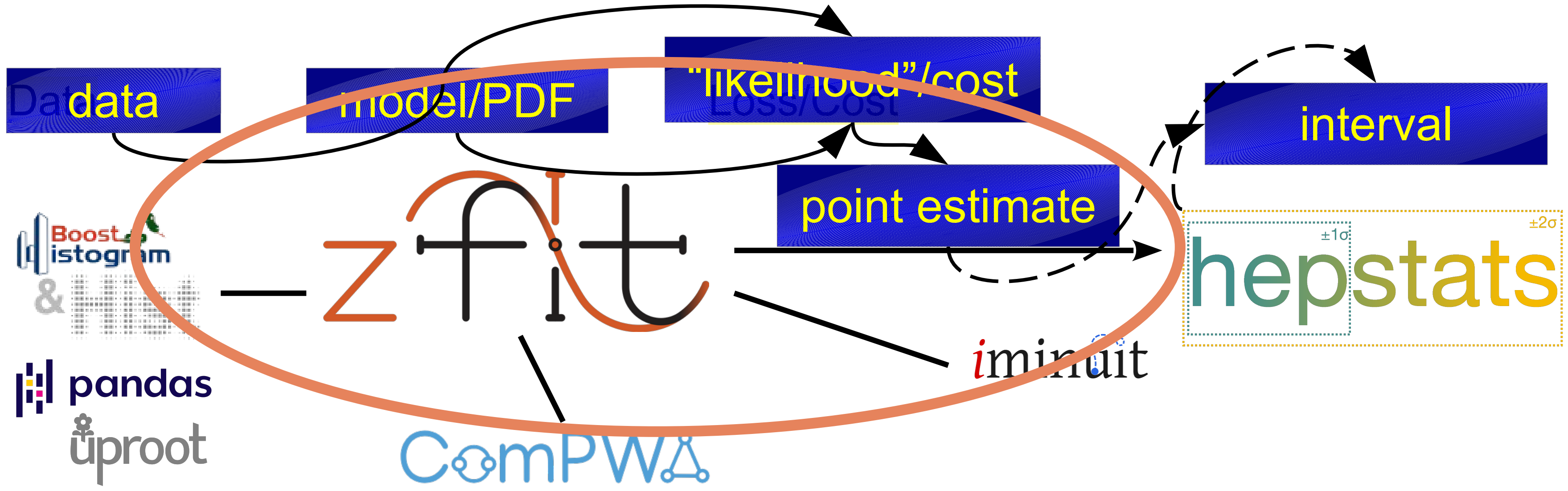


Build complicated physics models

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Python packages
- no advanced features
- *«Python too slow»*

TensorProb

TensorFlow Analysis

probfit

RooFit

carl

mlfit

scipy

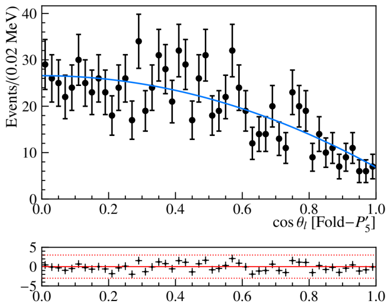
TensorFlow Probability

HEP Python

Non-HEP

2018

# HEP Model Fitting in Python

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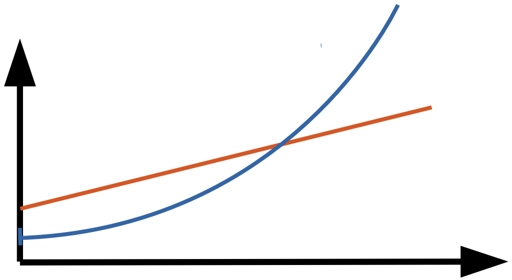

Scalable
large data, complex models

Pythonic
integrate into ecosystem, stable API

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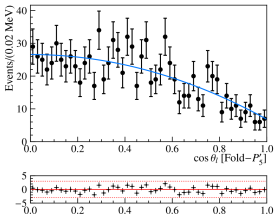


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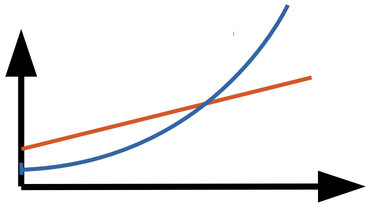

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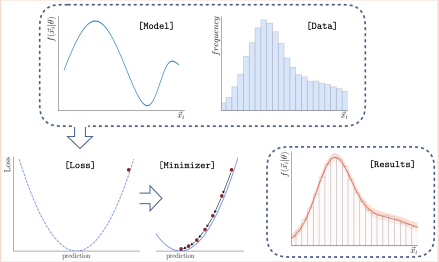
## Computing backend

## API & Workflow



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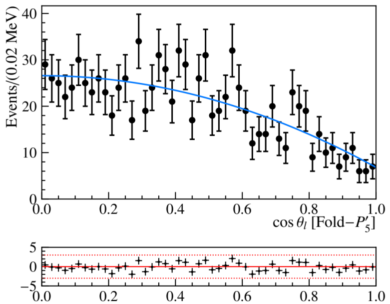


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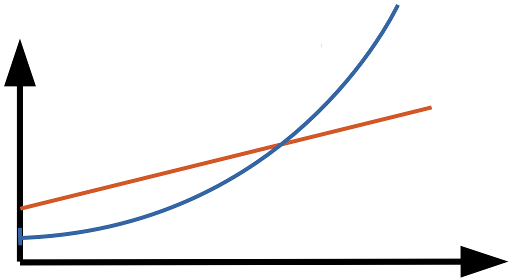

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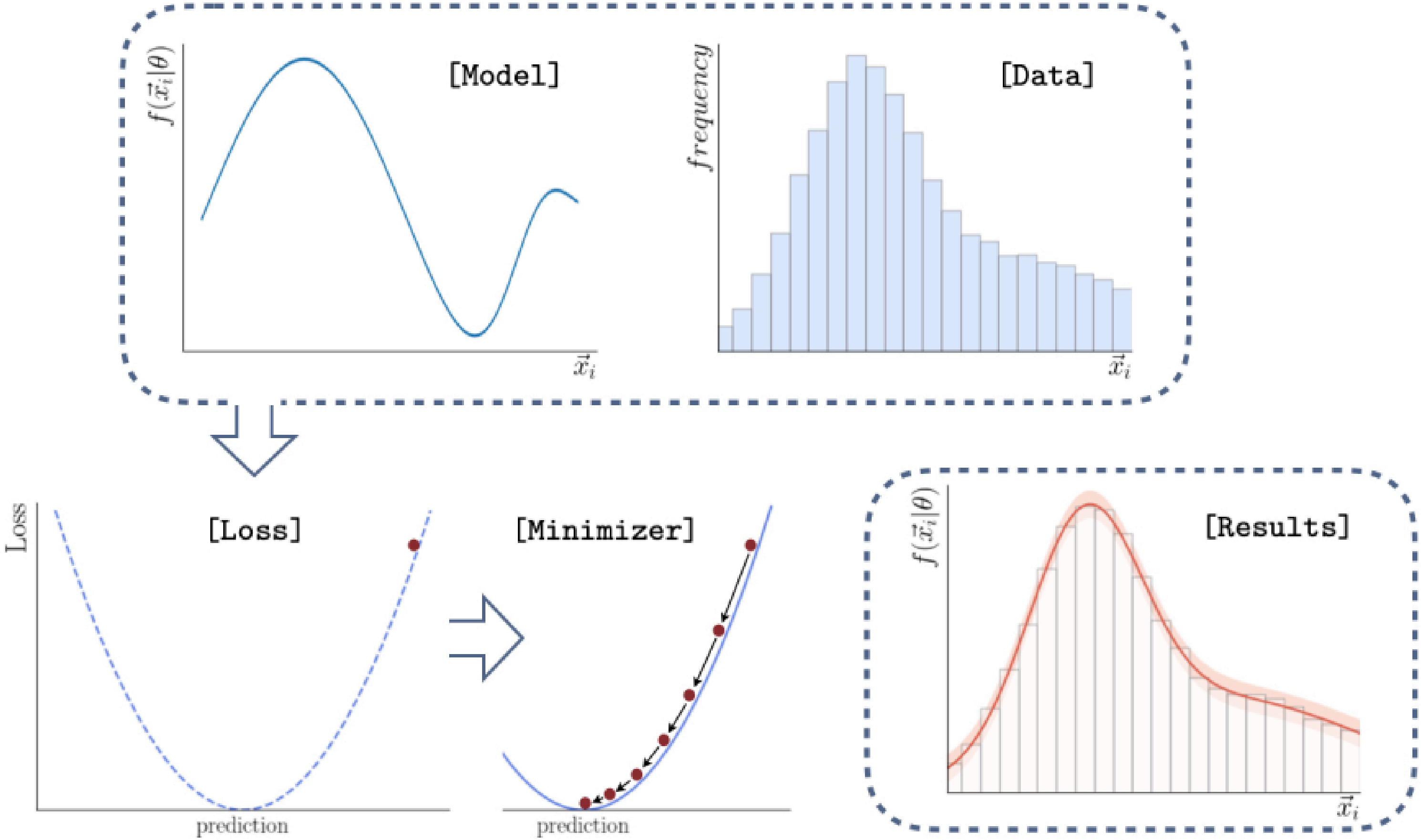
# API & Workflow

Five maximally independent parts

"Fits look always
 the same"



# Complete fit

```python
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
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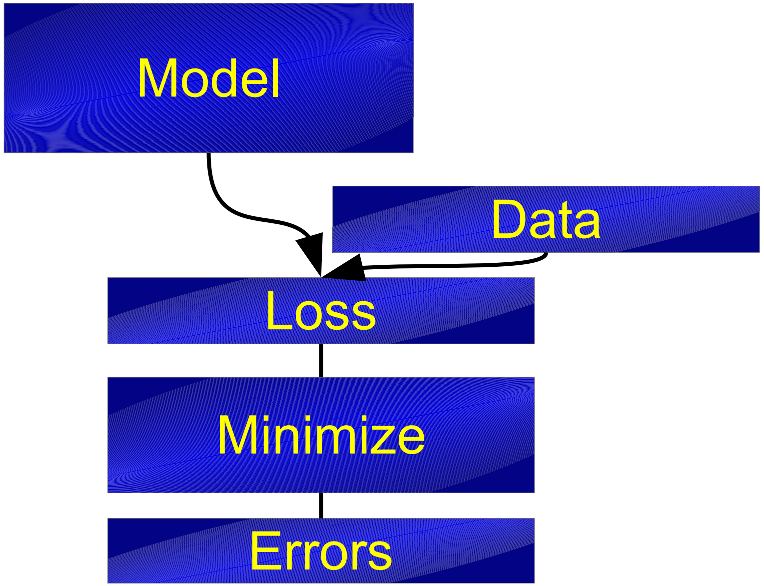

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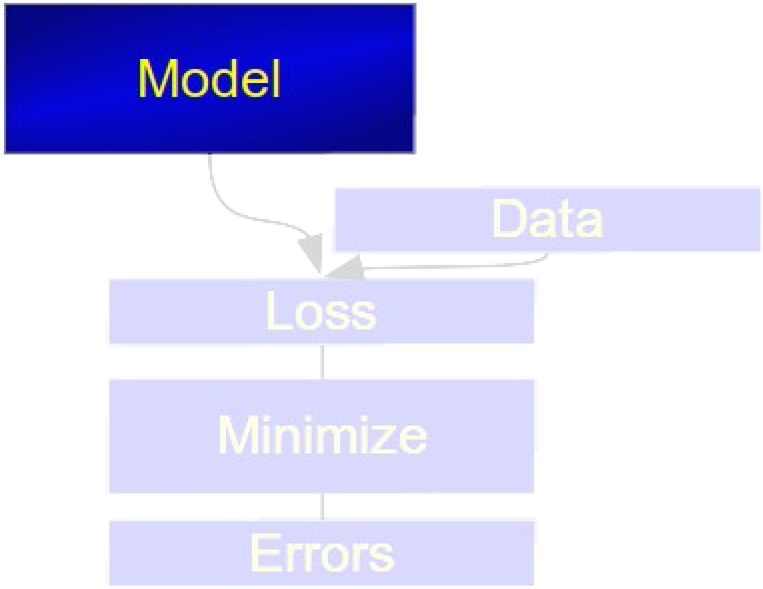

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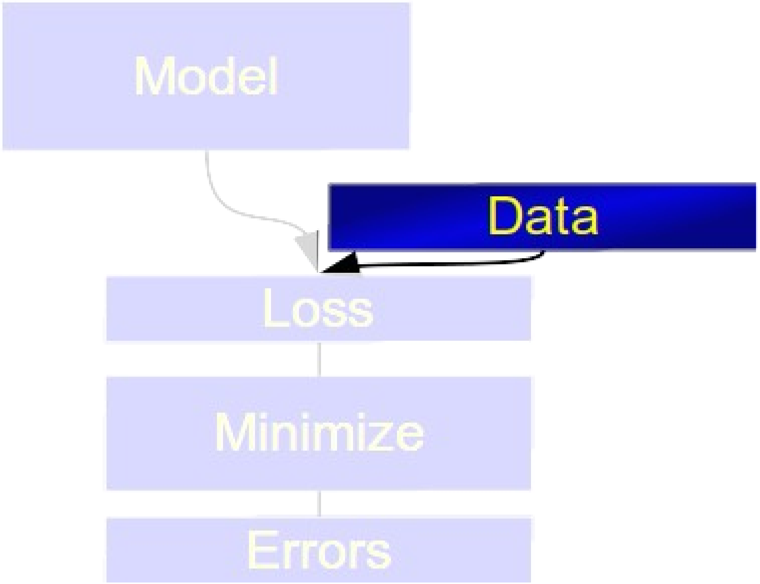

# Complete fit: Loss

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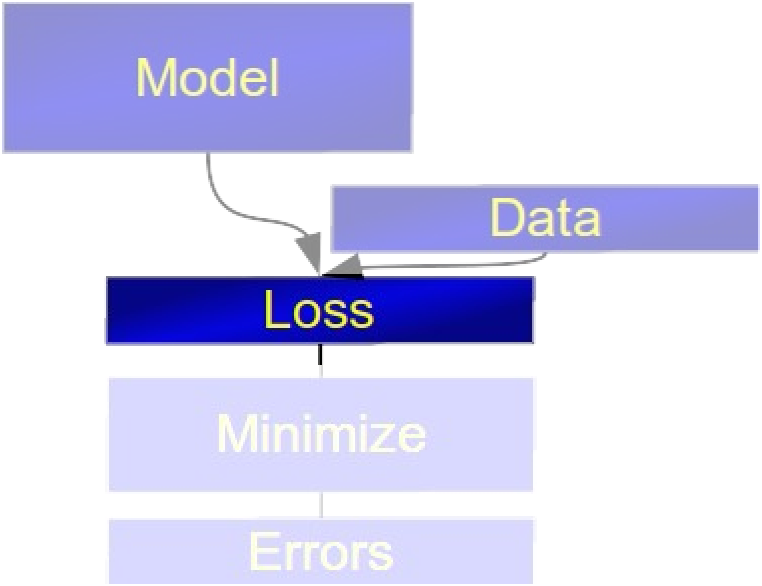

# Complete fit: Minimization

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param_errors_asymmetric, new_result = result.errors()
```
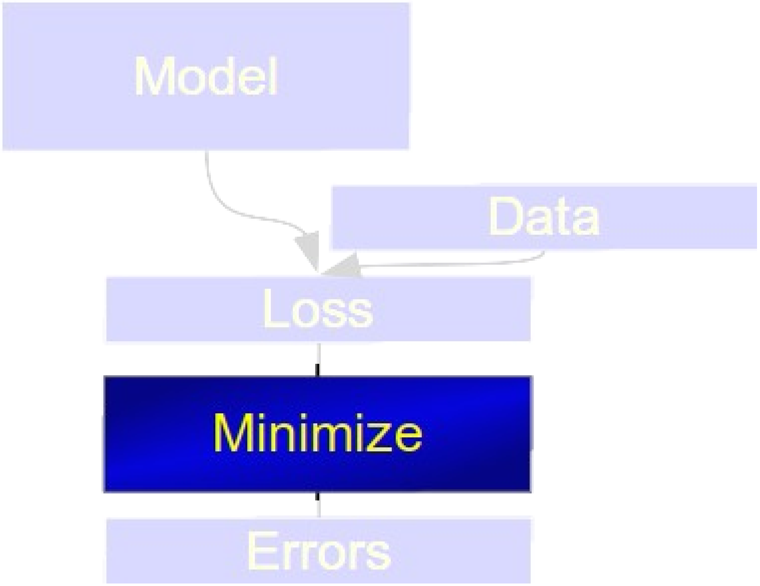
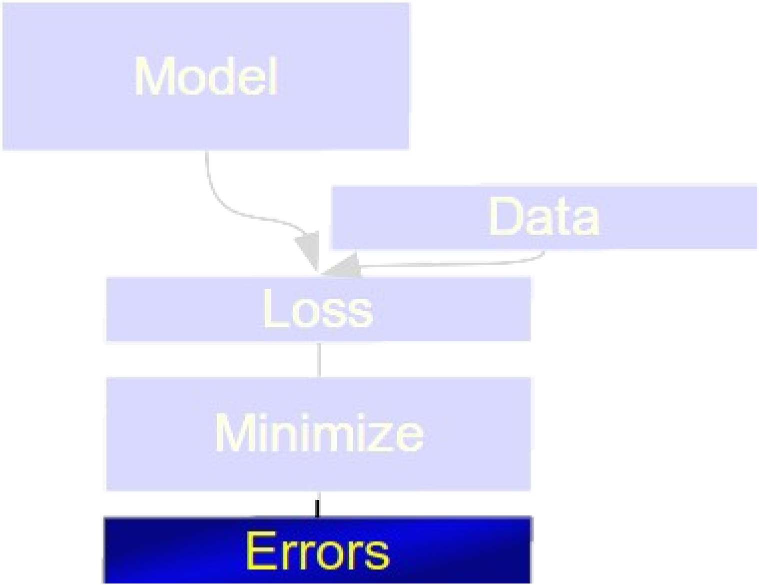



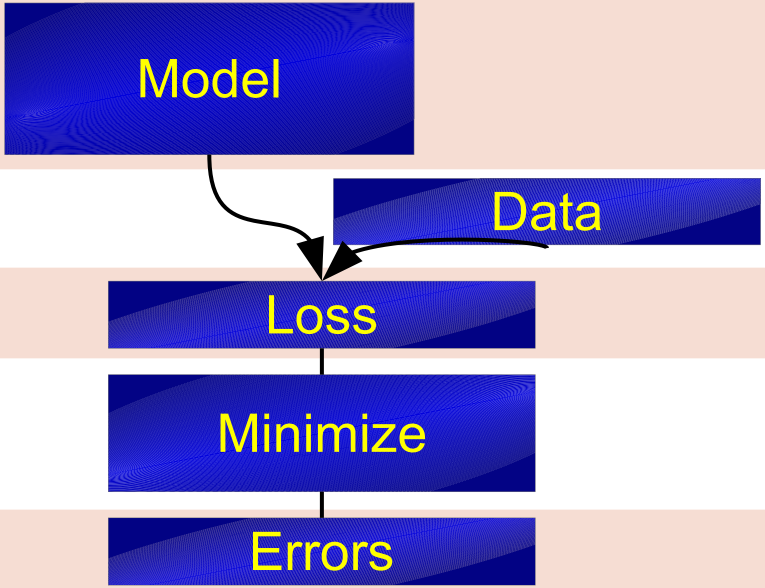
# Complete fit: Result

```python
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



# Basic API example

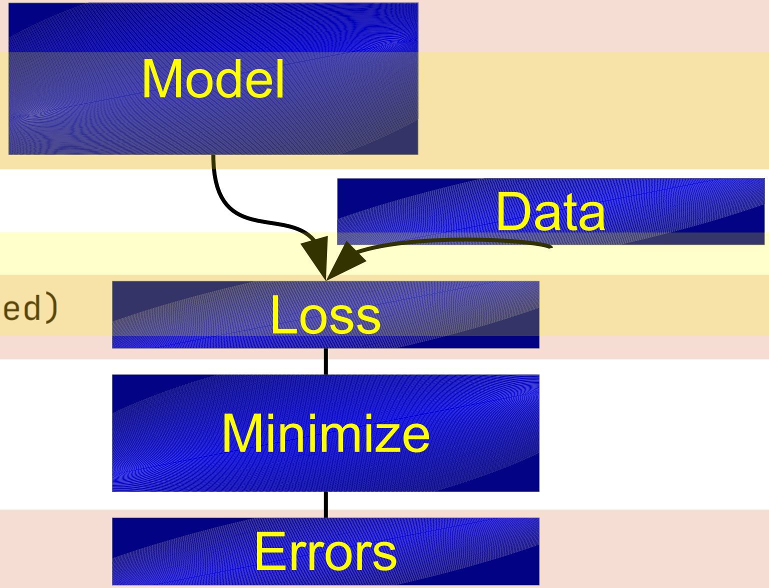
```python
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



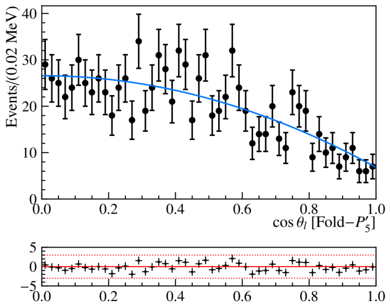
# Basic API example

## Going binned

```python
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)
obs_binned = obs.with_binning(30)
gauss_binned = gauss.to_binned(obs_binned)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)
data_binned = data.to_binned(obs_binned)
nll = zfit.loss.BinnedNLL(model=gauss_binned, data=data_binned)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```

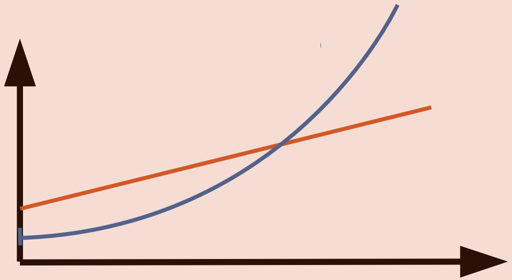


# HEP Model Fitting in Python




HEP

advanced features, simply extendable



Scalable

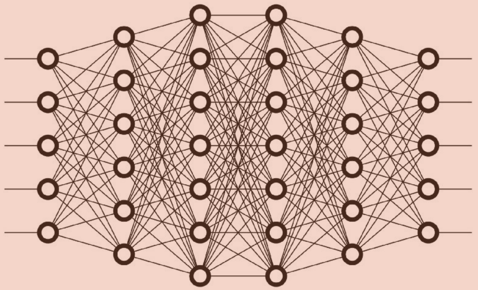
large data, complex models

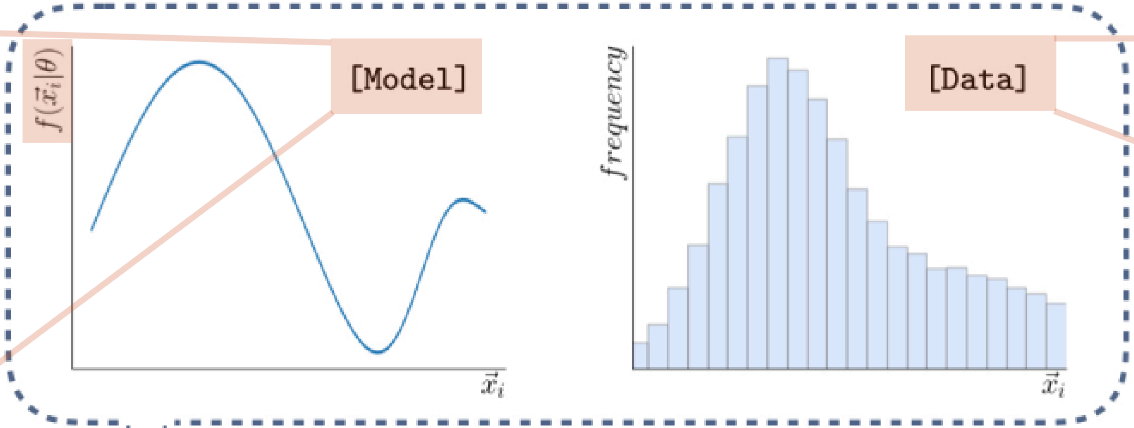
Pythonic

integrate into ecosystem, stable API

# Deep Learning

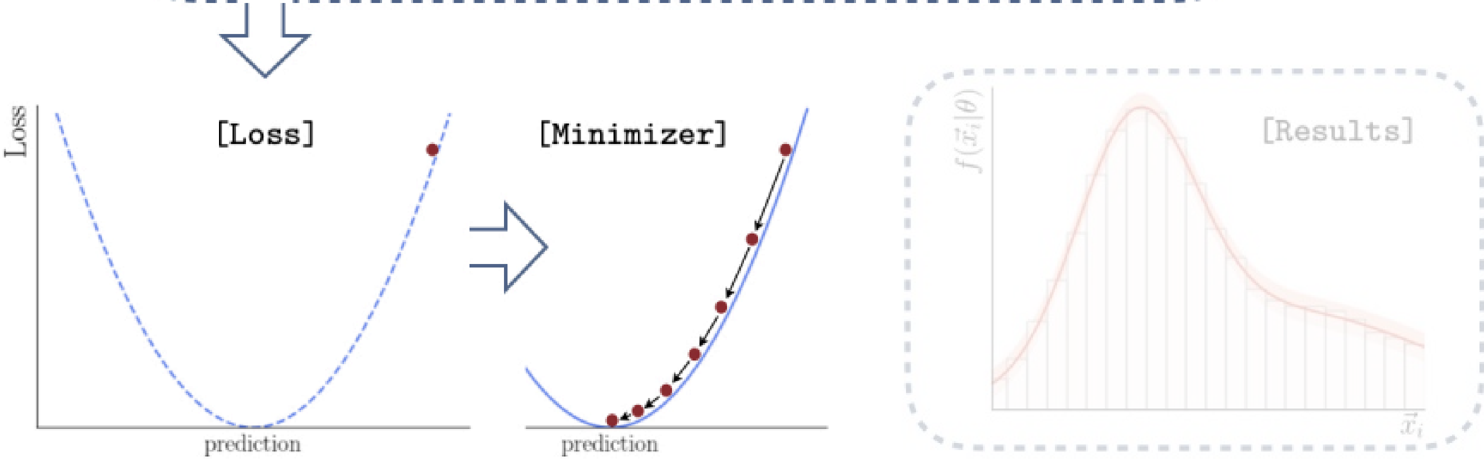
Neural Network






„Big Data“

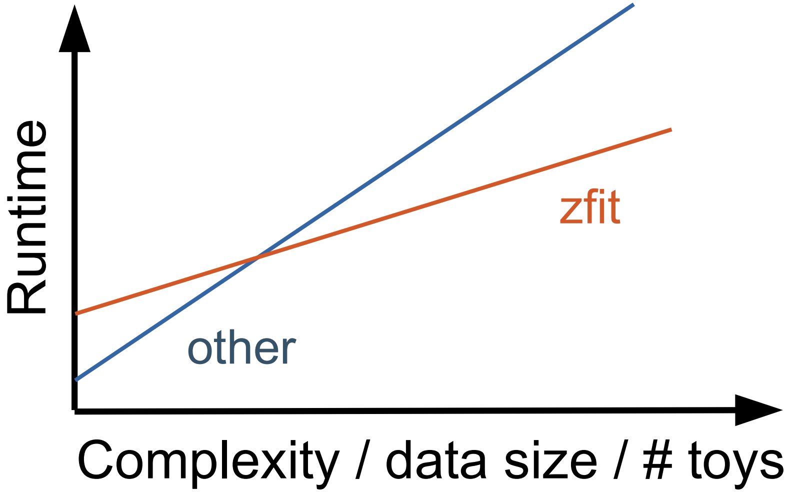
„One huge, complicated function“



# Scalable: Performance

*Use same backend as ML uses*

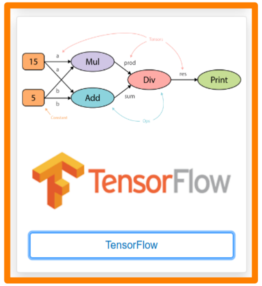
- Numpy-like backend TensorFlow *(JAX)*
  - JIT compiled, CPU or GPU
  - Automatic gradient




Single, simple fit "slow"

- 0.01 or 1 sec not relevant
- 1 or 10 hours relevant

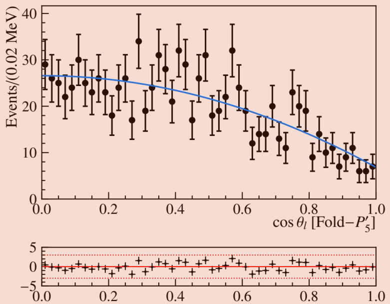
```python
import zfit.z.numpy as znp

ar = znp.linspace(0, 1, 10)
sin = znp.sin(ar)
sum_sin = znp.sum(sin)
```



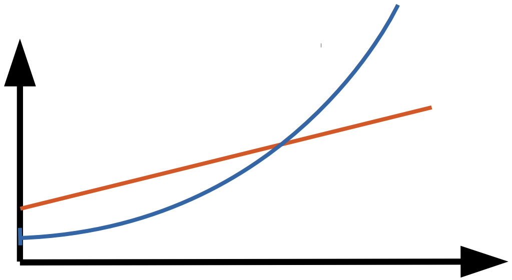
# Delegating the workload

| | C++ library | Numpy based | zfit |
|---|---|---|---|
| HEP specific content/API | | | |
| Models | | SciPy | TF Probability |
| Gradients | CLAD | | |
| Computational optimizations | | | |
| Parallelization/GPU | | Numba NumPy | TensorFlow intel NVIDIA |
| Low level handling | | python | |

# HEP Model Fitting in Python




HEP
advanced features, simply extendable

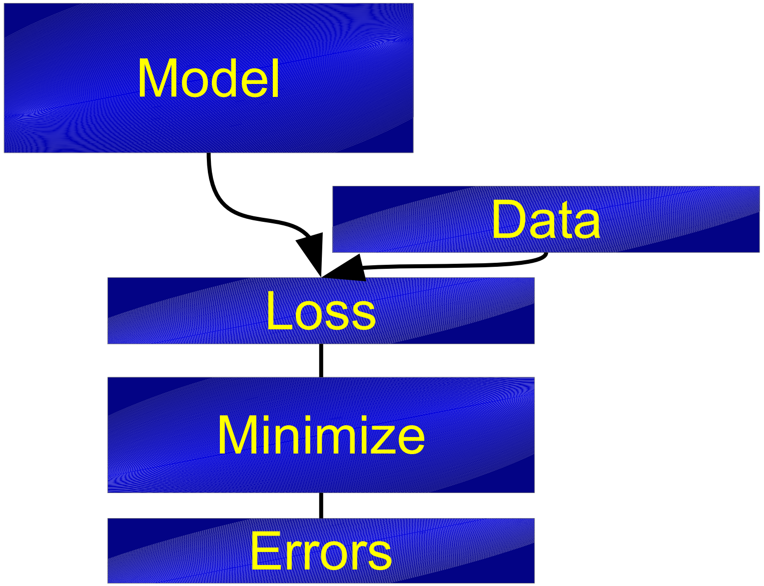


Scalable
large data, complex models

Pythonic
integrate into ecosystem, stable API

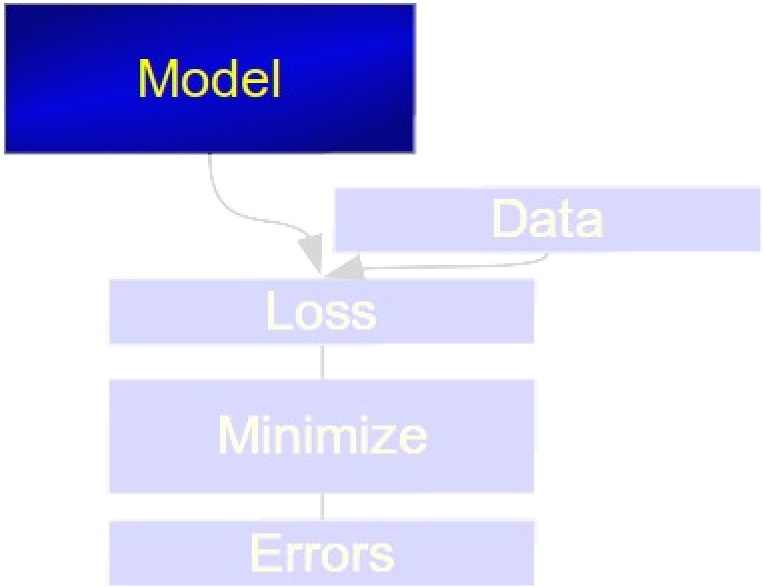
# Complete fit

```python
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



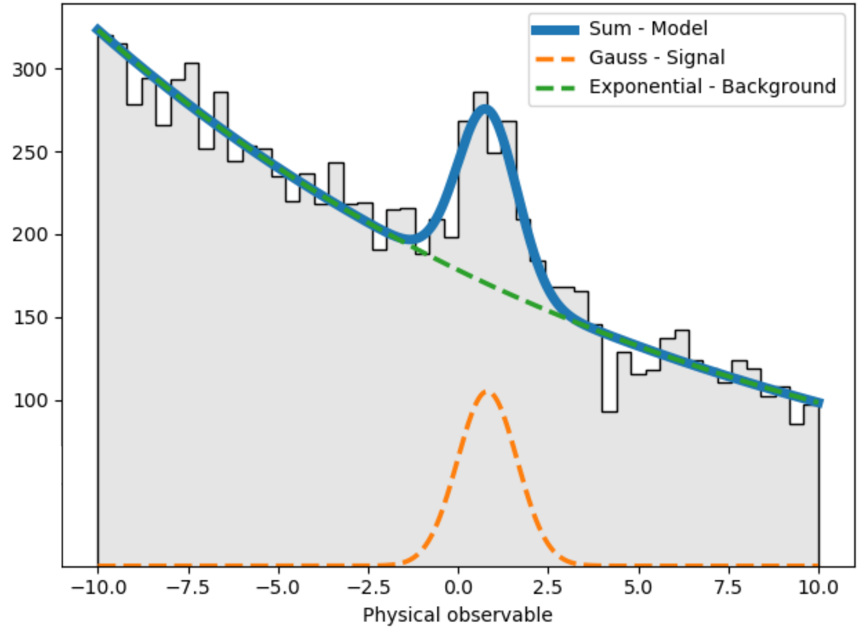
# Complete fit: Model

```python
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



# Example: Mass fit

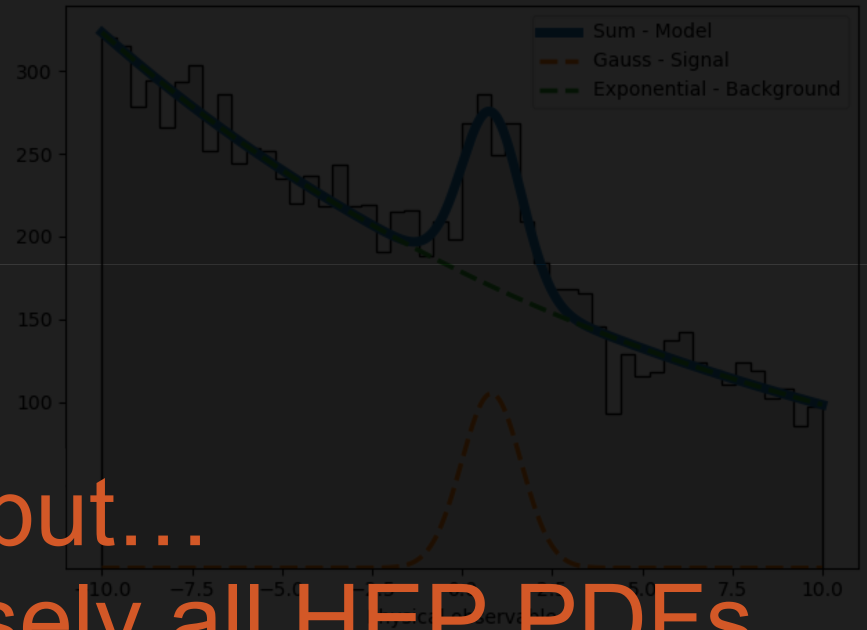
- Sum, Product, *(Convolution)*
- Gauss, (double) Crystalball,...
- Exponential, Polynomials,…
- Histograms, SplineInterpolation,...




```
lambd = zfit.Parameter("lambda", -0.06, -1, -0.01)
frac = zfit.Parameter("fraction", 0.3, 0, 1)

gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)
exponential = zfit.pdf.Exponential(lambd, obs=obs)
model = zfit.pdf.SumPDF([gauss, exponential], fracs=frac)
```

# Example: Mass fit

- Sum, Product, *(Convolution)*
- Gauss, (double) Crystalball,...
- Exponential, Polynomials,…
- Histograms, SplineInterpolation,...




```
lambd = zfit.Parameter("lambda", -0.06, -1, -0.01)
frac = zfit.Parameter("fraction", 0.5, 0, 1)

gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)
exponential = zfit.pdf.Exponential(lambd, obs=obs)
model = zfit.pdf.SumPDF([gauss, exponential], fracs=frac)
```

Good for out-of-the-box but…
does not cover even closely all HEP PDFs

# Custom PDF

```python
from zfit import z
from zfit.z import numpy as znp

class CustomPDF(zfit.pdf.ZPDF):
    _PARAMS = ['alpha']

    def _unnormalized_pdf(self, x):
        data = z.unstack_x(x)
        alpha = self.params['alpha']

        return znp.exp(alpha * data)
```

implement custom function

# Custom PDF

```python
from zfit import z
from zfit.z import numpy as znp

class CustomPDF(zfit.pdf.ZPDF):
    _PARAMS = ['alpha']

    def _unnormalized_pdf(self, x):
        data = z.unstack_x(x)
        alpha = self.params['alpha']

        return znp.exp(alpha * data)
```

```python
custom_pdf = CustomPDF(obs=obs, alpha=0.2)

integral = custom_pdf.integrate(limits=(-1, 2))
sample   = custom_pdf.sample(n=1000)
prob     = custom_pdf.pdf(sample)
```

} use functionality of model

# Custom PDF

```python
from zfit import z
from zfit.z import numpy as znp

class CustomPDF(zfit.pdf.ZPDF):
    _PARAMS = ['alpha']

    def _unnormalized_pdf(self, x):
        data = z.unstack_x(x)
        alpha = self.params['alpha']

        return znp.exp(alpha * data)
```

## Example of zfit Base Classes

Can also override:

- integrate → _integrate
- pdf → _pdf
- sample → _sample

Or register integral

```python
custom_pdf = CustomPDF(obs=obs, alpha=0.2)

integral = custom_pdf.integrate(limits=(-1, 2))
sample   = custom_pdf.sample(n=1000)
prob     = custom_pdf.pdf(sample)
```

} use functionality of model

# Arbitrary analytic shapes

```python
class P5pPDF(zfit.pdf.ZPDF):
    _PARAMS = ['FL', 'AT2', 'P5p']
    _N_OBS = 3

    def _unnormalized_pdf(self, x):
        FL = self.params['FL']
        AT2 = self.params['AT2']
        P5p = self.params['P5p']
        costheta_l, costheta_k, phi = ztf.unstack_x(x)

        sintheta_k = tf.sqrt(1.0 - costheta_k * costheta_k)
        sintheta_l = tf.sqrt(1.0 - costheta_l * costheta_l)

        sintheta_2k = (1.0 - costheta_k * costheta_k)
        sintheta_2l = (1.0 - costheta_l * costheta_l)

        sin2theta_k = (2.0 * sintheta_k * costheta_k)
        cos2theta_l = (2.0 * costheta_l * costheta_l - 1.0)

        pdf = ((3.0 / 4.0) * (1.0 - FL) * sintheta_2k +
                   FL * costheta_k * costheta_k +
                   (1.0 / 4.0) * (1.0 - FL) * sintheta_2k * cos2theta_l +
                   -1.0 * FL * costheta_k * costheta_k * cos2theta_l +
                   (1.0 / 2.0) * (1.0 - FL) * AT2 * sintheta_2k *
                   sintheta_2l * tf.cos(2.0 * phi) + tf.sqrt(FL * (1 - FL))
                   * P5p * sin2theta_k * sintheta_l * tf.cos(phi))

        return pdf
```

For example, create amplitude with ComPWA and zfit

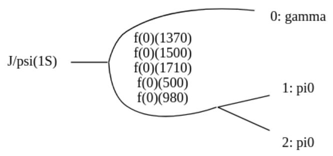
## Amplitude analysis with zfit

▶ Show code cell content

### Formulating the model

```python
import qrules

reaction = qrules.generate_transitions(
    initial_state=("J/psi(1S)", [-1, +1]),
    final_state=["gamma", "pi0", "pi0"],
    allowed_intermediate_particles=["f(0)"],
    allowed_interaction_types=["strong", "EM"],
    formalism="helicity",
)
```

▶ Show code cell source




```python
import ampform
from ampform.dynamics.builder import (
    create_non_dynamic_with_ff,
    create_relativistic_breit_wigner_with_ff,
)

model_builder = ampform.get_builder(reaction)
```

# Binned models

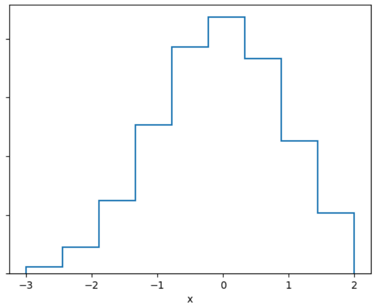
- Success story of Universal Histogram Interface (UHI)
- Modelled after/ compatible with **boost-histogram/hist/UHI**
  - Axes, names, ….

```
h = hist.Hist(hist.axis.Regular(3, -3, 3, name="x", flow=False),
              hist.axis.Regular(2, -5, 5, name="y", flow=False))
x = np.random.randn(1_000_000)
y = 0.5 * np.random.randn(1_000_000)
h.fill(x=x, y=y)

pdf = zfit.pdf.HistogramPDF(data=h)
```

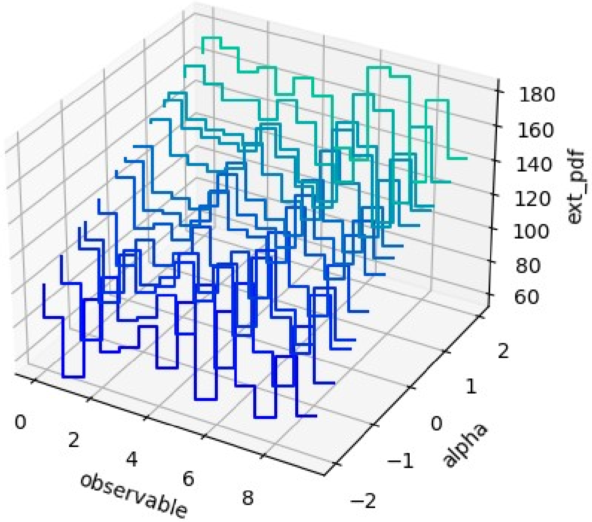
...and back

```
h_back = pdf.to_hist()
```

```
mplhep.histplot(h_back)
```

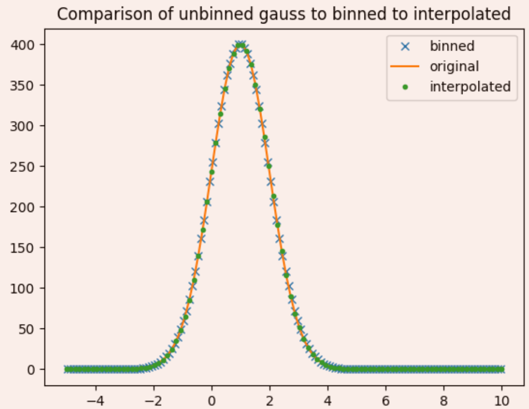


# More histograms



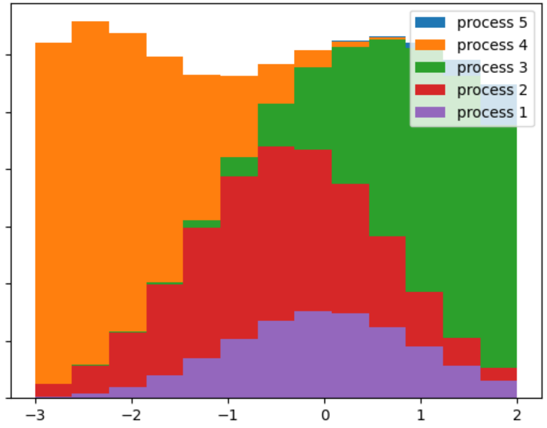

## Shape modifier

```python
pdf_syst = zfit.pdf.BinwiseScaleModifier(pdf, modifiers=True)
```




Unbinned → binned → interpolated

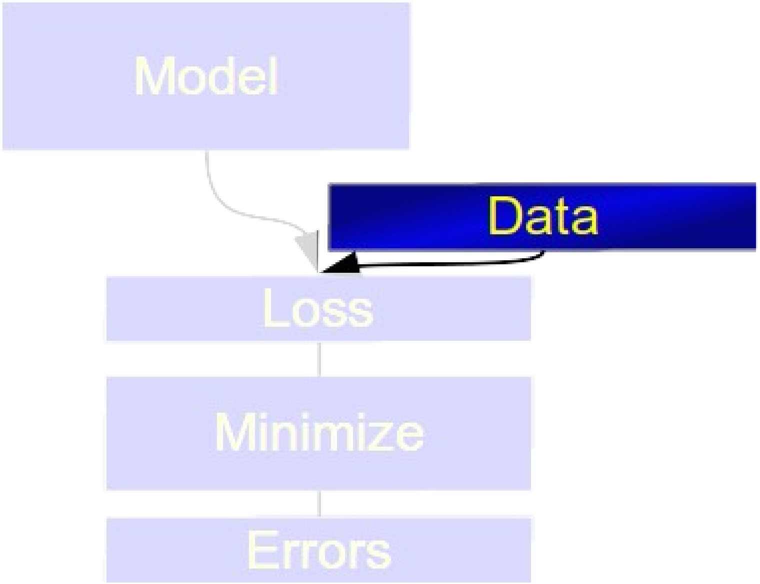
```python
pdfs = [zfit.pdf.HistogramPDF(h) for h in histos]
alpha = zfit.Parameter('alpha', 0, -5, 5)
morph = SplineMorphingPDF(alpha=alpha, hists=pdfs)
```




```python
pdfs = [zfit.pdf.HistogramPDF(h) for h in histos]
sumpdf = zfit.pdf.BinnedSumPDF(pdfs)
```

# Complete fit: Data

```
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



# Complete fit: Data

- From different sources
  - Hist, numpy, Pandas, ROOT, …
  - Can directly be given

Use the HEP/Python ecosystem for preprocessing

- Sampled from a model (toy studies)

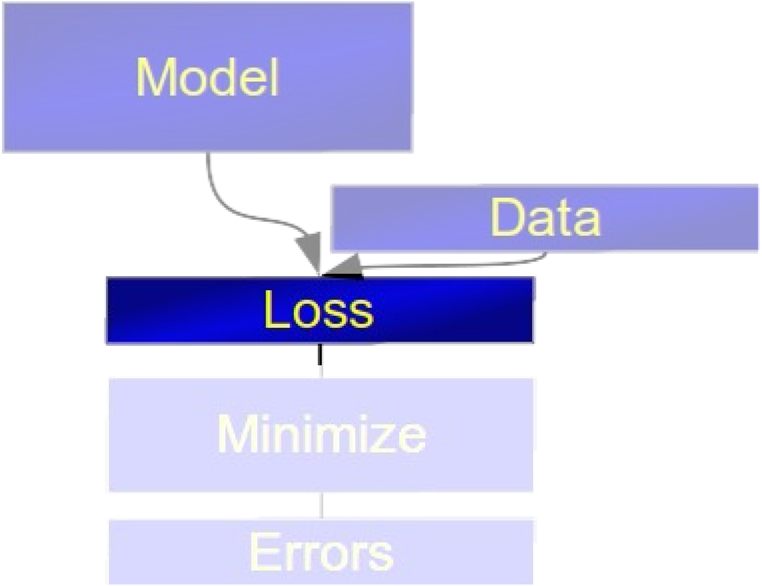
```
data = model.create_sampler(n_sample, limits=obs)
```

- UHI compatible!

```
binneddata = binnedpdf.sample()
mplhep.histplot(binneddata)
```

# Complete fit: Loss

```
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



# Loss

```python
nll_simultaneous = zfit.loss.UnbinnedNLL(model=[gauss1, gauss2],
                                          data=[data1, data2])

nll1 = zfit.loss.UnbinnedNLL(model=gauss1, data=data1)
nll2 = zfit.loss.UnbinnedNLL(model=gauss2, data=data2)
nll_simultaneous2 = nll1 + nll2
```

Equivalent

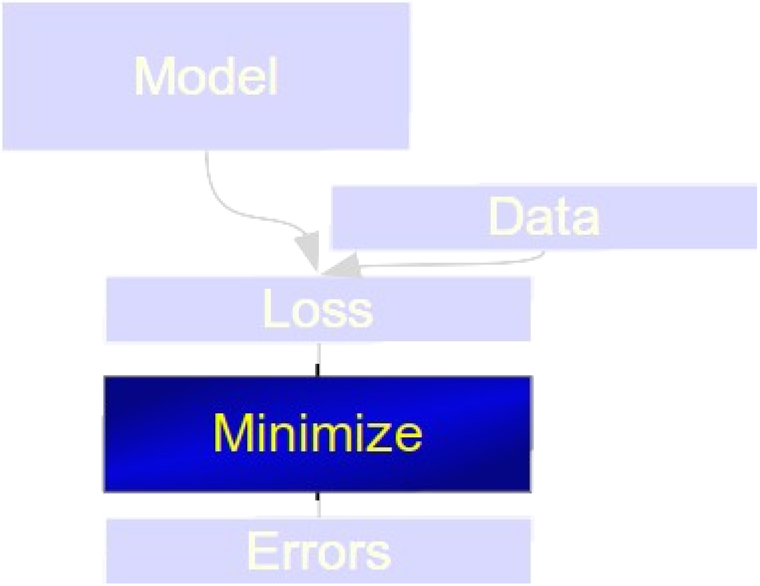
(arbitrary) constraints supported, added to loss

```python
constr = GaussianConstraint(params=params, observation=observed, uncertainty=sigma)
nll = zfit.loss.BinnedNLL(model=model, data=data, constraint=constr)
```

*Directly compatible with iminuit*

# Complete fit: Minimization

```python
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



# Minimize

- Problem: many, non-unified minimizer APIs
  - SciPy inferface "a bit messy", different convergence criterion, etc...
- Unified API: zfit minimizers, simply switch

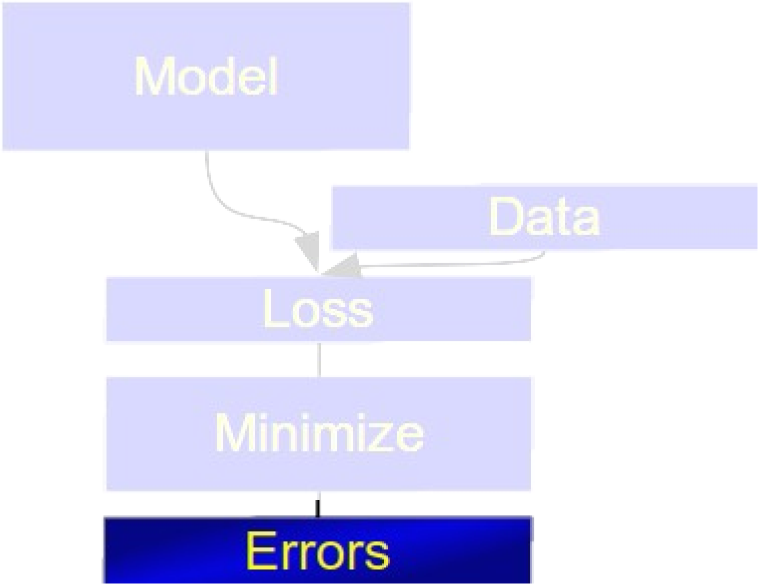
```
minimizer = zfit.minimize.IpyoptV1()
minimizer = zfit.minimize.Minuit()
minimizer = zfit.minimize.ScipyTrustConstrV1()
minimizer = zfit.minimize.NLoptLBFGSV1()
```

- Can use zfit loss, but also ***pure Python function***

```
result = minimizer.minimize(func, params)
```

# Complete fit: Result

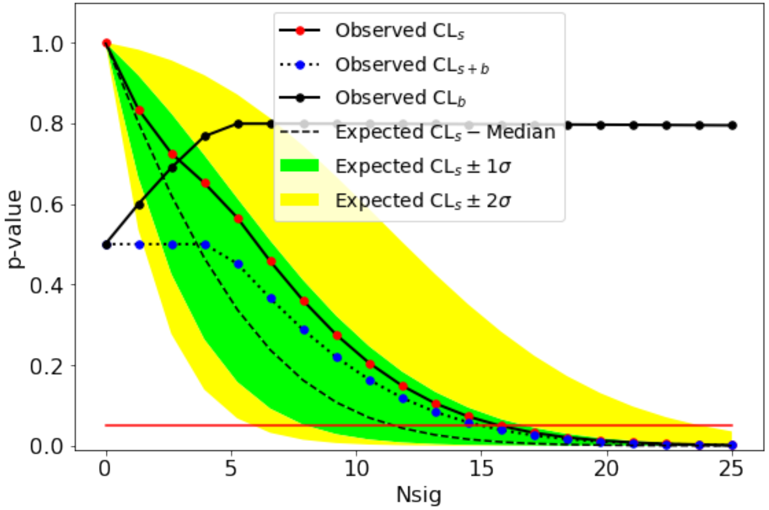
```python
normal_np = np.random.normal(2., 3., size=10_000)

obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



# hepstats

- Inference library for hypothesis tests
- Takes model, data, loss from zfit
- sWeights, CI, limits, …
- asymptotic or toys calculator

```
calculator = AsymptoticCalculator(loss, minimizer)
poinull = POIarray(Nsig, np.linspace(0.0, 25, 20))
poialt = POI(Nsig, 0)
ul = UpperLimit(calculator, poinull, poialt)
ul.upperlimit(alpha=0.05, CLs=True)
```



# $HS^3$

## HEP Statistics Serialization Standard

# Preservation and interoperability

- Goal: restore and exchange likelihood information
  - Use different frameworks (connect across languages)
  - Easily modify likelihoods (theorists!)
- Question: how? Which format?
  - Human-readable vs binary, scripts vs description,  
    virtual machines vs software dependencies, paper vs electronic,…

easy/complex — restoring difficulty/analysis complexity — hard/simple

hard — storing difficulty — easy

# HS3

HEP Statistics Serialization Standard
*Human-readable & preservable format for HEP statistics*

- By RooFit, zfit, pyhf and bat.jl; developing stage
- Explore and define common ground
  - What is a Gaussian/Gauss/Normal? Sum? Variable?
  - Defining channels and nuisance parameter (HistFactory-like)
- Best effort base: «What works for all, works»

easy/complex — restoring difficulty /analysis complexity — hard/simple

hard — storing difficulty — easy

# zfit serialization - HS3

1) Can dump/load (some) PDFs HS3-like

2) Custom functions currently pickled, in future as SymPy/Mathematica

- Project already achieved that
- ComPWA for amplitudes in Sympy

```
'pdfs': {'SumPDF': {'pdfs': [{'extended': 'n_sig',
                              'mu': 'mu',
                              'sigma': 'sigma',
                              'type': 'Gauss',
                              'x': 'x'},
                             {'extended': 'n_bkg',
                              'lam': 'lambda',
                              'type': 'Exponential',
                              'x': 'x'}],
                    'type': 'SumPDF'}},
'variables': {'lambda': {'max': -0.009999999776482582,
                         'min': -1.0,
                         'name': 'lambda',
                         'step_size': 0.001,
                         'value': -0.06294756382703781},
```

easy/complex restoring difficulty /analysis complexity hard/simple

hard 1) 2) storing difficulty easy

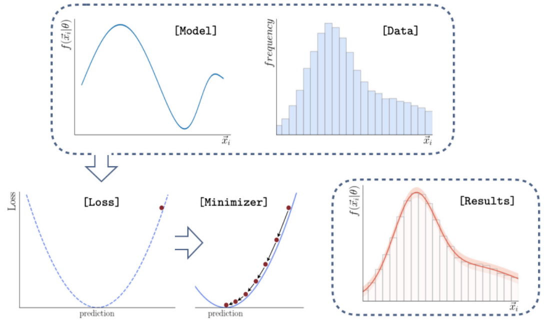
# Conclusion

- Python HEP fitting ecosystem
built from multiple libraries

- zfit «open-world» fitter,
well integrated with the ecosystem

- Interoperability & building on existing
Python scientific ecosystem is key

- HS³ likelihood serialization standard



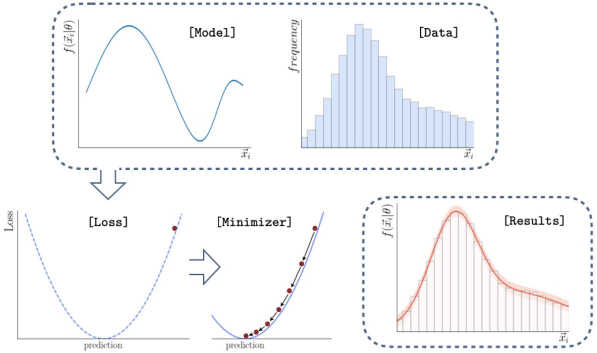
# Conclusion

build stable model fitting ecosystem for HEP

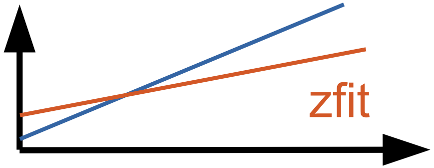
- Recent addition of binned/mixed fits
- Human-readable serialization

  HS3 JSON serialization (WIP)
  Pickling of results
  Custom  dumping simple
  Serialization of toys

- Planning for zfit V2




```
'pdfs': {'SumPDF': {'pdfs': [{'extended': 'n_sig',
                               'mu': 'mu',
                              'sigma': 'sigma',
                               'type': 'Gauss',
                               'x': 'x'},
                              {'extended': 'n_bkg',
                               'lam': 'lambda',
                               'type': 'Exponential',
                               'x': 'x'}],
                     'type': 'SumPDF'}},
```



# Backup Slides

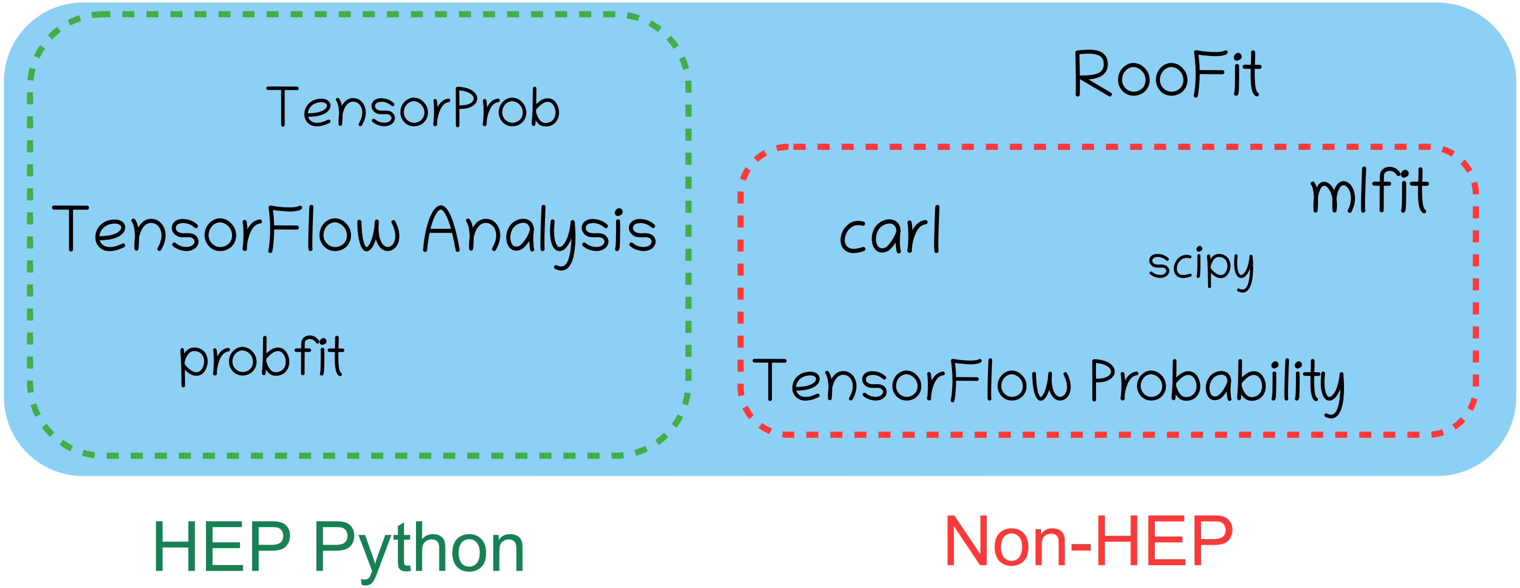
- Backend & TF
- Amplitude
- K*ll toys
- K*mumu Wilson coeffs
- Other fitting packages
- Zfit (associated) packages
- Zfit project
- Zfit elements examples

# zfit features

- Extended fits, Chi2, binned, unbinned, mixed
- PDFs convertable binned ↔ unbinned (including to hist), mixed
- Multidimensional
- Any backend supported (numpy-like), optimal with TF currently
- Sample from PDF
- Arbitrary constraints (custom made)
- Custom PDF: define shape → auto normalized, sampling etc.
- Automatic/numerical gradient
- Different minimizers, optimized API
- JIT/eager support

# Fitting in Python

A lot of projects are around



# Backend & TensorFlow

# Backend: a comparison

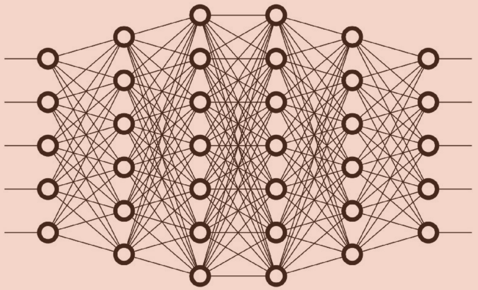
- TensorFlow: supports the most features to this day
- PyTorch: missing advanced math (complex support, …)
- Numpy/SciPy: Too slow, no gradient, no GPU
- JAX: very promising, but *no globals (cache,…)*,
  only static known shapes (adaptive algorithms, accept-reject...), only
  JAX/Numpy arrays compatible
- SymPy: limited to mathematical expressions (no control-flow,…)
  but can convert to any other backend (used by TensorWaves)

# *Deep Learning*

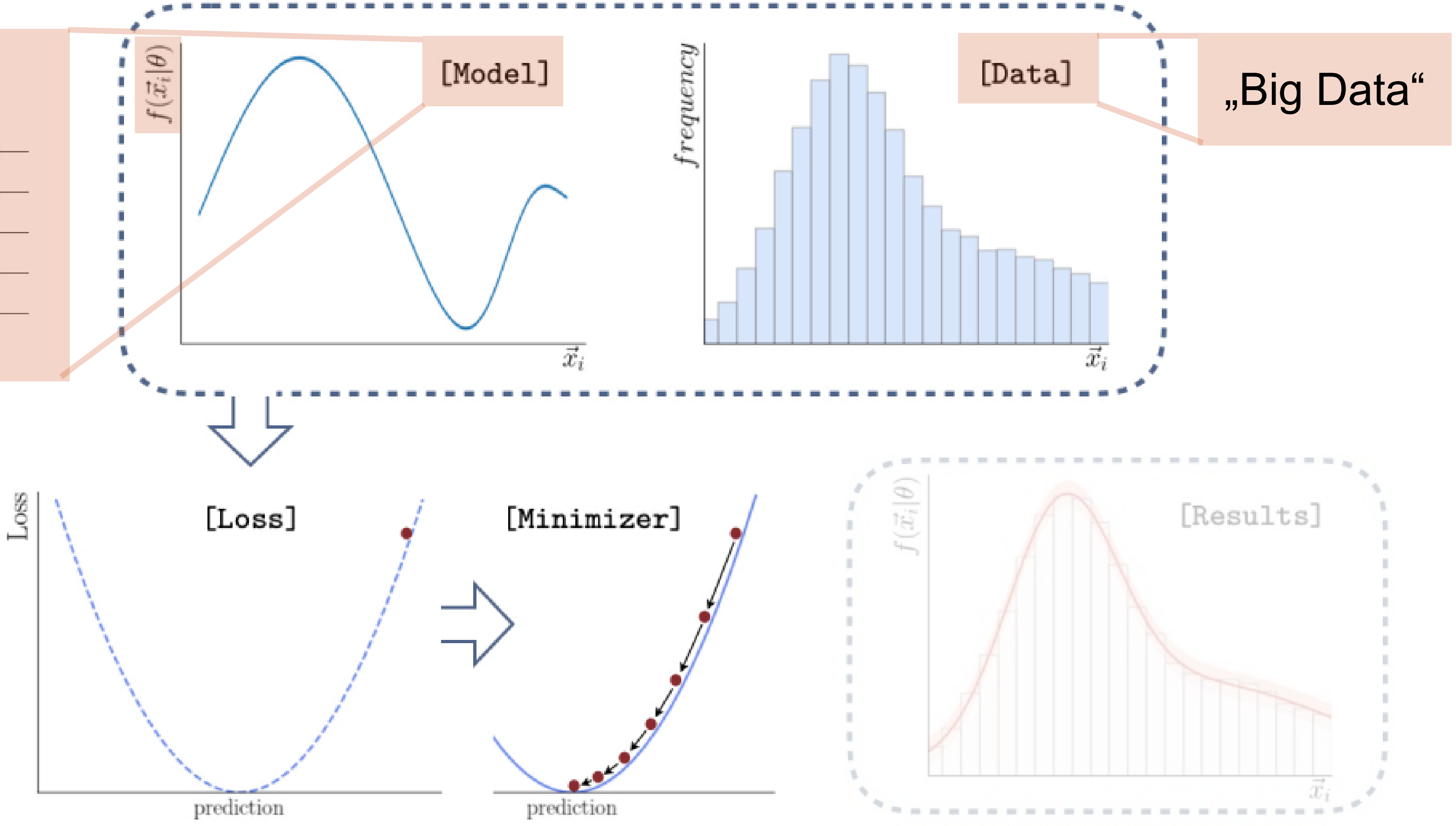
lessons for model fitting

# Deep Learning

Neural Network



„One huge, complicated function"



*Can* we express model fitting as static graphs?

***Yes!***

# HPC perspective

1) Definition of computation, shape etc. (add static knowledge)
2) Compilation of the graph
3) Execution of computation (re-use optimized graph)

Inside TF, hidden to end-user

HPC: the more is know *before* the execution, the better

TensorFlow takes care of *how* to use this knowledge

# Graph elements

*… do not have to be constant!*

**Parameters**

Can change their value

**Random numbers**

Generate newly on every graph execution: MC integration,…

**Control flow (if, while)**

Steer the execution: Accept-reject sampling (while), etc.

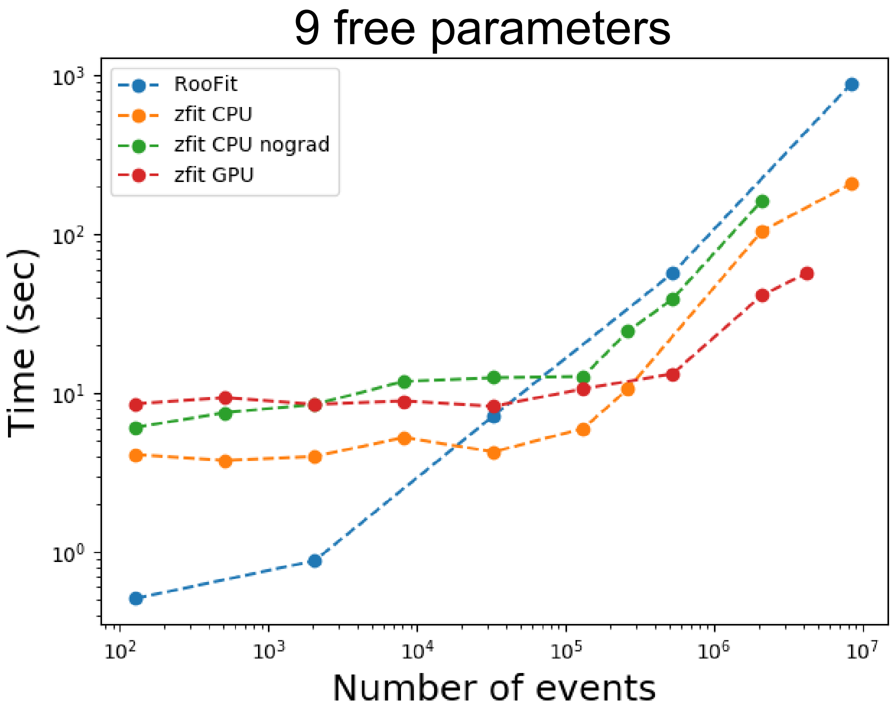
Static, not constant

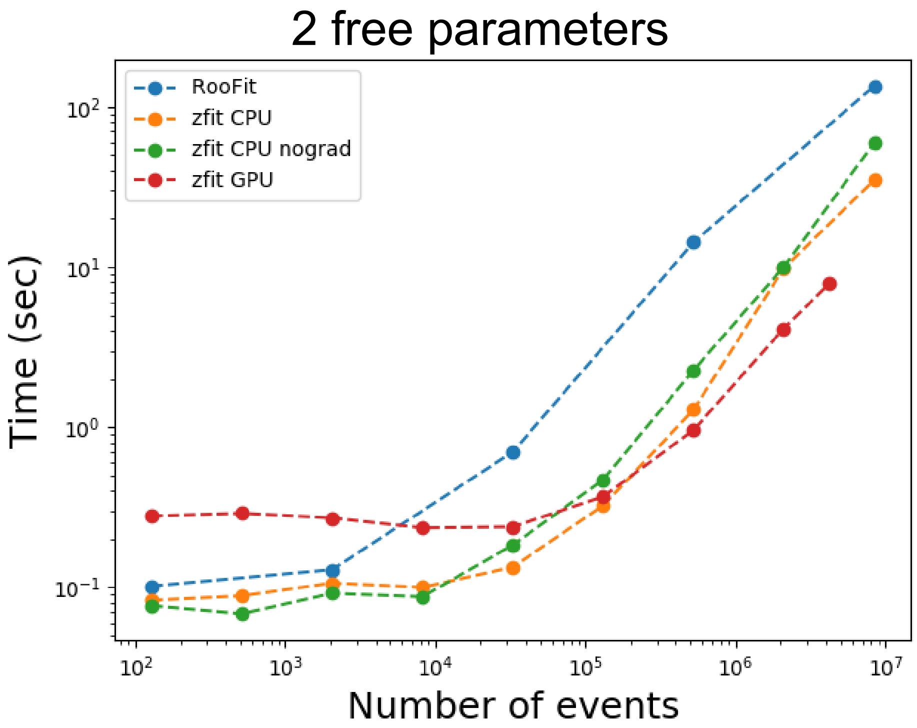
# Deep Learning vs. Model Fitting

| Similarity | Complicated Models | Large Data | Composed loss | Minimization | Results and uncertainties |
|---|---|---|---|---|---|
| HEP | Non-trivial functions | Whole Dataset | simultaneous, constraints | Global min, $2^{nd}$ derivative algorithm | Hesse, profiling |
| Deep Learning | Combine many, trivial functions | Many, small Batches | *Anything! (GANs, RL,...)* | Local (!) min, $1^{th}$ derivative, many steps | None |
| Conclusion | | | | | |

# Scalability: Performance

Fitting time (lower is better): **RooFit** vs. **zfit**



# Amplitude

# Angular toys

# $B^0 \to K^{*0} l^+ l^-$ angular: toy study

Sensitivity study

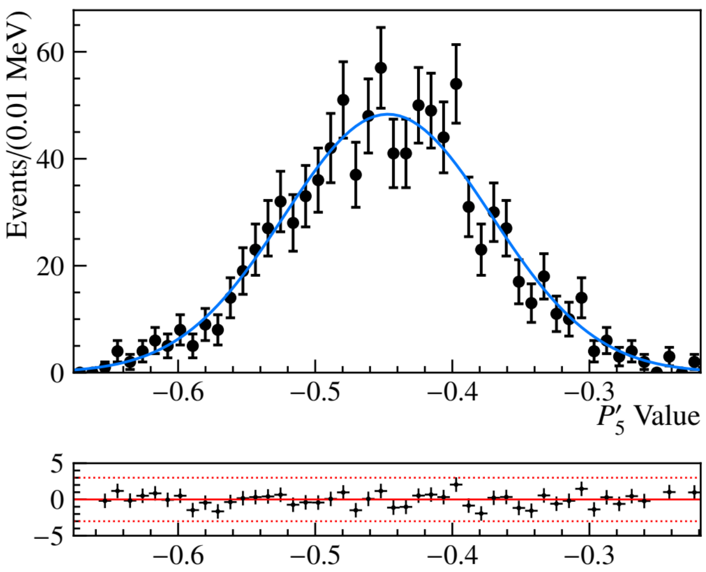
- draw toys (sample) from PDF
- Fit to sample

```python
for i in range(ntoys):

    # set initial sampling values
    for param in params:
        param.set_value(...)

    sampler.resample()

    # set random initial values
    for param in params:
        param.set_value(...)

    result = minimizer.minimize(nll)

    if result.converged:
        ...
```

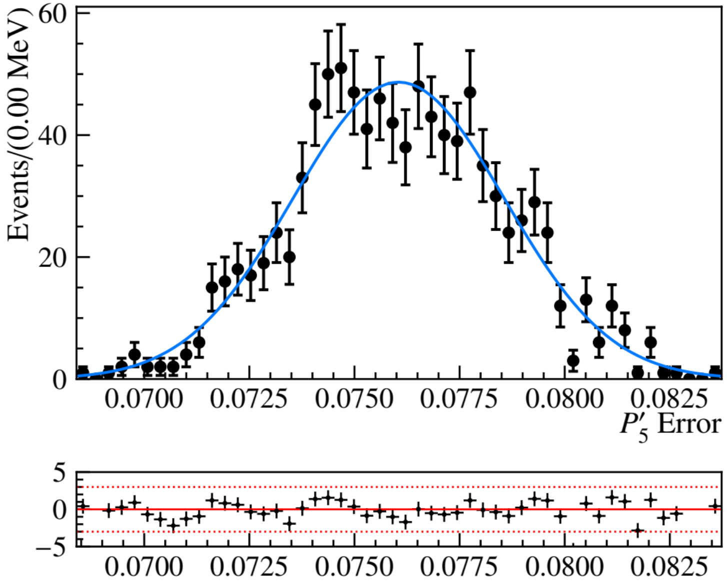
# $B^0 \to K^{*0} l^+ l^-$ angular: toy study

## Result of toy study

### P5' value




### P5' error



# Extending with a mass shape

```python
# Create mass pdf
mu = zfit.Parameter("mu", 5279, 5200, 5400)
sigma = zfit.Parameter("sigma", 30, 0, 300)
a0 = zfit.Parameter("a0", 1.0, 0, 10)
a1 = zfit.Parameter("a1", 1.0, 0, 10)
n0 = zfit.Parameter("n0", 5, 0, 10)
n1 = zfit.Parameter("n1", 5, 0, 10)

mass = zfit.Space("mass", limits=(4900, 5600))

massPDF = zfit.pdf.DoubleCB(obs=mass, mu=mu, sigma=sigma,
                            alphal=a0, nl=n0, alphar=a1, nr=n1)

pdf = massPDF * angularPDF
```

Build model

# Fitting libraries and comparison

# Python model fitting in HEP

- Scalable: large data, complex models
- Pythonic: use Python ecosystem/language
- Specific HEP functionality:
  - Normalization: specific range, numerical integration,...
  - Composition of models
  - Multiple dimensions
  - Custom models
  - Non-trivial loss (constraints, simultaneous,…)

# HEP Python projects

Probfit, TensorProb,…

- Lack generality and extendibility
- “experimental”, but great proof of concept
  - API and Python in general
  - Computational backends (e.g. Cython, TensorFlow)
  - Building an ecosystem (iminuit,…)

General impression in comparison with other HEP packages

# Non-HEP

Scipy, lmfit, TensorFlow Probability,...

- Lack of specific HEP features
  - *Normalization: specific range, numerical integration,...*
  - *Composition of models*
  - *Multiple dimensions*
  - *Custom models*
- Irrelevant functionality supported in API
  - Survival function, …

# zfit related packages

# phasespace

- Package for phasespace generation of particles
- Covers functionality of TGenPhaseSpace (and more)
- Pure Python (& TensorFlow), integrates seemless with zfit

```
pion = GenParticle('pi+', PION_MASS)
kaon = GenParticle('K+', KAON_MASS)
kstar = GenParticle('K*', KSTARZ_MASS).set_children(pion, kaon)
gamma = GenParticle('gamma', 0)
bz = GenParticle('B0', B0_MASS).set_children(kstar, gamma)

weights, particles = bz.generate(n_events=1000)
```

# Zfit: project description

# Ecosystem: API & Workflow

## Establish a stable API

- High level libraries (statistics, plotting,...)
  - „code against an interface, not an implementation“
- Replace each component
  - Allow other libraries to implement custom parts

**Many discussions with community to avoid splitting/duplication**

# Pythonic

- Pure Python («pip install zfit»)
- Integrated into python ecosystem
    - Load ROOT files (uproot,no ROOT dependence!)
    - Use Minuit for minimization (iminuit)
    - Data preprocessing with Pandas DataFrame
    - Plotting with matplotlib
    - High level statistics (lauztat, more WIP)
- Extendable classes
    - e.g. custom PDF

# Scalable: TensorFlow

- Deep Learning framework by Google
- Modern, declarative graph approach
- Built for highly parallelized, fast communicating CPU, GPU, TPU,… clusters
- Built to use «Big Data»

# Zfit library examples

# Minimize Python function

```python
def func(x):
    x = np.array(x)  # make sure it's an array
    return np.sum((x - 0.1) ** 2 + x[1] ** 4)

func.errordef = 0.5

params = [1, -3, 2, 1.4, 11]

result = minimizer.minimize(func, params)
```

# Model, loss building

## sum of two pdfs

```
sum_pdf = zfit.pdf.SumPDF([gauss, exponential], fracs=frac)
```

## shared parameters

```
mu_shared = zfit.Parameter("mu_shared", 1., -4, 6)

gauss1 = zfit.pdf.Gauss(mu=mu_shared, sigma=sigma1, obs=obs)
gauss2 = zfit.pdf.Gauss(mu=mu_shared, sigma=sigma2, obs=obs)
```

## simultaneous loss

```
nll1 = zfit.loss.UnbinnedNLL(model=gauss1, data=data1)
nll2 = zfit.loss.UnbinnedNLL(model=gauss2, data=data2)
nll_simultaneous2 = nll1 + nll2
```

From classical

to more TensorFlow

# Model, loss building

## Simple combinations

```
func_n = zfit.func.ZFunc(...)  # pseudo code
func = func_1 + func_2 * func_3
```

## Composite Parameter

```
pdf = zfit.pdf.Gauss(mu=tensor1, sigma=4)
```

## Custom Loss

```
loss = zfit.loss.SimpleLoss(lambda: tensor_loss)
```

up to pure TensorFlow

=> use all of zfit functionality like minimizers

# Model building

```python
obs = zfit.Space("x", limits=(-10, 10))

mu =    zfit.Parameter("mu",          1,  -4,  6)
sigma = zfit.Parameter("sigma",       1, 0.1, 10)
lambd = zfit.Parameter("lambda",     -1,  -5,  0)
frac =  zfit.Parameter("fraction", 0.5,   0,   1)

gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)
exponential = zfit.pdf.Exponential(lambd, obs=obs)
```

parameters

models

# Simultaneous fit

```python
mu_shared = zfit.Parameter("mu_shared", 1., -4, 6)
sigma1 = zfit.Parameter("sigma_one", 1., 0.1, 10)
sigma2 = zfit.Parameter("sigma_two", 1., 0.1, 10)

gauss1 = zfit.pdf.Gauss(mu=mu_shared, sigma=sigma1, obs=obs)
gauss2 = zfit.pdf.Gauss(mu=mu_shared, sigma=sigma2, obs=obs)
```

shared parameters

```python
nll_simultaneous = zfit.loss.UnbinnedNLL(model=[gauss1, gauss2],
                                         data=[data1, data2])

nll1 = zfit.loss.UnbinnedNLL(model=gauss1, data=data1)
nll2 = zfit.loss.UnbinnedNLL(model=gauss2, data=data2)
nll_simultaneous2 = nll1 + nll2
```

Completely equivalent