

# scalable pythonic fitting

**Jonas Eschle** on behalf of zfit  
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SWISS NATIONAL SCIENCE FOUNDATION



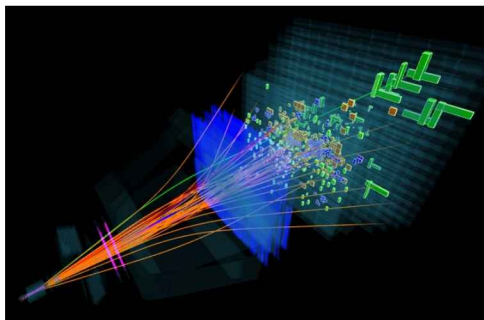
**University of  
Zurich** <sup>UZH</sup>

# Statistical inference in HEP



Analysis: from collecting data to extracting statistical statement

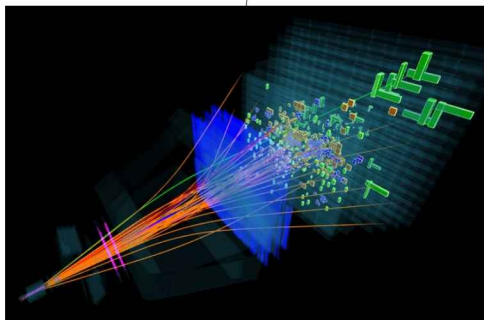
Reconstruction,  
stripping, ...



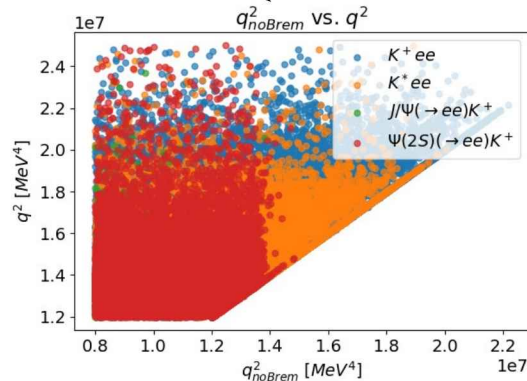
# Statistical inference in HEP

Analysis: from collecting data to extracting statistical statement

Reconstruction,  
stripping, ...



Selection,  
corrections, ...

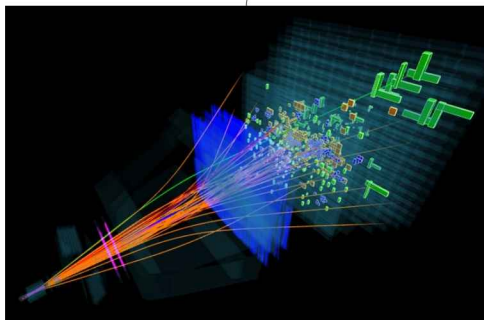


# Statistical inference in HEP

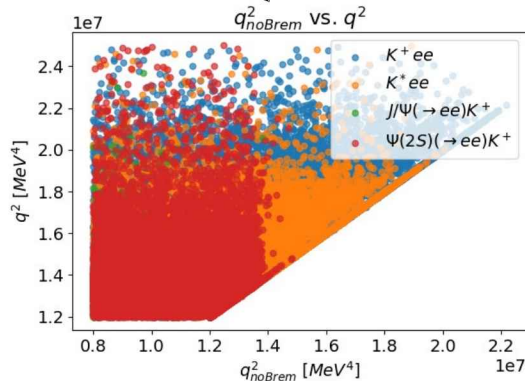
Analysis: from collecting data to extracting statistical statement

Involves often likelihood fitting and hypothesis testing

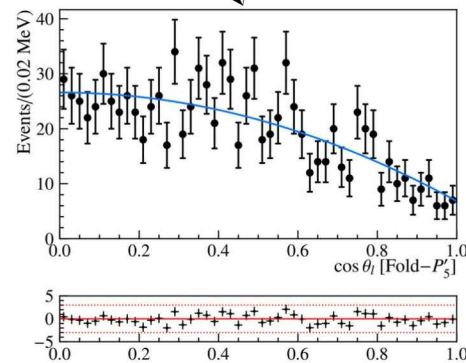
Reconstruction,  
stripping, ...



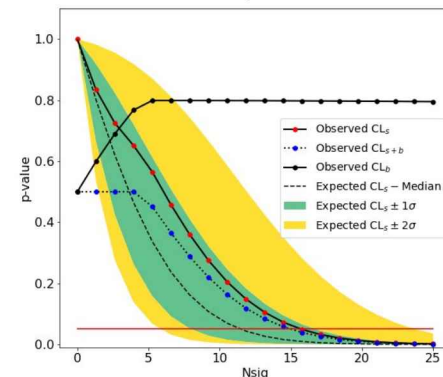
Selection,  
corrections, ...



Model and fit



Hypothesis testing





# Statistical inference in HEP



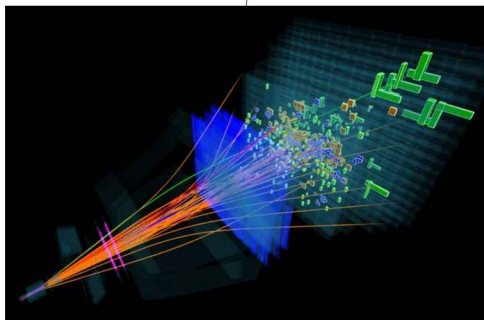
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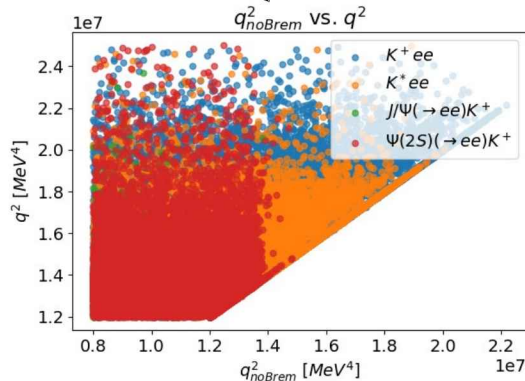
How to use Python for analysis?



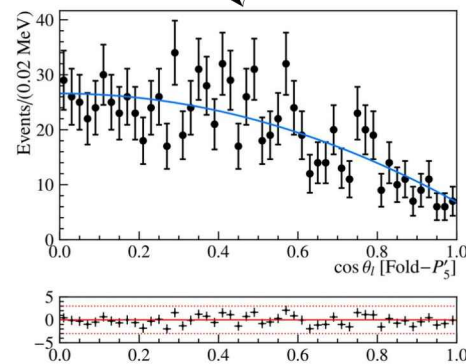
Reconstruction,  
stripping, ...



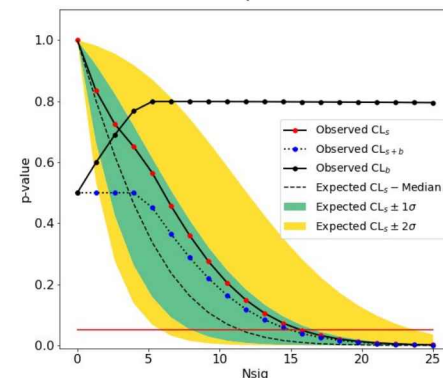
Selection,  
corrections, ...



Model and fit



Hypothesis testing

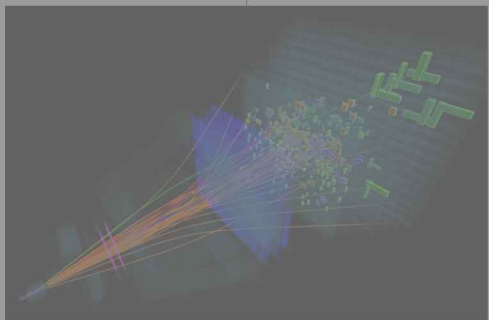


# Statistical inference in HEP



Analysis: from collecting data to extracting statistical statement  
Involves often likelihood fitting and hypothesis testing

Reconstruction,  
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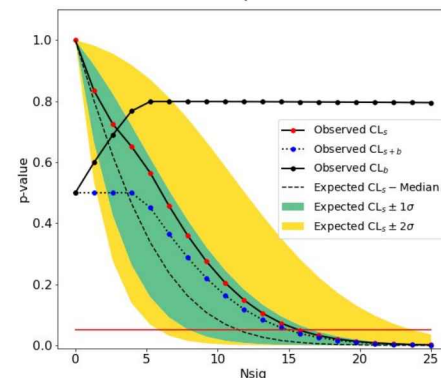
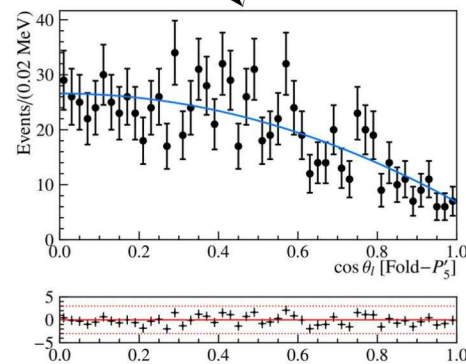
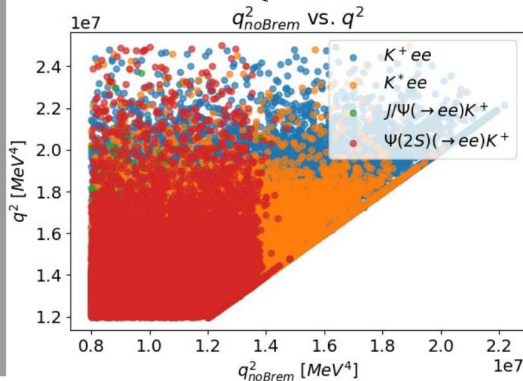
Selection,  
corrections, ...



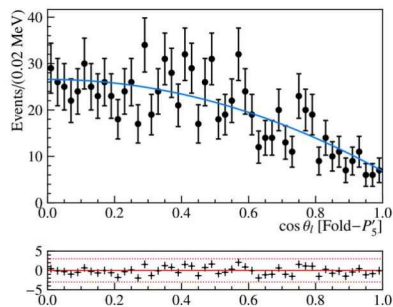
zfit  
Model and fit



Hypothesis testing



# HEP Model Fitting in Python



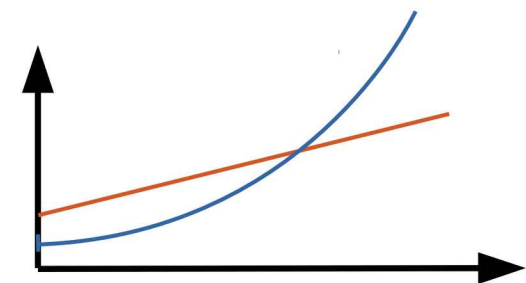
**HEP**

advanced features,  
simply extendable

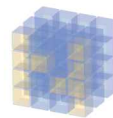


**Scalable**

large data, complex models



**Pythonic**



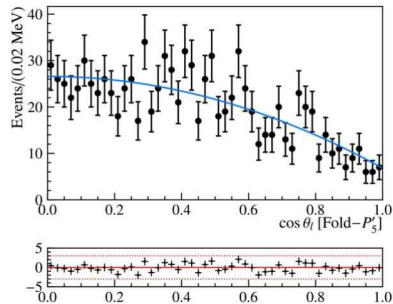
NumPy



python™

integrate into ecosystem, stable API

# HEP Model Fitting in Python



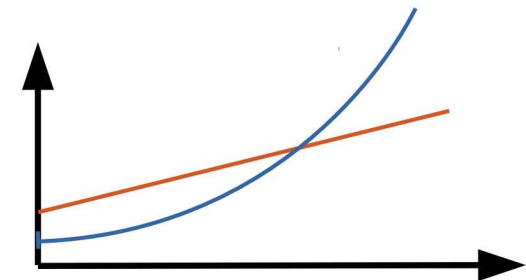
HEP

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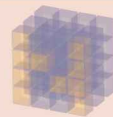


Scalable

large data, complex models



Pythonic



NumPy



python™

integrate into ecosystem, stable API

# Complete fit

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

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

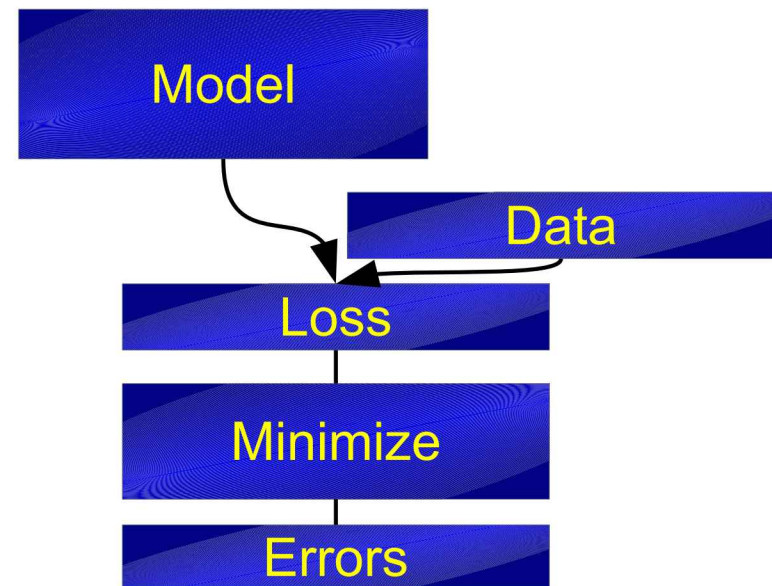
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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

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

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

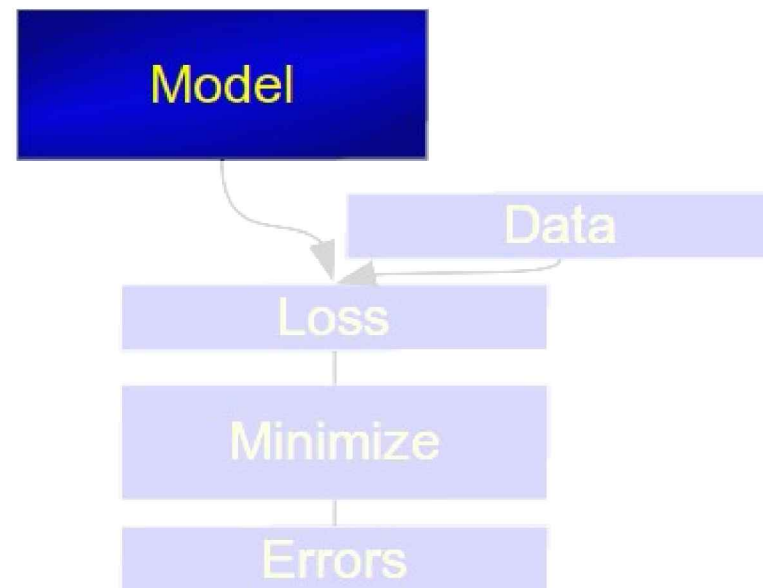
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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

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

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

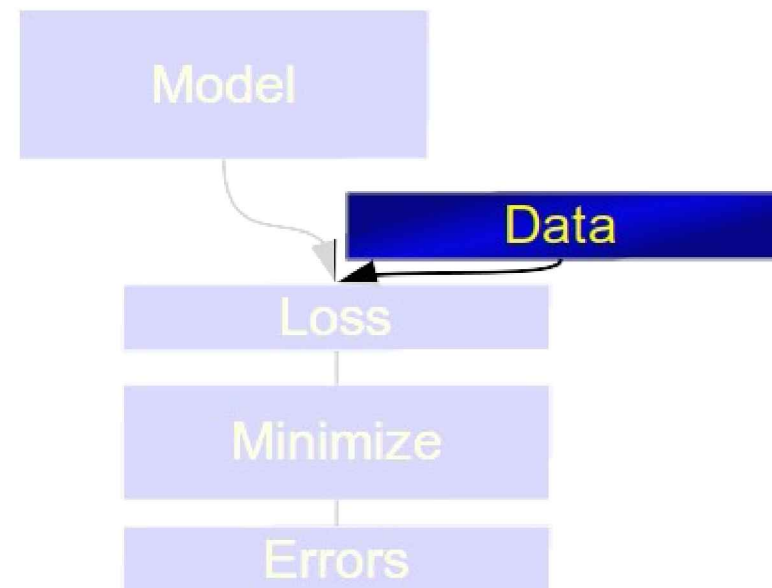
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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)

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





# Complete fit: Loss

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

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

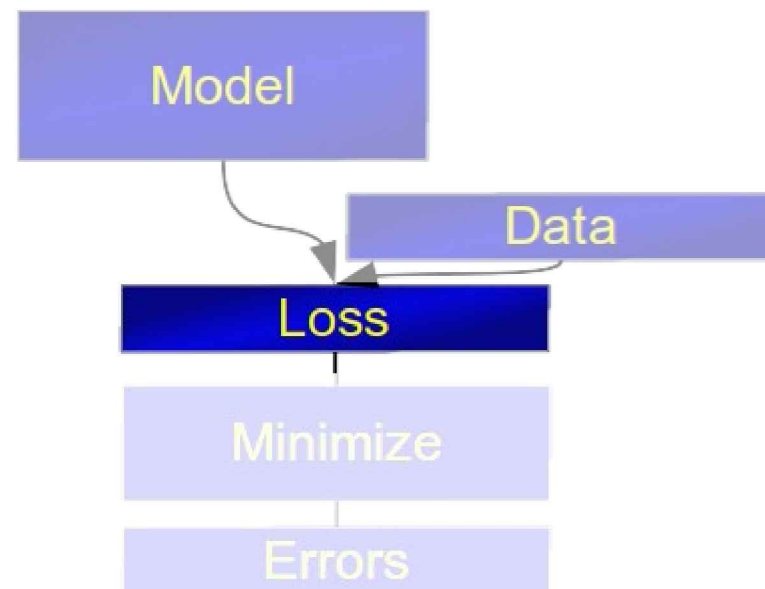
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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()
```



# Complete fit: Minimization

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

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

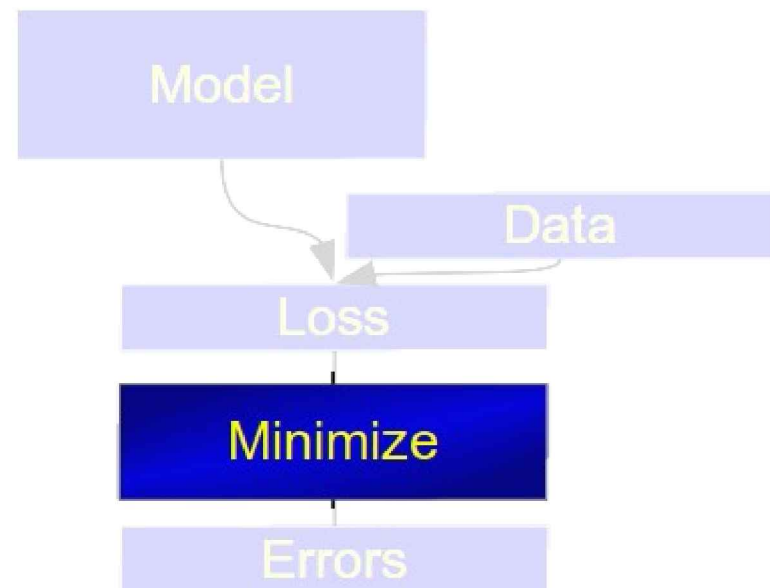
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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: Result

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

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

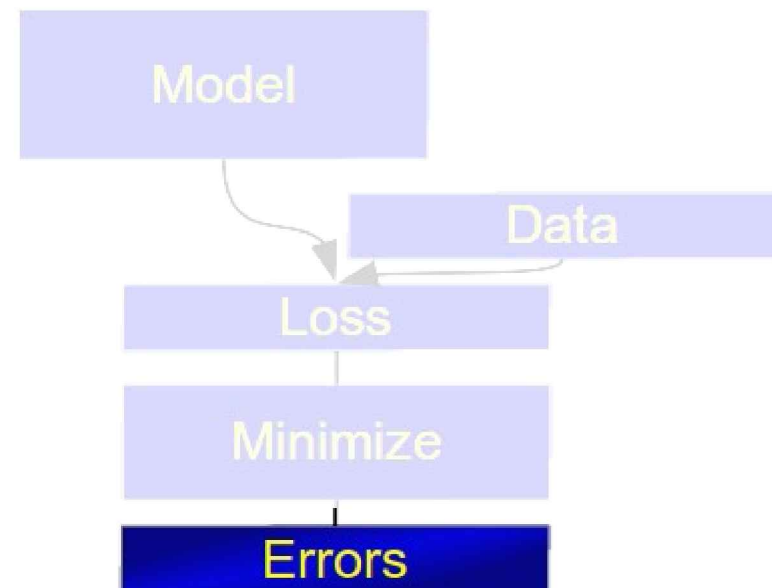
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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

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

param_errors = result.hesse()
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```



# Basic API example

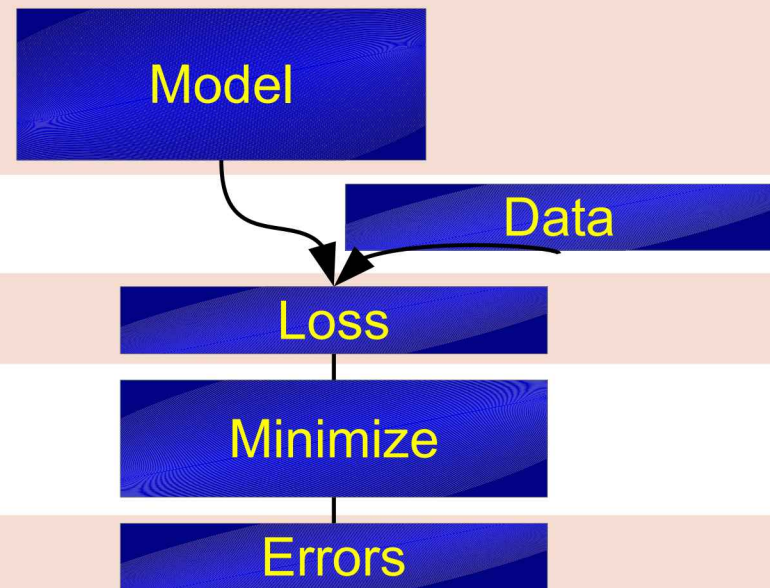
```
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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minimizer = zfit.minimize.Minuit()
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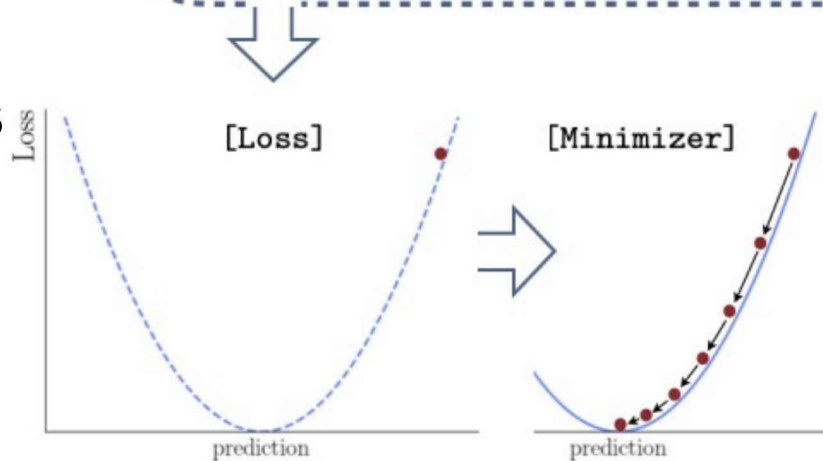
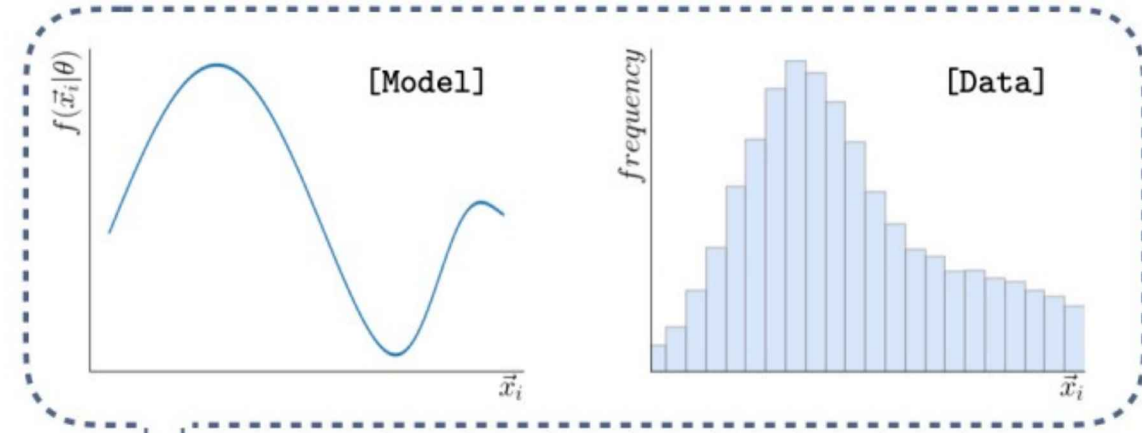
param_errors = result.hesse()
param_errors_asymmetric, new_result = result.errors()
```



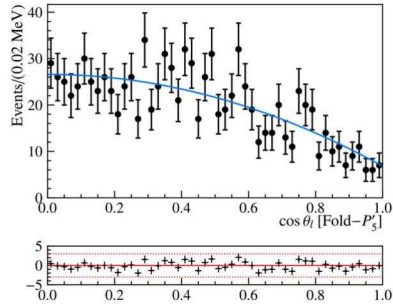
# Workflow

Five maximally independent parts

"Fits look always the same"



# HEP Model Fitting in Python



**HEP**

advanced features,  
simply extendable



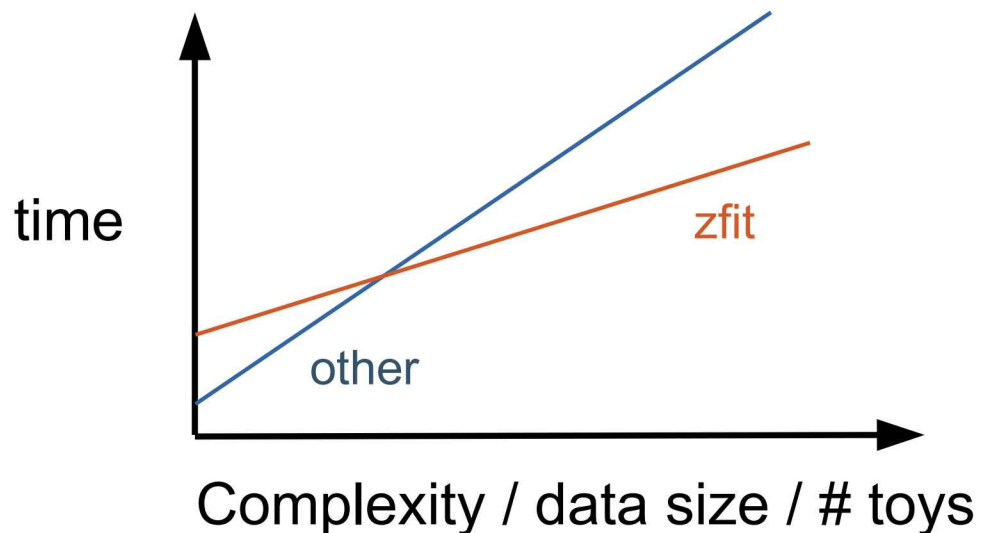
**Scalable**  
large data, complex models

**Pythonic**  NumPy  python™  
integrate into ecosystem, stable API

# Scalable: Performance

*There is no free lunch*

- Initial overhead, flat increase
  - TensorFlow (JAX, ...) backend
  - JIT compiled, CPU or GPU
- Single, simple fit "slow"
    - 0.01 or 1 sec not relevant
    - 1 or 10 hours relevant





# Scalable: Performance



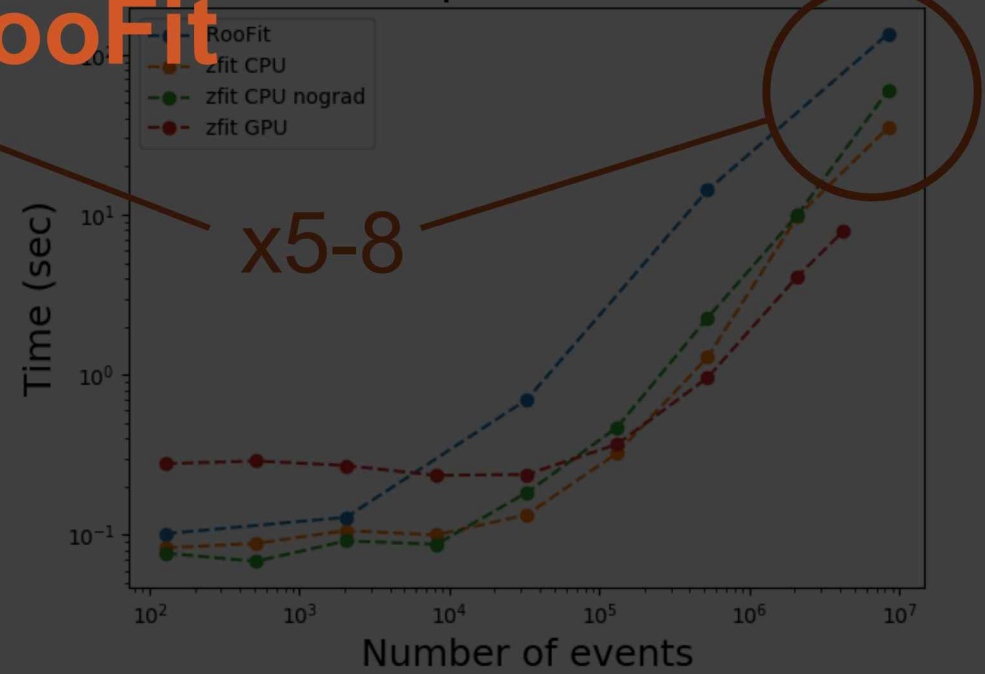
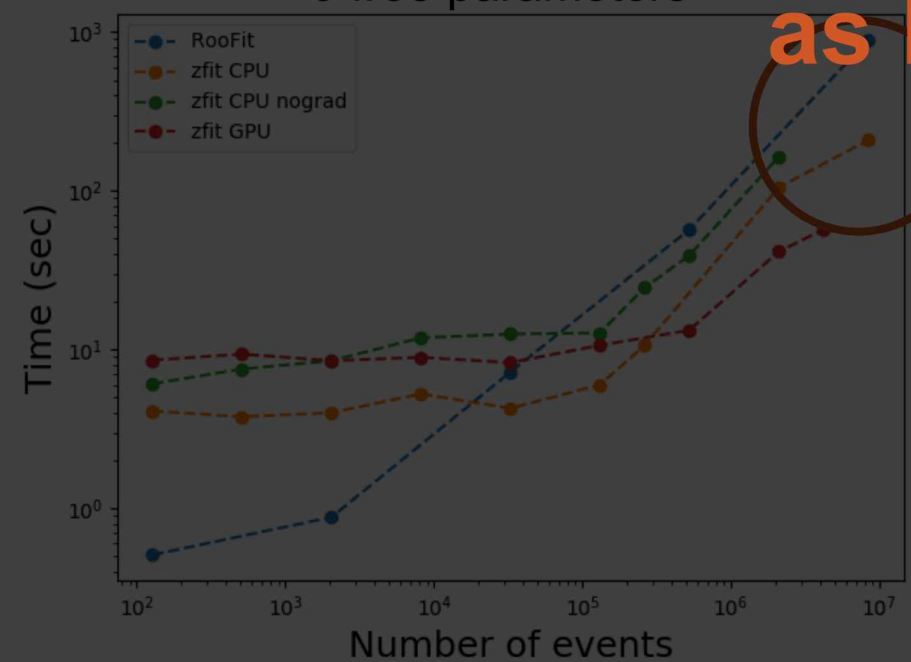
Sum of 9 Gaussians, toy fitting time, 6 core CPU: RooFit vs. zfit

**Same order of magnitude**

**as RooFit**

9 free parameters

2 free parameters



x5-8

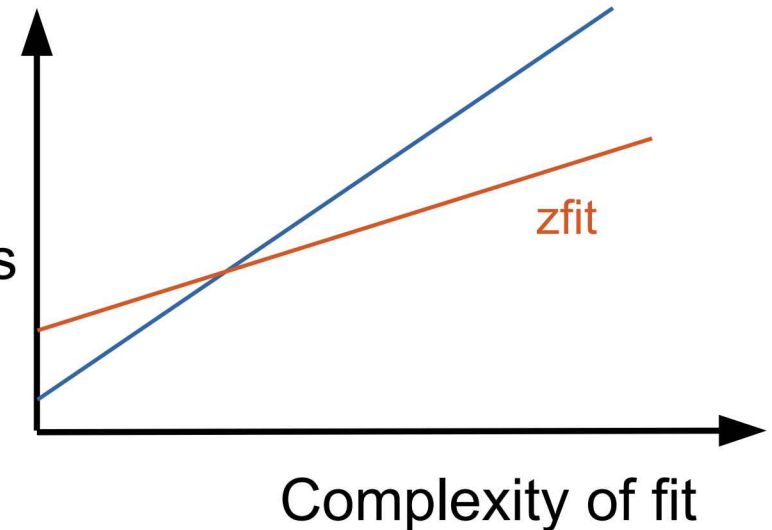
# Scalable: Usability



*Things should not be easy or hard,  
but consistent*

- Code lines
  - 5 or 10: irrelevant
  - 50 or 300: matters

Difficulty /  
# code lines



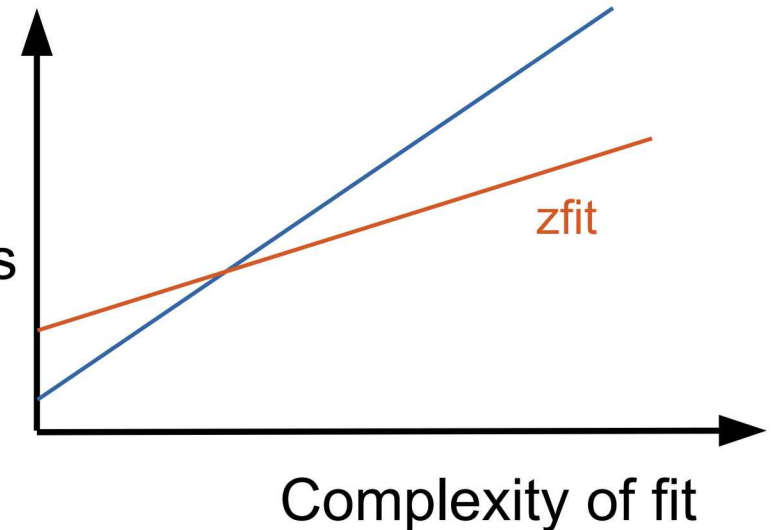
# Scalable: Usability



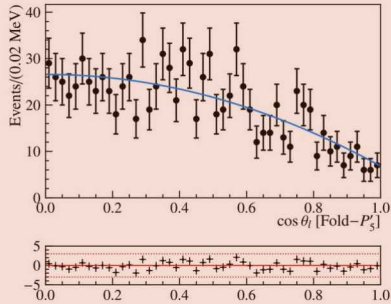
*Things should not be easy or hard,  
but consistent*

- Code lines
  - 5 or 10: irrelevant
  - 50 or 300: matters
- Cover all usecases out of the box is impossible
  - Convenient base classes, allow full control
  - Modular structure; provide all elements (e.g. shapes)

Difficulty /  
# code lines



# HEP Model Fitting in Python



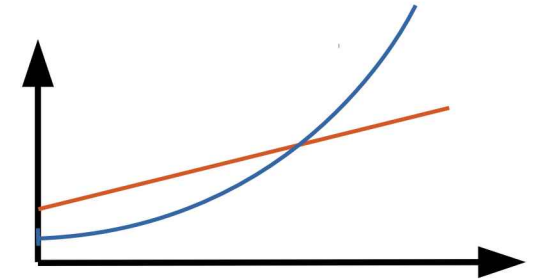
HEP

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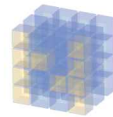


Scalable

large data, complex models



Pythonic



NumPy



python™

integrate into ecosystem, stable API

# Complete fit

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

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

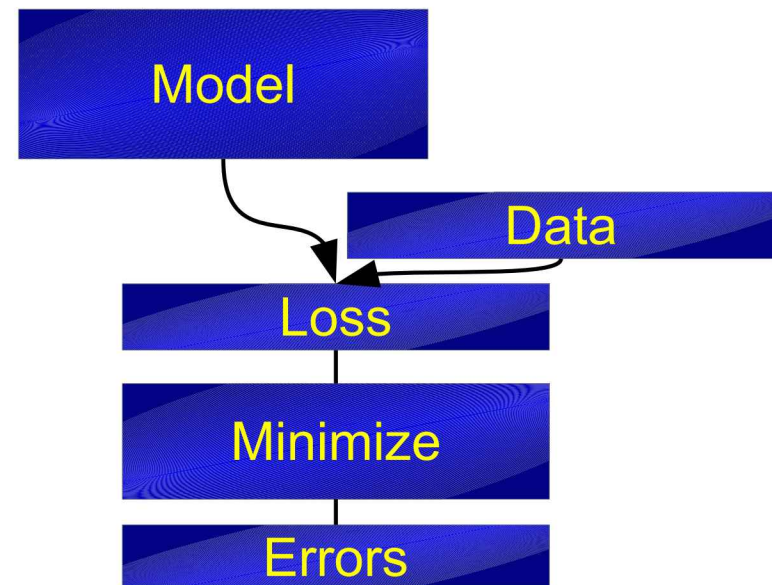
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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

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

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

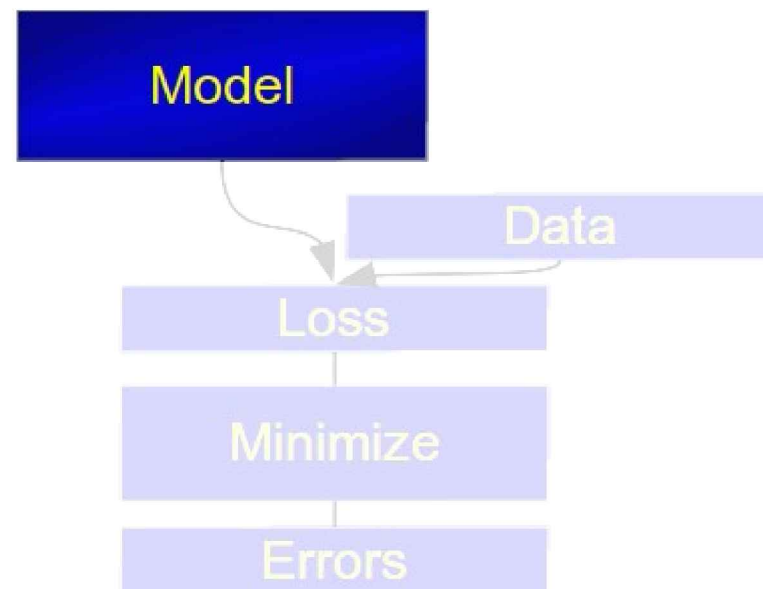
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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

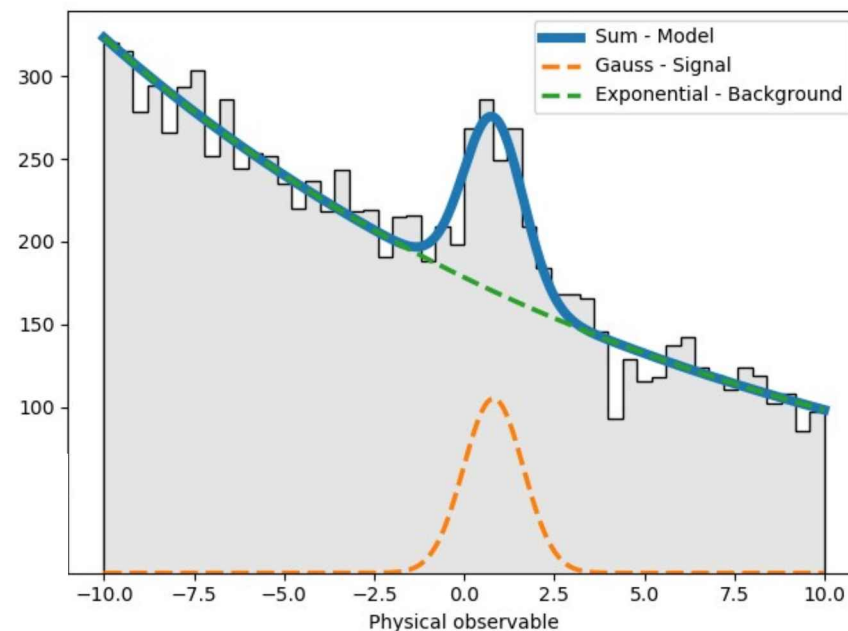
- Sum, Product, (*Convolution*)
- Gauss, (double) Crystalball,...
- Exponential, Polynomials,...

```

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,...



```

lambda = zfit.Parameter("lambda", -0.06, -1, -0.01)
frac = zfit.Parameter("frac", 0, 0, 1)

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



```
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

```
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)
```

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

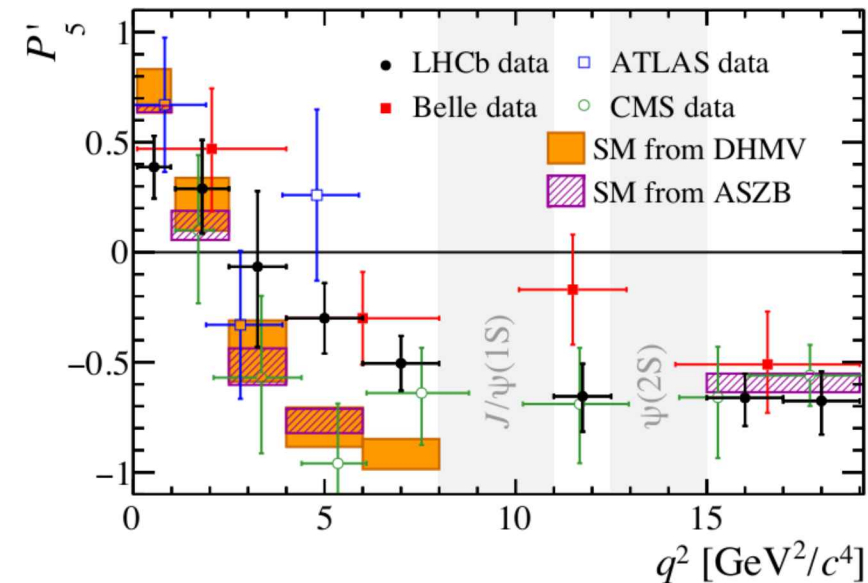
```
integral = custom_pdf.integrate(limits=(-1, 2))
```

```
sample = custom_pdf.sample(n=1000)
```

```
prob = custom_pdf.pdf(sample)
```

} use functionality of model

# $B^0 \rightarrow K^{*0} l^+ l^-$ angular: P5'



P5': optimised observable  
Fit of P5', from [1, 2]

```
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 +
```

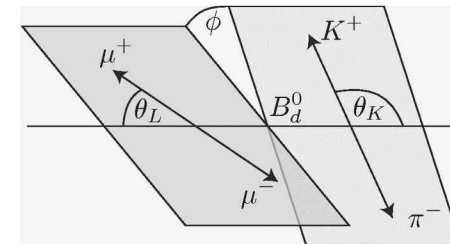
```
           -1.0 * FL * costheta_k * costheta_k * cos2theta_l +
```

```
           (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
```

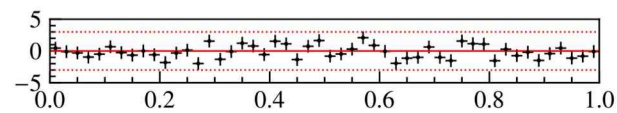
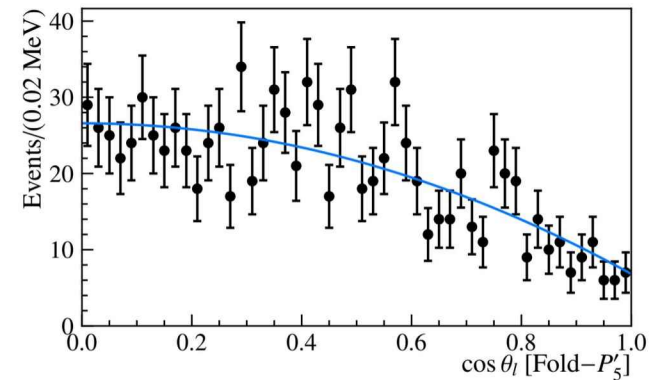
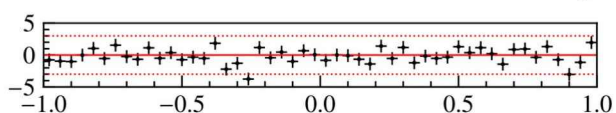
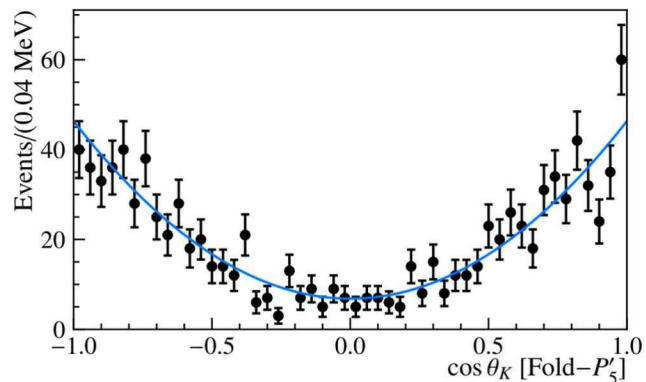
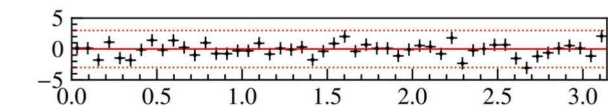
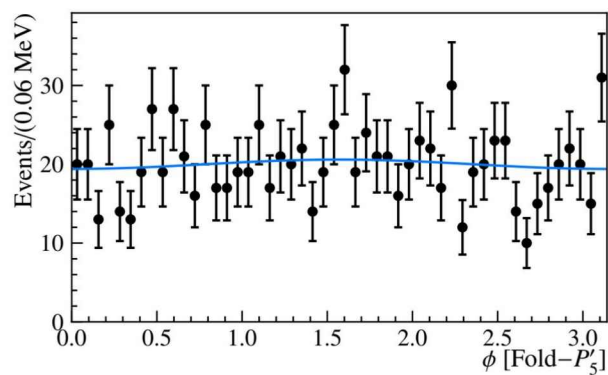


# $B^0 \rightarrow K^{*0} l^+ l^-$ angular: fitted P5'



Projections of three angles

Plot with mplhep, matplotlib



# Complete fit: Data

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

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

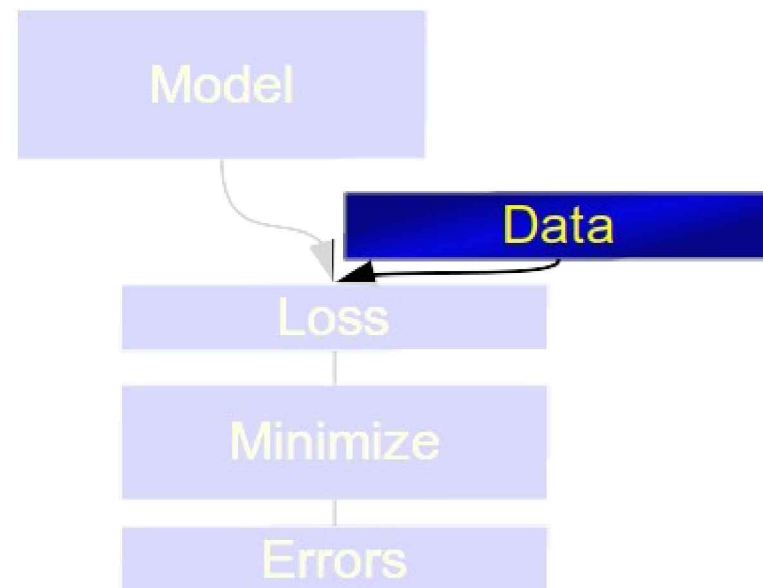
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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
  - Numpy, Pandas, ROOT, ...

Use the HEP/Python ecosystem for preprocessing

- Sampled from a model (toy studies)

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

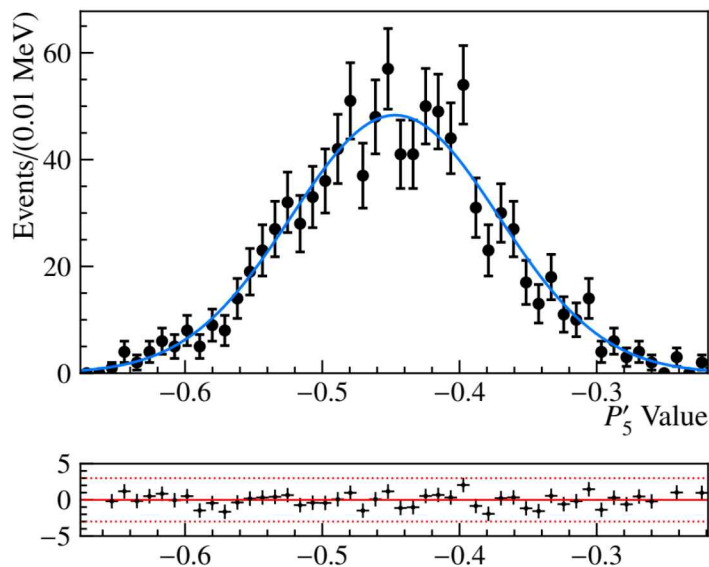


# $B^0 \rightarrow K^{*0} l^+ l^-$ angular: toy study

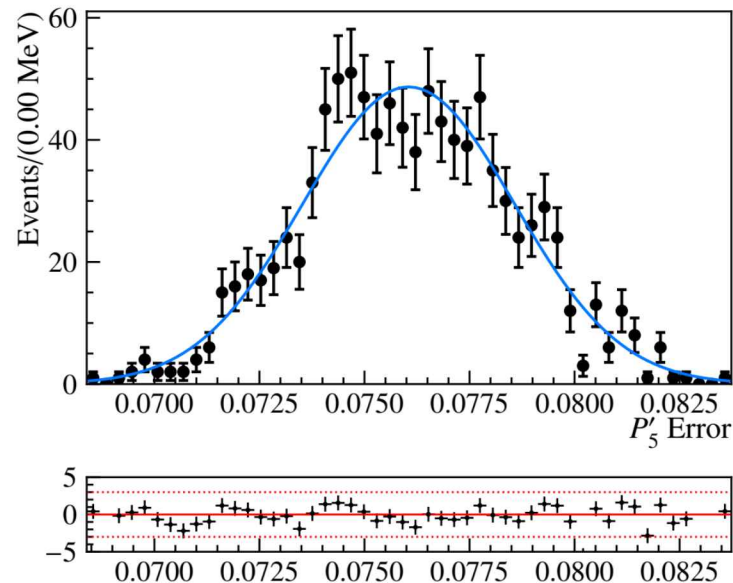


## Result of toy study

### P5' value



### P5' error



# Complete fit: Loss

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

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

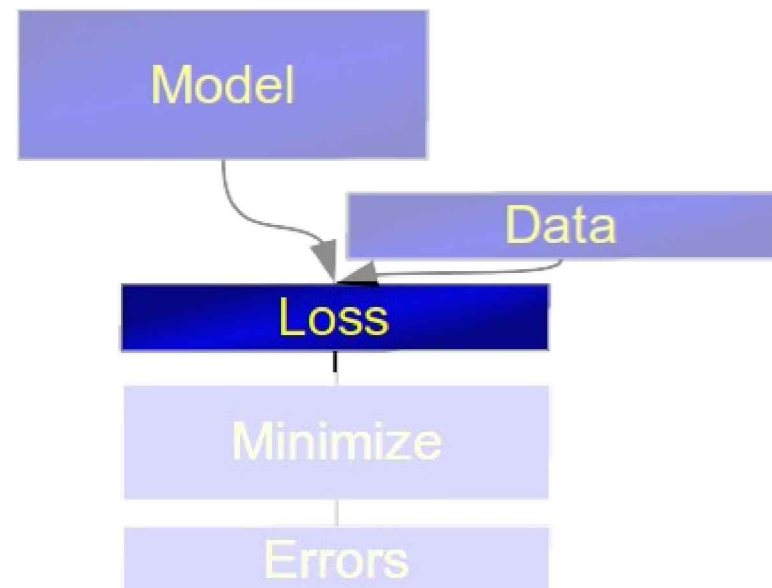
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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



```
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

```
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

Constraints (also arbitrary) are fully supported

# Complete fit: Minimization

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

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

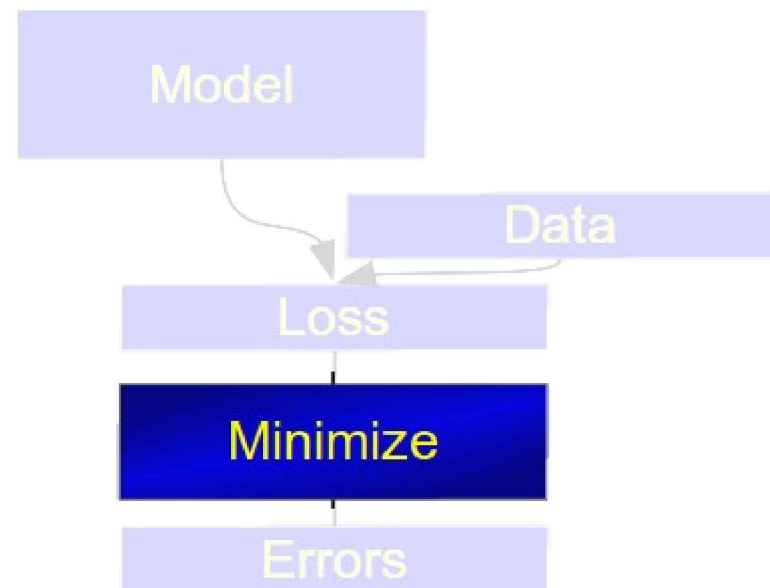
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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



- Many different minimizers available, 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

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

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

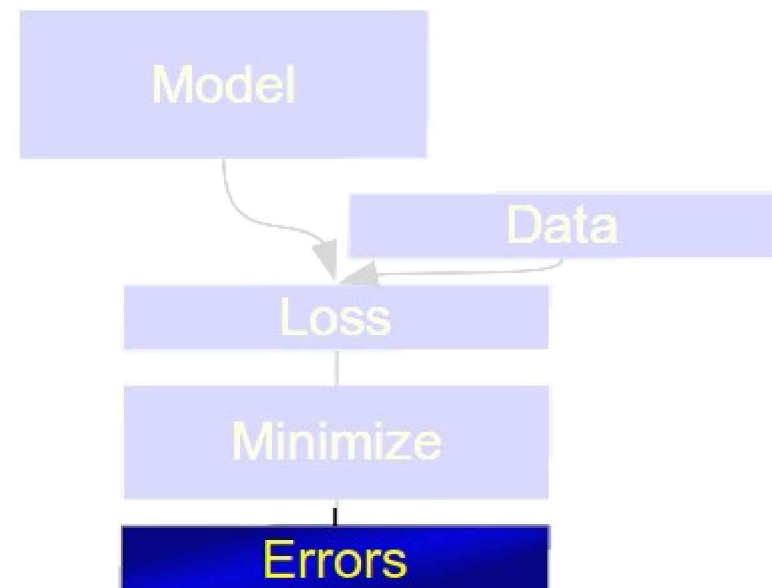
mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.5, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

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()
```





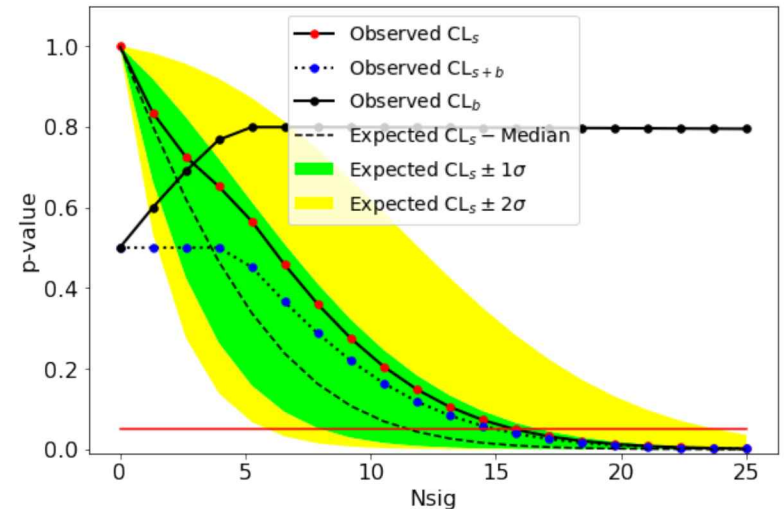
# Back to HEP ecosystem: hepstats



- High level statistics library for hypothesis tests
- Takes model, data, loss from zfit
- sWeights, CI, limits, ...  
asymptotic or toys



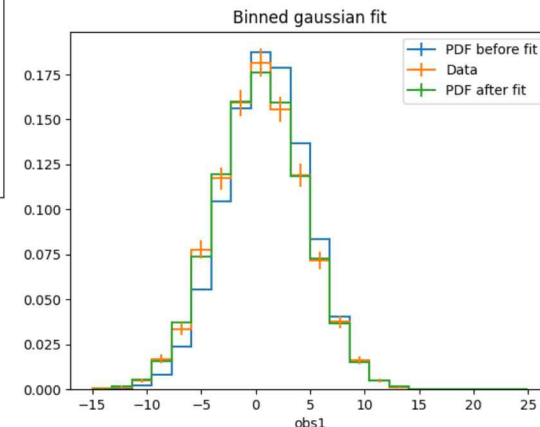
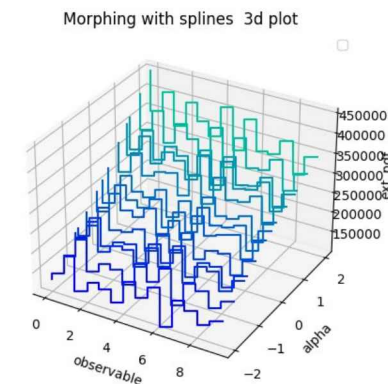
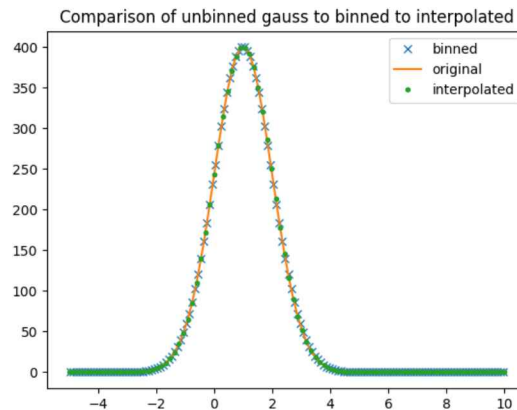
```
calculator = AsymptoticCalculator(loss, minimizer)
poinull = POIarray(Nsig, np.linspace(0.0, 25, 20))
poialt = POI(Nsig, 0)
ul = UpperLimit(calculator, poinull, poialt)
ul.upperlimit(alpha=0.05, CLs=True)
```



# Close future: binned fits

- Integrate with boost\_histogram, hist and mplhep
- Dedicated method "counts" (returns histogram)
- Features (expected):
  - Morphing of templates
  - Systematics of any kind
  - Interpolate (-> unbinned)
  - Irregular binning

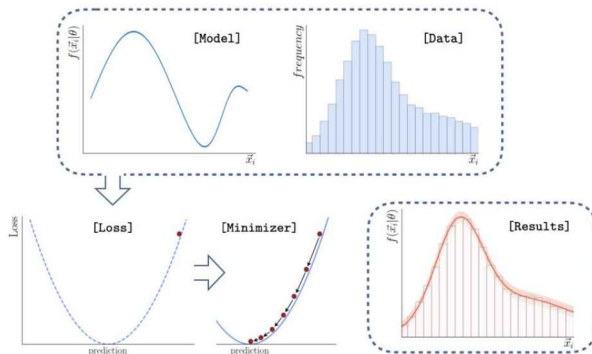
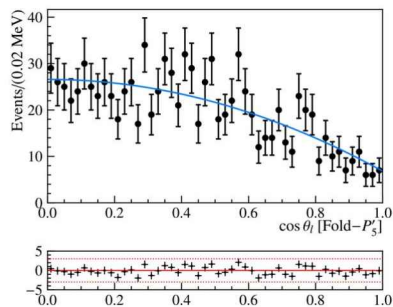
Expected in ~ 1 months:  
Discussion welcome! Ideas? Use-cases?



# Conclusions

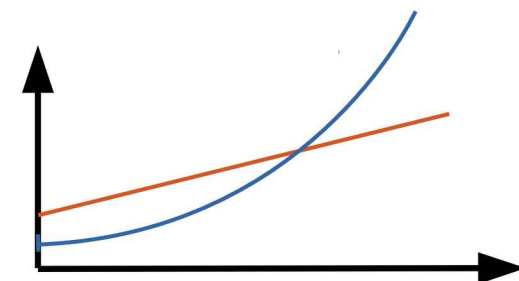
**HEP**

advanced features,  
simply extendable

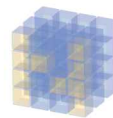


**Scalable**

large data, complex models



**Pythonic**



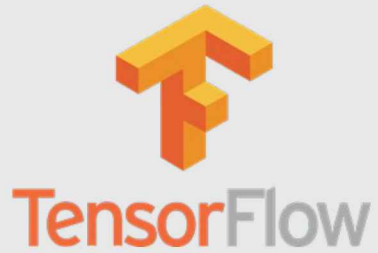
NumPy



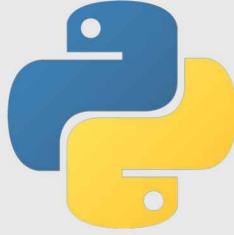
python™

integrate into ecosystem, stable API

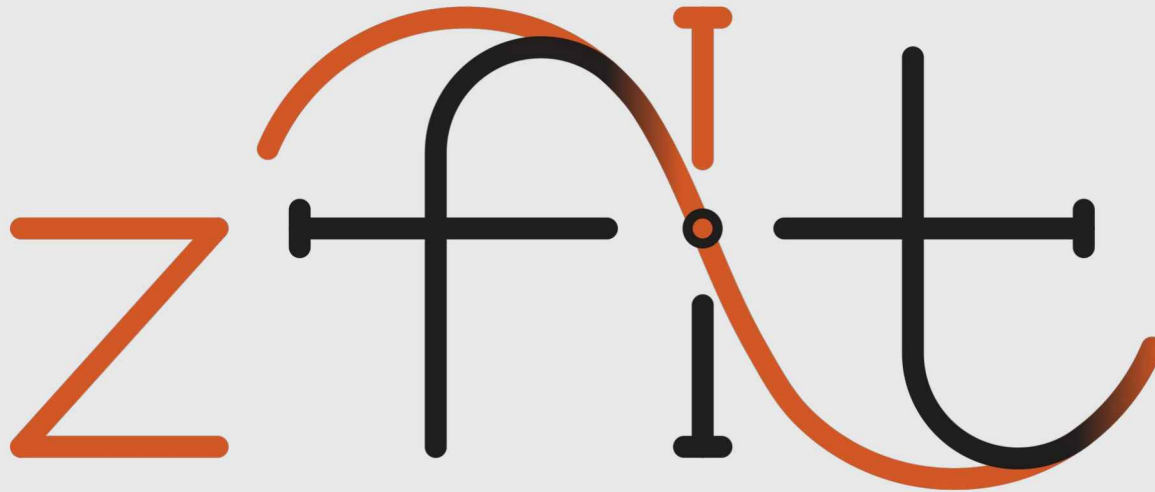
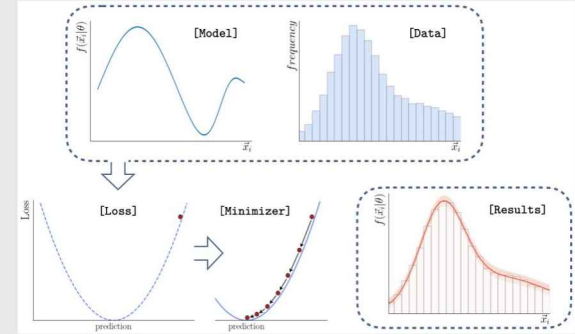
scalable



pythonic



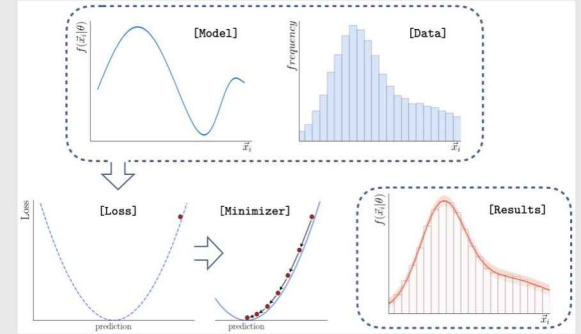
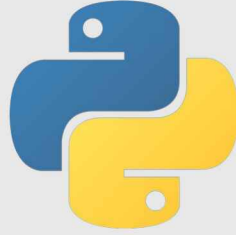
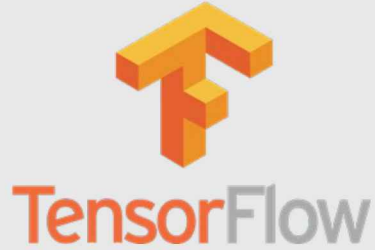
fitting



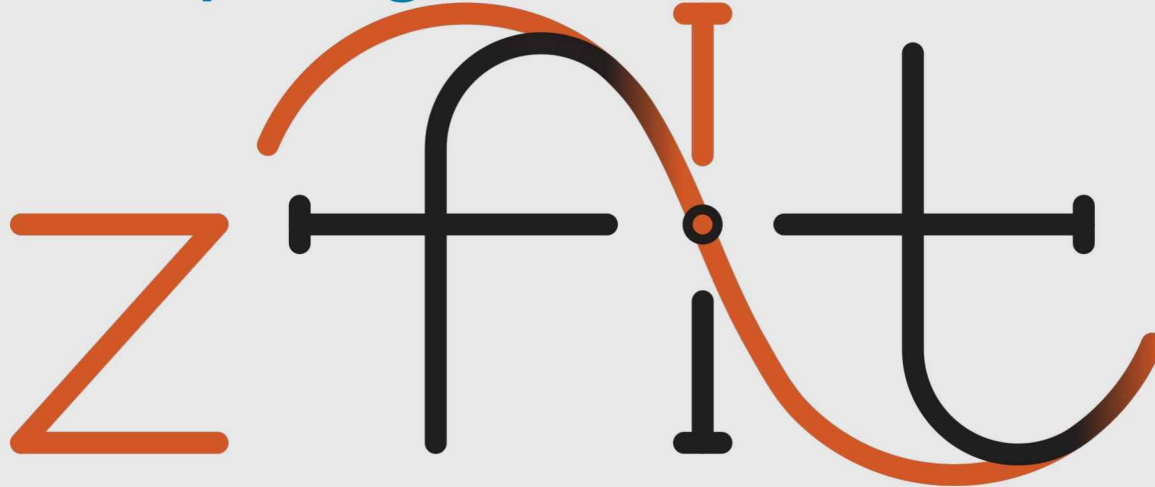
scalable

pythonic

fitting



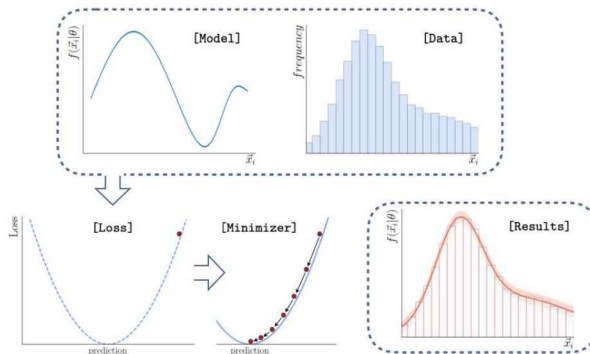
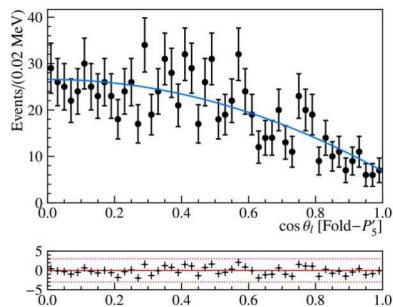
Try it out: <https://github.com/zfit/zfit-tutorials>



# Conclusions

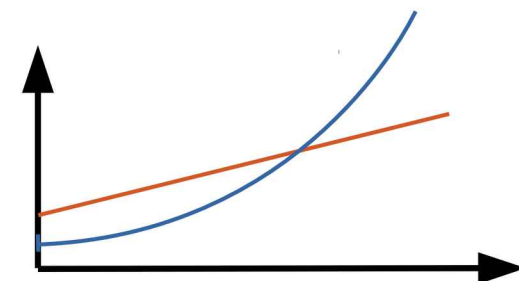
**HEP**

advanced features,  
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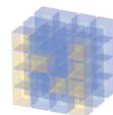


**Scalable**

large data, complex models



**Pythonic**



NumPy



python™

integrate into ecosystem, stable API



- LHCb collision: <https://physicsworld.com/wp-content/uploads/2018/08/LHCb-collision.png>

# Backup Slides

<https://zfit.github.io/zfit/>

zfit@GitHub



Gitter channel



zfit@physik.uzh.ch

**Join the discussion!**

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

# Backend & TensorFlow

# Backend: tracing and autograd



Tracing

*execute Python once, remember (algebraic) computation*

Autograd

*"analytic" gradient of function*



Recent rise of big data industry created libraries that support this

Includes GPU support, optimizations, caching,...





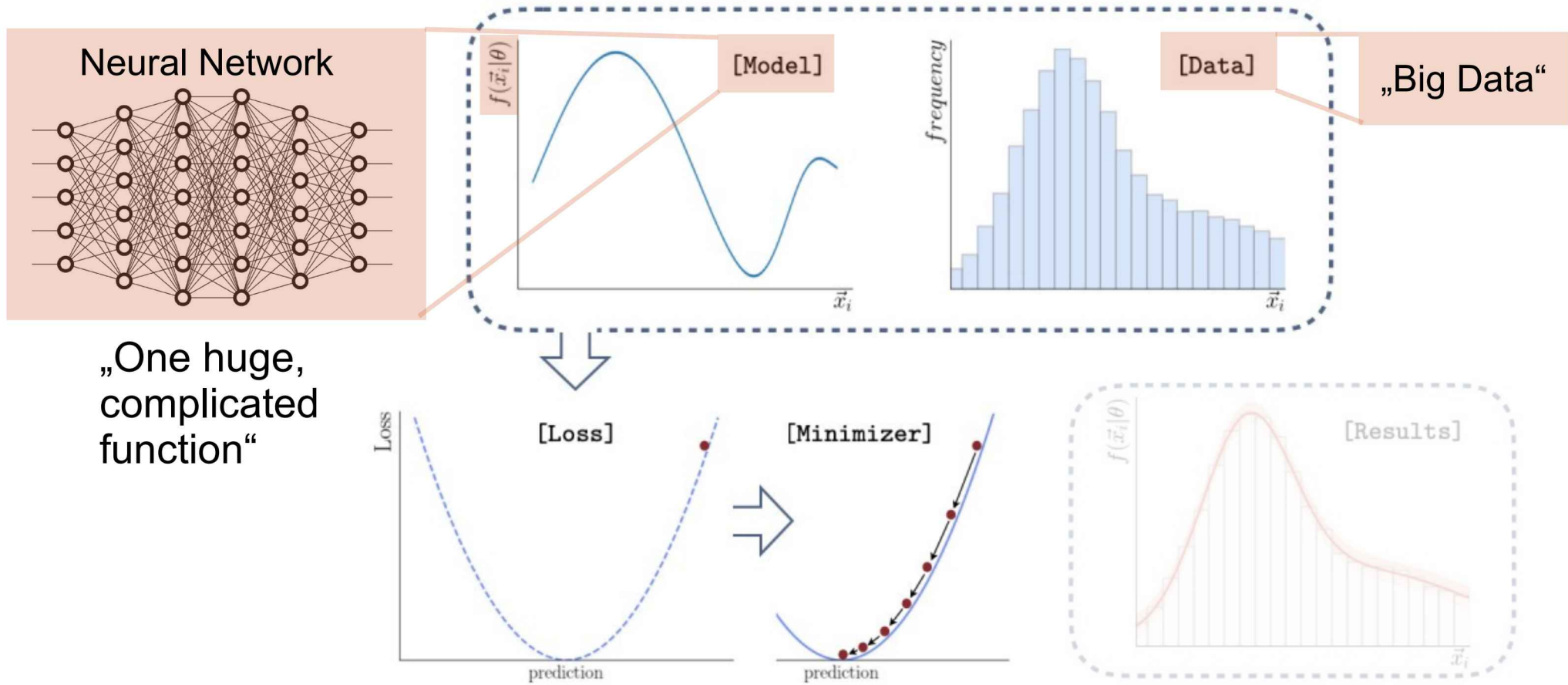
build *the* stable model fitting ecosystem for HEP

- Integrate into HEP ecosystem
  - functionality limited; stable API
- Technical requirements
  - performance; maintainability
- HEP requirements
  - advanced features; simply extendable code


# Deep Learning

lessons for model fitting

# Deep Learning



# Main backend: TensorFlow

- By Google, highly popular (130k★, 4<sup>th</sup> on )
- Used in multiple physics libraries and analyses




# Main backend: TensorFlow



- By Google, highly popular (150k★, 4<sup>th</sup> on )



# Main backend: TensorFlow

- By Google, highly popular (130k★, 4<sup>th</sup> on )
  - Used in multiple physics libraries and analyses
  - Consists of "two parts":
    - High level API for building neural networks (*NOT used!*)
    - **Low level API** with Numpy-style syntax  
`tf.sqrt`, `tf.random.uniform`,...
  - Two modes:
    - "numpy"-like (full Python flexibility)
    - "compiled" (very performant)
- } GPU/Multi CPU support



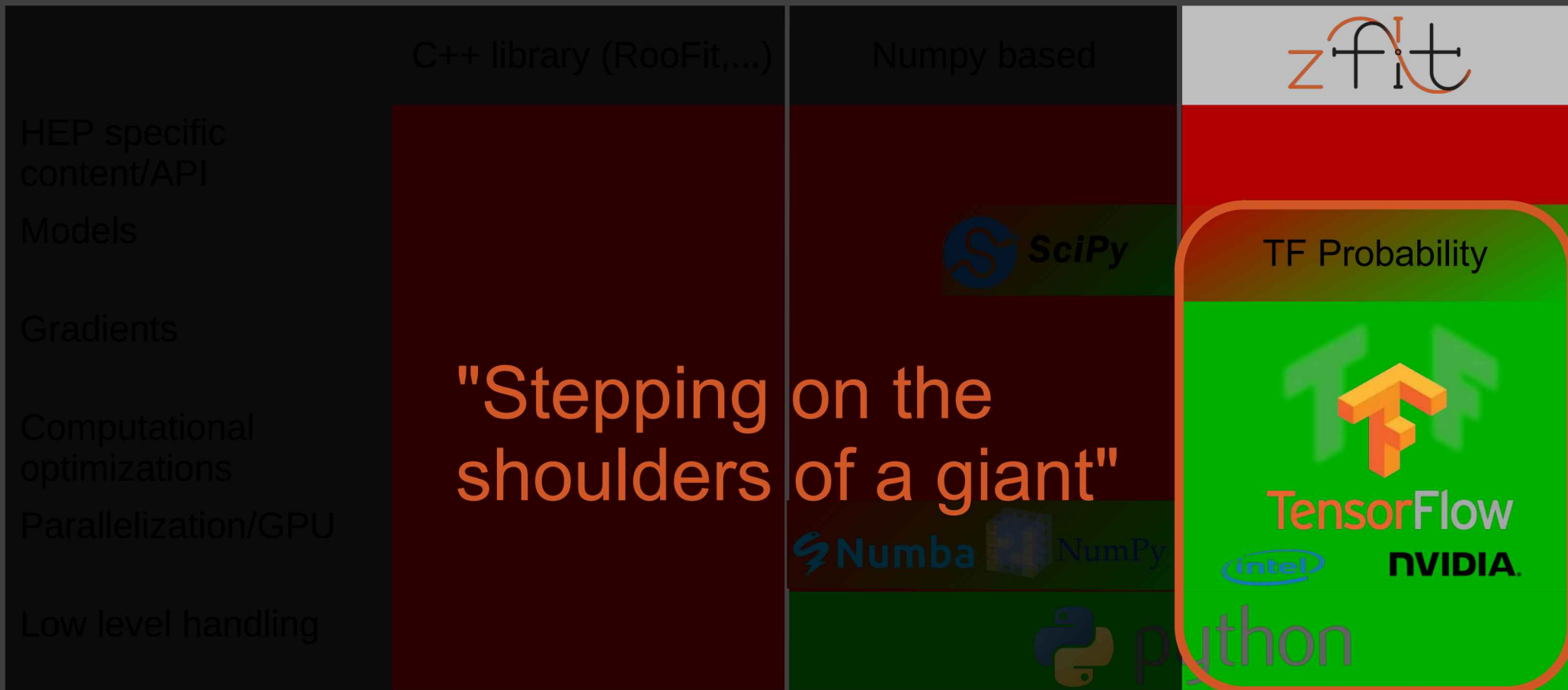


# Delegating the workload



	C++ library (RooFit,...)	Numpy based	zfit	
HEP specific content/API				
Models				TF Probability
Gradients				
Computational optimizations				
Parallelization/GPU				
Low level handling				

# Delegating the workload



# Delegating the workload



*Can* we express model fitting as  
static graphs?

***Yes!***

- 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

*... 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 <sup>nd</sup> derivative algorithm	Hesse, profiling
Deep Learning	Combine many, trivial functions	Many, small Batches	<i>Anything!</i> (GANs, RL,...)	Local (!) min, 1 <sup>th</sup> derivative, many steps	None
Conclusion					



# Deep Learning vs. Model Fitting



But...

what *is* a Deep Learning library?

Similarity`	Complicated Models	Large Data	Composed loss.	Minimization	Results and uncertainties
HEP	Non-trivial functions	Whole Dataset	simultaneous, constraints	Global min, 2 <sup>nd</sup> derivative algorithm	Hesse, profiling
Deep Learning	Combine many, trivial functions	Many, small Batches	<i>Anything!</i> (GANs, RL,...)	Local (!) min, 1 <sup>th</sup> derivative, many steps	None
Conclusion	No real impact	Optimizations for OOM calculations	HEP trivial special case	Optimizers Free „analytic“ derivatives!	No support, but simple

# Deep Learning vs. Model Fitting



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# Deep Learning vs. Model Fitting



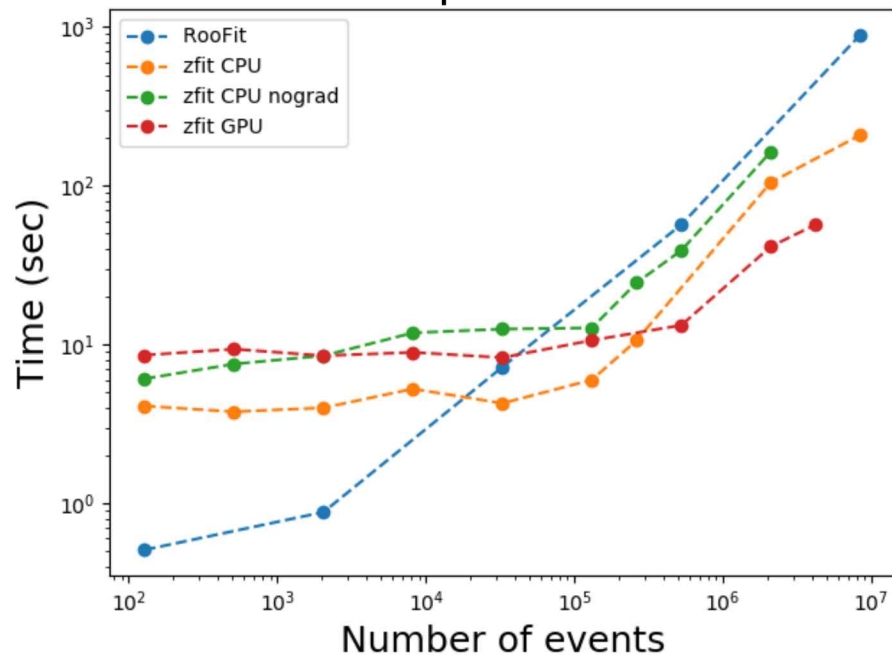
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Modern, high performance computing

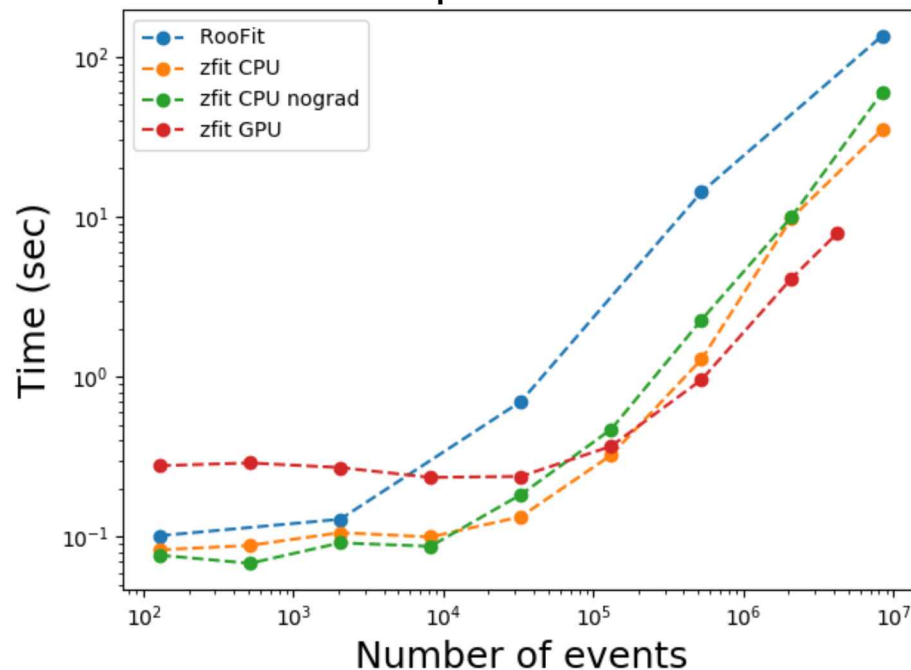
# Scalability: Performance

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

9 free parameters



2 free parameters



# Amplitude

# Example amplitude

```

RESONANCES = [('rho(770)', ('pi-', 'pi0'), bw_amplitude),
              ('K(2)*(1430)0', ('K+', 'pi-'), bw_amplitude),
              ('K(0)*(1430)+', ('K+', 'pi0'), bw_amplitude),
              ('K*(892)+', ('K+', 'pi0'), bw_amplitude),
              ('K(0)*(1430)0', ('K+', 'pi-'), bw_amplitude),
              ('K*(892)0', ('K+', 'pi-'), bw_amplitude)]

COEFFS = {...}

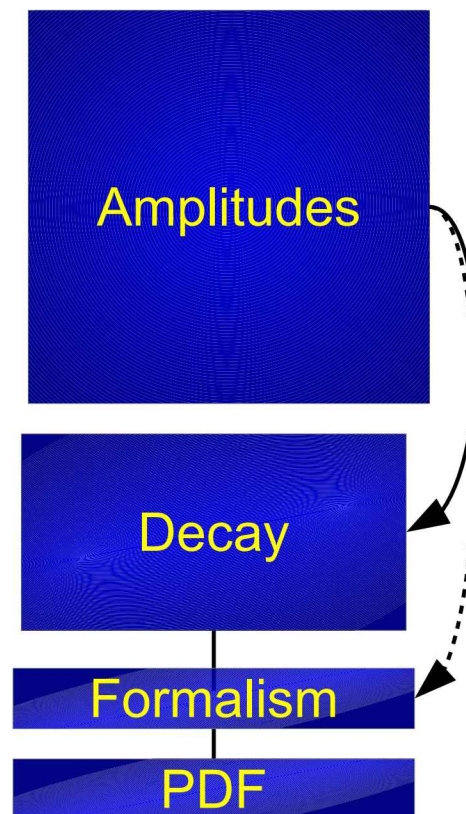
D2Kpipi0 = Decay('D0', ['K+', 'pi-', 'pi0'])

for res, children, amp in RESONANCES:
    D2Kpipi0.add_amplitude(res, children, amp, COEFFS[res])

formalism = ThreeBodyDalitzFormalism("Zemach B Frame")

pdf = D2Kpipi0.create_pdf(name="D2Kpipi0", formalism=formalism)

```



# Angular toys



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



## Sensitivity study

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

```
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:  
        ...
```

## Sensitivity study

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

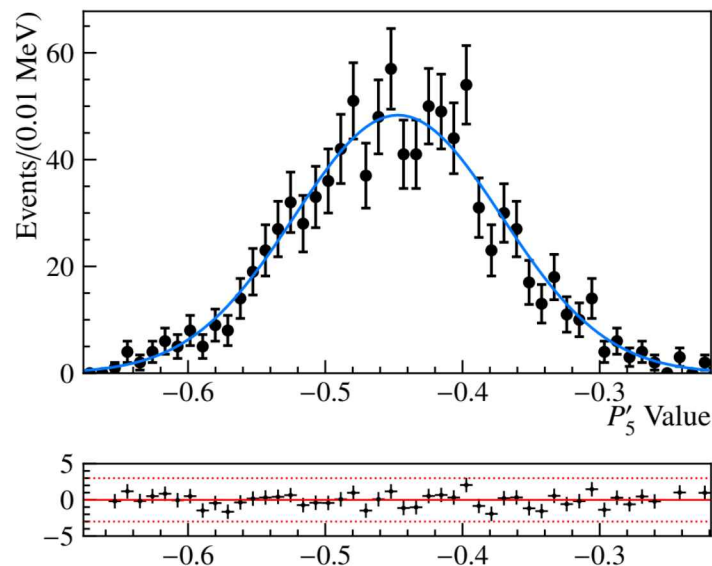
```
for i in range(ntoys):  
  
    # set initial sampling values  
    for param in params:  
        param.set_value(...)  
  
    sampler.resample()  
  
    # set random initial values  
    for param in params:  
        param.set_value(...)  
  
    result = minimizer.minimize(nll)  
  
    if result.converged:  
        ...
```

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

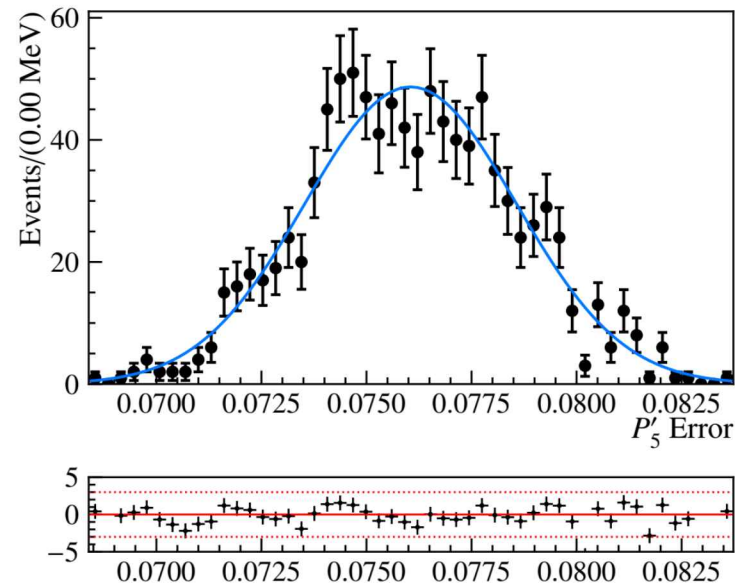


## Result of toy study

### P5' value



### P5' error



# Extending with a mass shape

```
# 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,  
|                             alphas=a0, nls=n0, alphas=a1, nrs=n1)
```

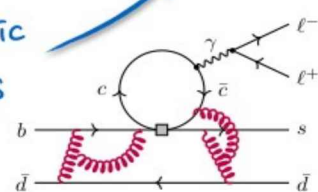
```
pdf = massPDF * angularPDF
```

Build model

# $B^0 \rightarrow K^{*0} \mu^+ \mu^-$ full amplitude

- Measuring the full differential decay ratio [1, 2]

- Angular,  $q^2$  distribution  $\frac{d^4\Gamma}{dq^2 d\cos\theta_\ell d\cos\theta_K d\phi} \propto \sum J_i(q^2) f(\cos\theta_\ell, \cos\theta_K, \phi)$
- Branching ratio information

$$\mathcal{A}_\lambda^{L,R} = \mathcal{N}_\lambda \left\{ \underbrace{[(C_9 \pm C'_9) \mp (C_{10} \pm C'_{10})]}_{\text{Wilson coeff.}} \underbrace{[\mathcal{F}_\lambda(q^2)]}_{\text{Form Factors}} + \frac{2m_b M_B}{q^2} \left[ \underbrace{(C_7 \pm C'_7)}_{\text{Wilson coeff.}} \underbrace{[\mathcal{F}_\lambda^T(q^2)]}_{\text{Form Factors}} - 16\pi^2 \frac{M_B}{m_b} \underbrace{[\mathcal{H}_\lambda(q^2)]}_{\text{non-local hadronic matrix elements "charm-loop"}} \right] \right\}$$


# 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,...)



- *Limited customization and extendibility*
- *Sub-optimal scalability for ever larger datasets and modern computing infrastructure*
- **Isolated, aging ecosystem,** no cutting-edge software
- **Not Python native**
  - *Memory allocation errors*
  - *Arbitrary C++ limitations*
  - *No real integration into the Python ecosystem*

Probfitt, TensorProb,...

- Lack **generality** and extensibility
- “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

## Scipy, Imfit, 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, ...

# TFA: approach & differences

- Build «optimized» TensorFlow
  - accept-reject as `tf.while_loop`, Dataset input,...
- ...and hide the tedious, unambiguous parts
  - automatic normalization, Tensor cache, ...
- Well defined structures, e.g.
  - String name order (like columns) in PDFs, data, limits,...
  - $\text{pdf}(„x“)$  \*  $\text{pdf}(„y“)$   $\Rightarrow$   $\text{pdf}(„x“, „y“)$ 
    - 1-dim      1-dim      2-dim
  - Local/recursive dependency resolution of Parameters

# Zfit related packages

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



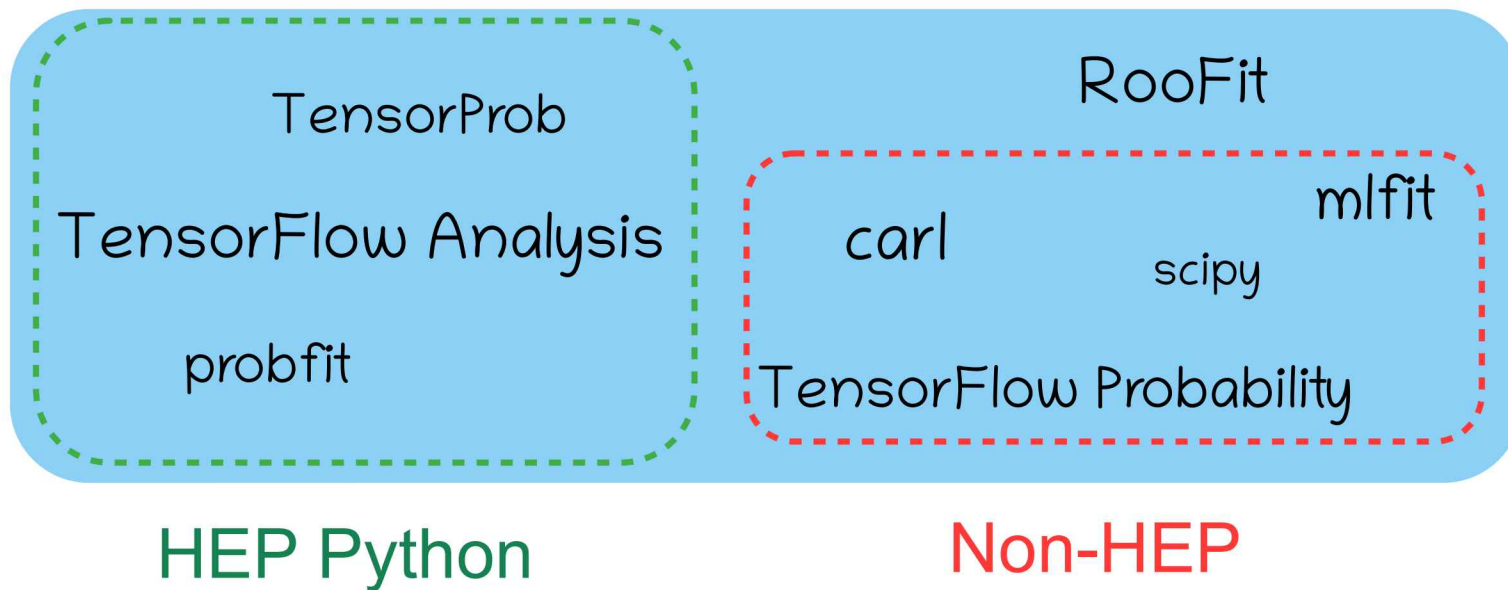
- zfit: stable core
  - Unbinned fits, binned WIP
  - n-dim models with integral, pdf, sample
- zfit-physics: HEP specific content
  - BreitWigner, DoubleCB,...
  - Faster development, more content
  - Ideal for contributions
    - Auto testing of new pdfs/func
    - Contribution guidelines

## build stable model fitting ecosystem for HEP

- **Integrate into HEP ecosystem**
  - functionality limited; stable API
- **Technical requirements**
  - performance; maintainability
- **Analysis requirements**
  - advanced features; simply extendable code

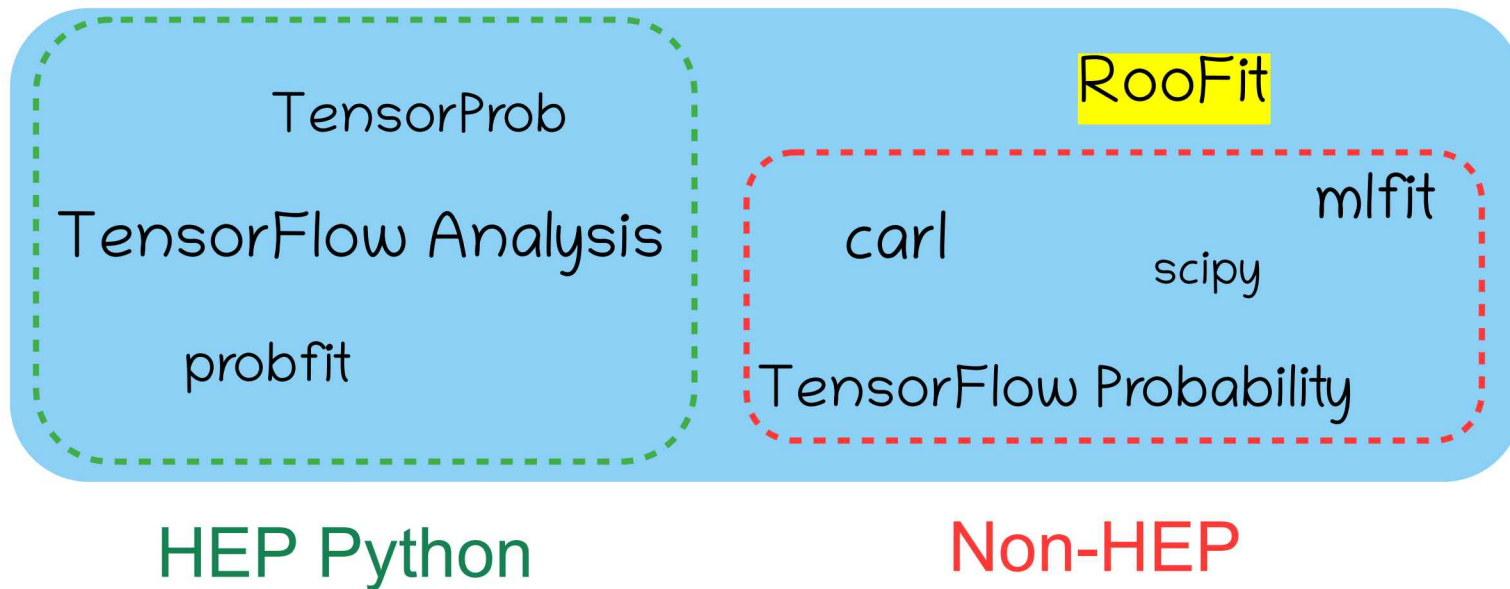
# Fitting in Python

A lot of projects are around

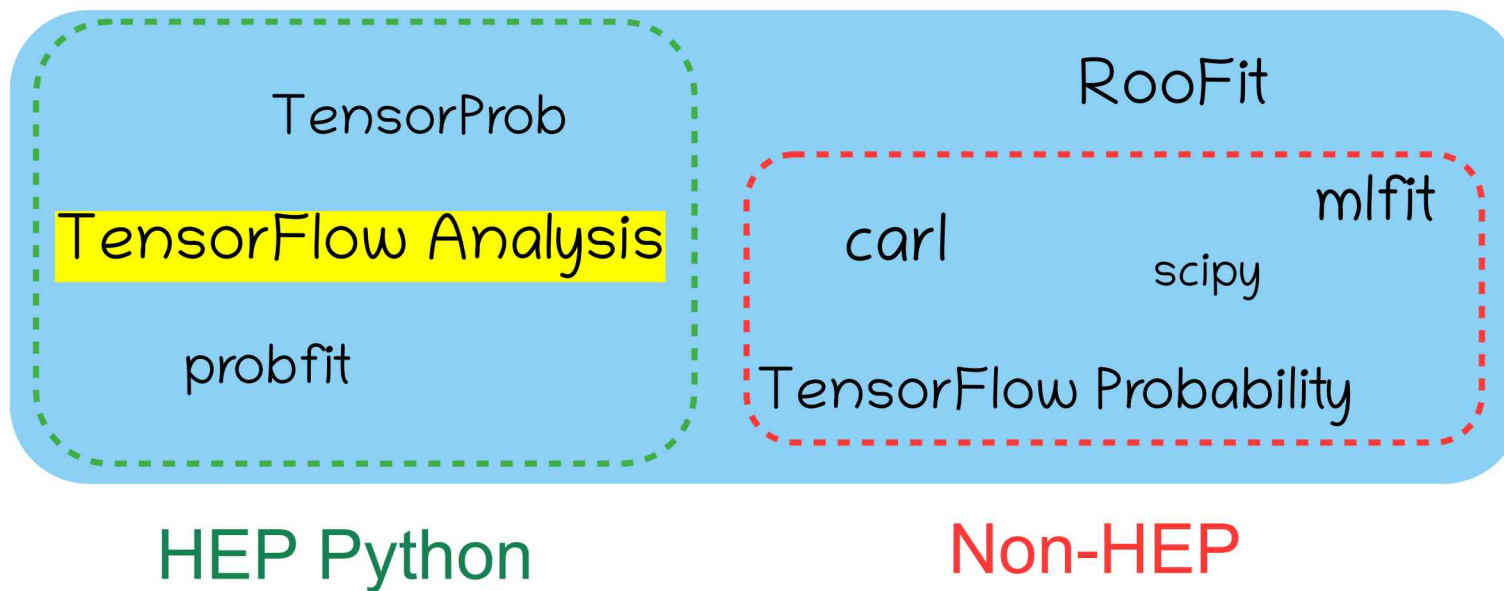


# Fitting in Python

A lot of projects are around



A lot of projects are around



# Fitting in Python



A lot of projects are around!

- RooFit
- ~~HEP Python fitting projects~~
- ~~Non-HEP~~

A lot of projects are around

- RooFit
- ~~HEP Python~~
- ~~Non-HEP~~

No optimised model fitting library for HEP  
that is well integrated into Python

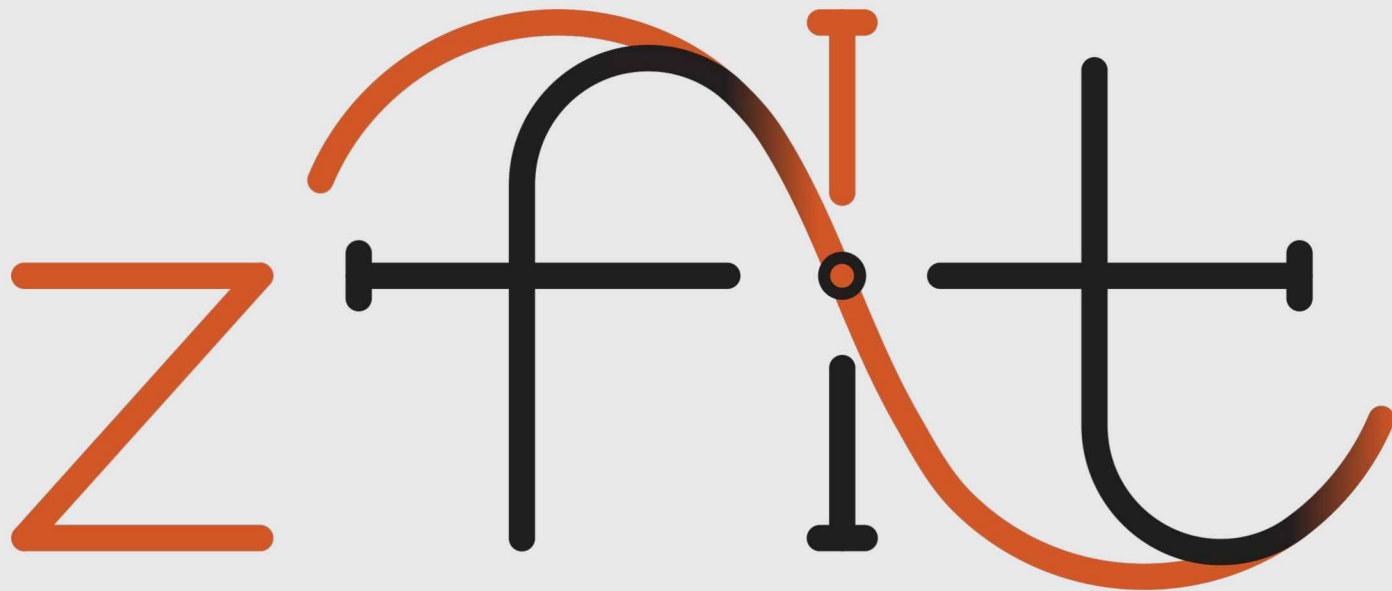


A lot of projects are around

- RooFit
- ~~HEP Python~~
- ~~Non-HEP~~

No optimised model fitting library for HEP  
that is well integrated into Python

... but a lot to learn and build from!



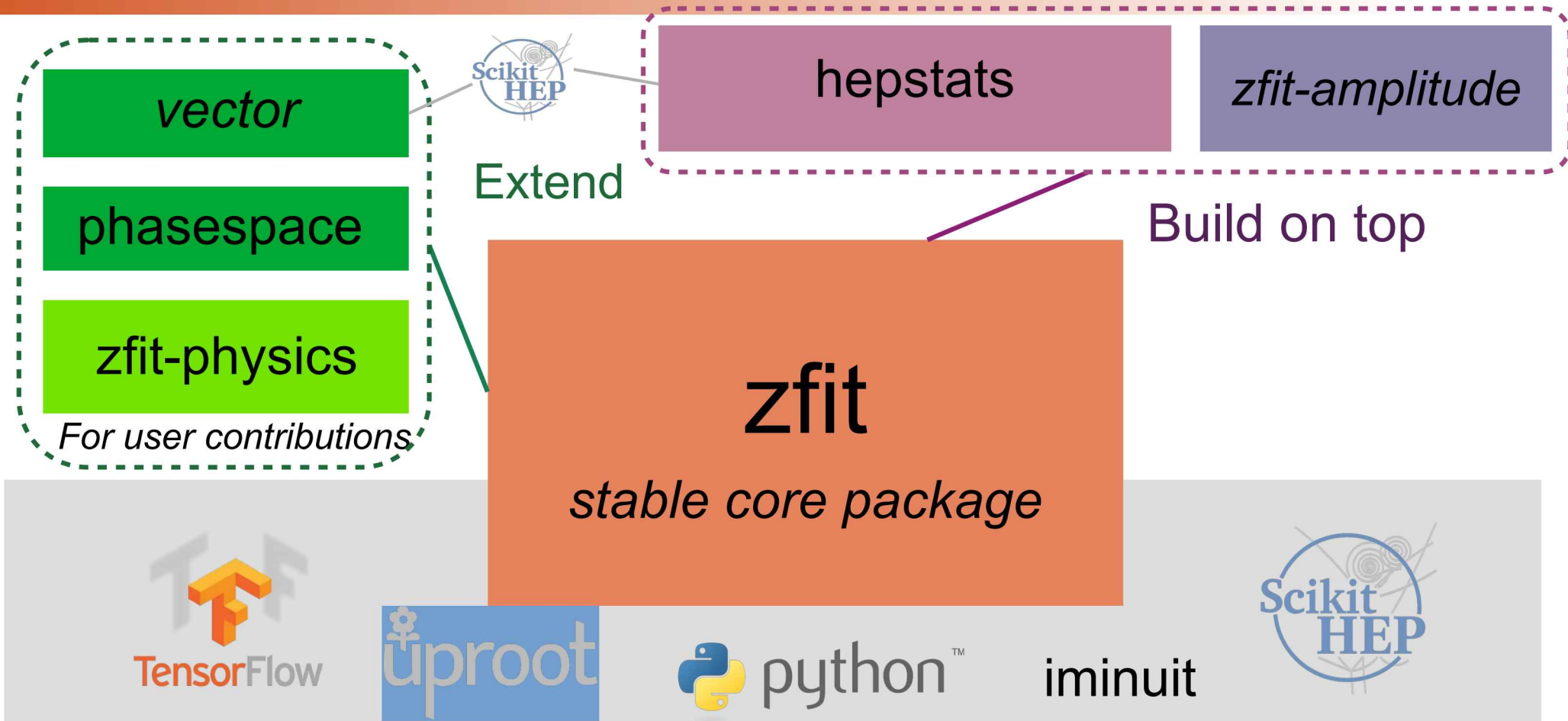
scalable pythonic fitting

build *the* stable model fitting ecosystem for HEP  
...the time has come

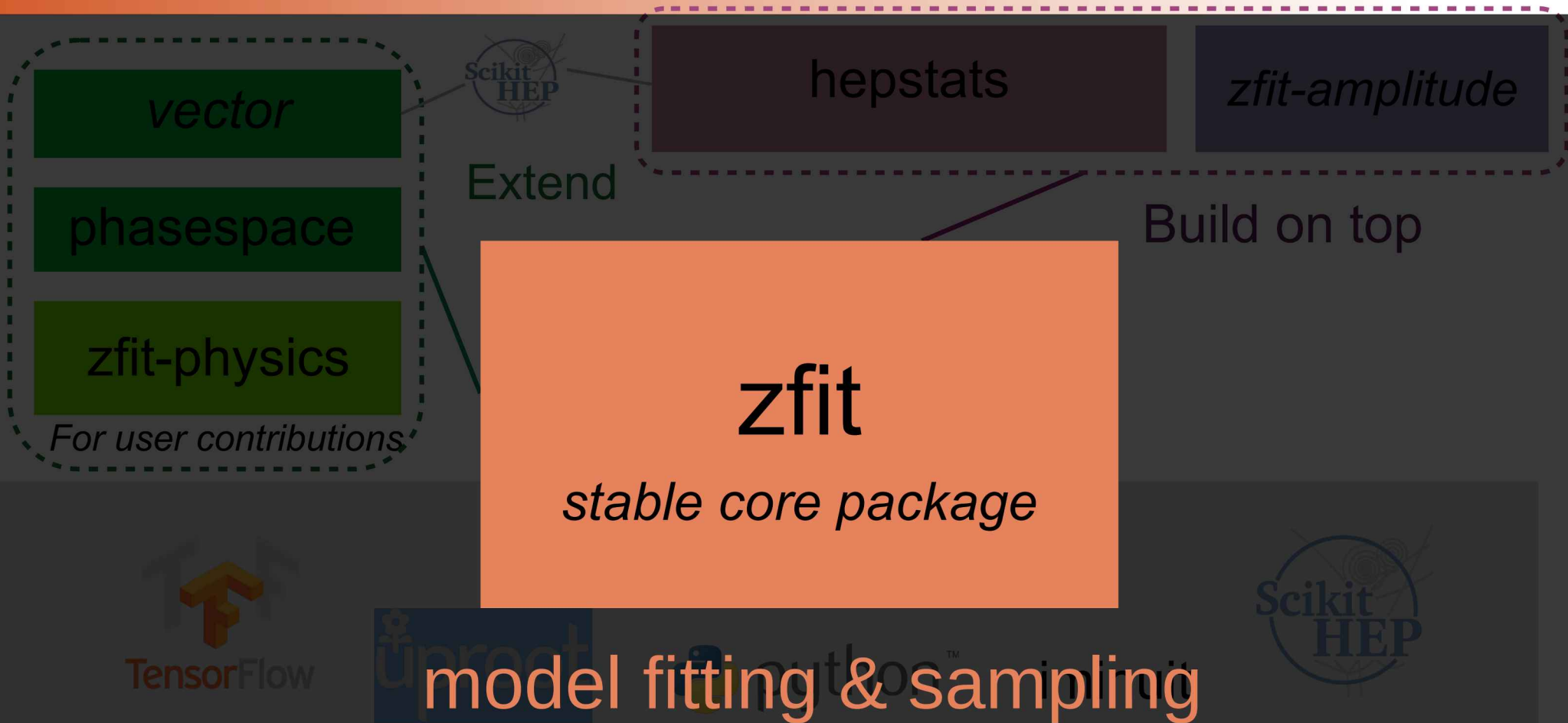
build *the* stable model fitting ecosystem for HEP

- Integrate into HEP ecosystem  
functionality limited; stable API
- Technical requirements  
performance; maintainability
- Analysis requirements  
advanced features; simply extendable code

# Ecosystem



# Ecosystem



## 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

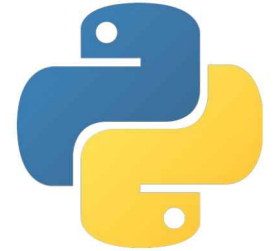
**Many discussions with community  
to avoid splitting/duplication**



# 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



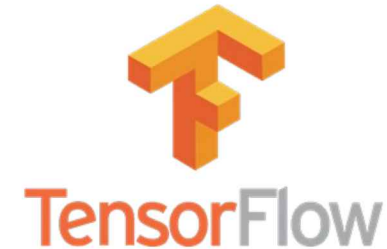
- TensorFlow **hidden** backend, uses graphs
  - numpy-like syntax
  - parallelization on CPU/GPU, analytic gradient,...
- Writing functions simple for users *and* developers
  - No Cython, MPI, CUDA,... for *state-of-the-art performance*
  - No low-level maintenance required!
- Used in multiple physics libraries and analyses



# 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



```
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)
```

=> use all of zfit functionality like minimizers

up to pure  
TensorFlow



# Model building

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

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

} parameters

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

} models

# Simultaneous fit

```
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

```
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