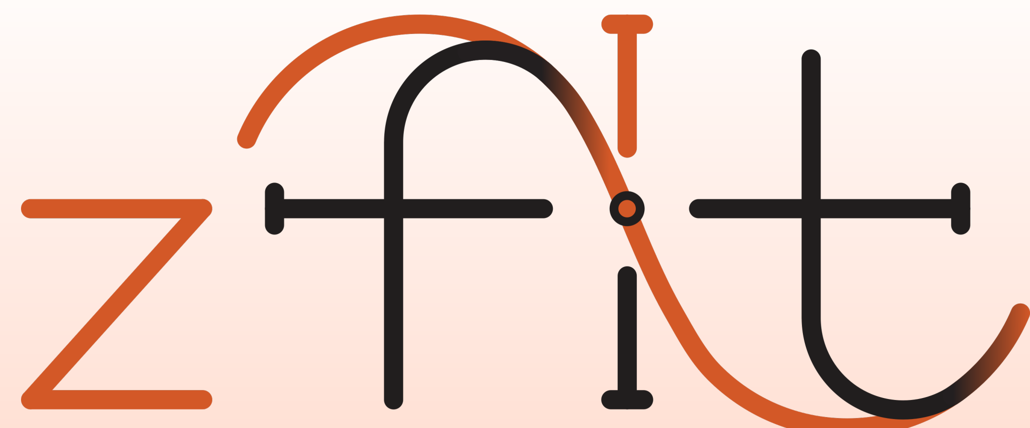
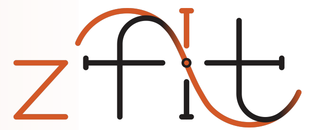


scalable pythonic fitting

Jonas Eschle on behalf of zfit
jonas.eschle@cern.ch

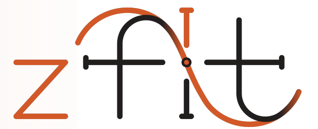
HEP Model Fitting in Python

HEP Model Fitting in Python



- Scalable: large data, complex models
- Pythonic: use Python ecosystem/language
- HEP specific functionality

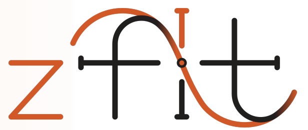
Fitting in Python



A lot of projects are around!

- RooFit
- HEP Python fitting projects
- Non-HEP

Fitting in Python



A lot of projects are around!

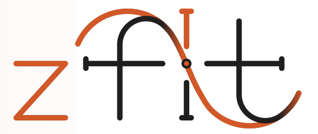
- ~~RooFit~~
- ~~HEP Python fitting projects~~
- ~~Non-HEP~~

No feasible Python model fitting library for HEP

… but a lot to learn and build from!

zfit

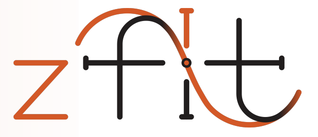
zfit: the project



build *the* stable model fitting ecosystem for HEP

...the time has come

- Functionality limited to model fitting & sampling
- Use power & knowledge of existing libraries
- Build fresh from scratch
- Community invokation



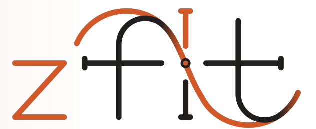
API & workflow definition

Computational backend

(reference) implementation

API & Workflow

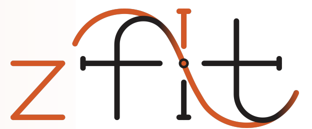
API & Workflow: why



- High level libraries (statistics packages, amplitude fitters,...)
  - „code against an interface, not an implementation“
- Replace each component
  - Allow other libraries to implement custom parts
  - Provide reference implementation for all parts

Allows ecosystem to grow "by itself"

Workflow



Five maximally independent parts

Well defined API implemented as interfaces

[Model]

$f(\vec{x}_i|\theta)$

$\vec{x}_i$

[Data]

frequency

$\vec{x}_i$

[Loss]

Loss

prediction

[Minimizer]

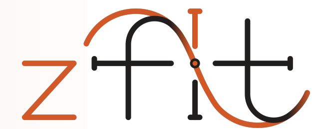
prediction

[Results]

$f(\vec{x}_i|\theta)$

$\vec{x}_i$

Workflow



Five maximally independent parts

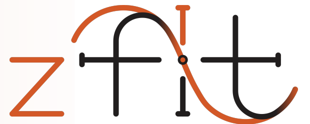
Well defined API implemented as interfaces

Example:
Library as "loss builder"

[Model] [Data] [Loss] [Minimizer] [Results]

Your function here

Workflow/API implemented



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```

Model

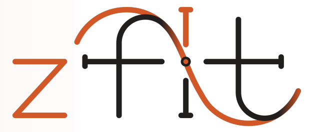
Data

Loss

Minimize

Errors

Workflow



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$\vec{x}_i$

[Data]

$frequency$

$\vec{x}_i$

[Loss]

Loss

prediction

[Minimizer]

prediction

[Results]

$f(\vec{x}_i|\theta)$

$\vec{x}_i$

Computational Backend

~~Computational Backend~~

“And now for something completely different.”
Monty Python

~~Computational Backend~~

(very brief) introduction to

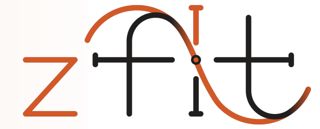
Deep Learning

or Neural Networks

or Machine Learning

or Big Data…

Deep Learning



Neural Network

„One huge, complicated function“

[Model]

[Data]

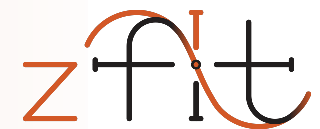
„Big Data“

[Loss]

[Minimizer]

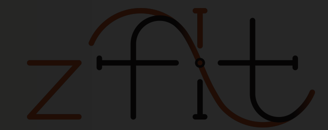
[Results]

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, 2nd derivative algorithm	Hesse, profiling
Deep Learning	Combine many, trivial functions	Many, small Batches	*Anything! (GANs, RL,...)*	Local (!) min, 1th derivative, many steps	None
Conclusion					

Deep Learning vs. Model Fitting



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Conclusion	No real impact	Optimizations for OOM calculations	HEP trivial special case	~~Optimizers~~ Free „analytic“ derivatives!	No support, but simple

But...

what *is* a Deep Learning library?

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, 2nd derivative algorithm	Hesse, profiling
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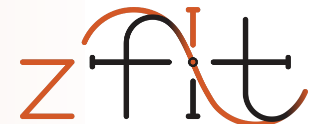
Conclusion	No real impact	Optimizations for OOM calculations	HEP trivial special case	~~Optimizers~~ „analytic“ derivatives!	No support, but simple

Modern, high performance computing

TensorFlow

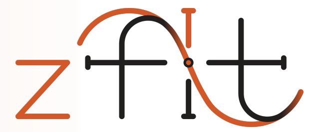


- By Google, highly popular (130k★, 4th on GitHub)
- Used in multiple physics libraries and analyses
- Consists of "two parts":
  - High level API for building neural networks *(NOT used!)*
  - Low level API with Numpy-style syntax

    tf.sqrt, tf.random.uniform,...

...but many Deep Learning frameworks are similar

Advantages

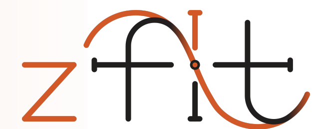


- Autograd: automatic gradient calculation
- Native CPU/GPU/distributed support
- Optimizations (graphs,…)

Used (+ maintained!) by industry
where performance is money

huge financial interest

Delegating the workload



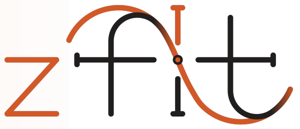
	C++ library (RooFit,...)	Numpy based	zfit
HEP specific content/API			
Models		SciPy	TF Probability
Gradients			TensorFlow
Computational optimizations			
Parallelization/GPU		Numba NumPy	intel NVIDIA
Low level handling		python	

Delegating the workload

	C++ library (RooFit,...)	Numpy based	zfit
HEP specific content/API			API & Workflow
Models		SciPy	TF Probability
Gradients			TensorFlow
Computational optimizations			
Parallelization/GPU		Numba NumPy	intel NVIDIA
Low level handling		python	python

"Stepping on the shoulders of a giant"

Performance



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

Same order of magnitude as RooFit

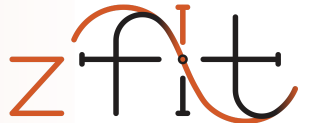
9 free parameters

2 free parameters

x5-8

Implementation

Complete fit

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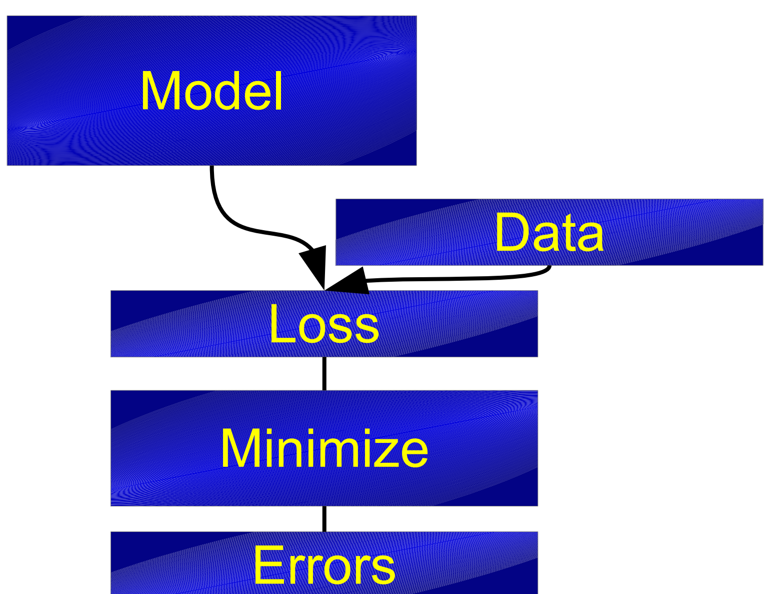
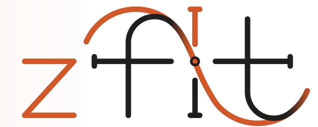


Complete fit: Model

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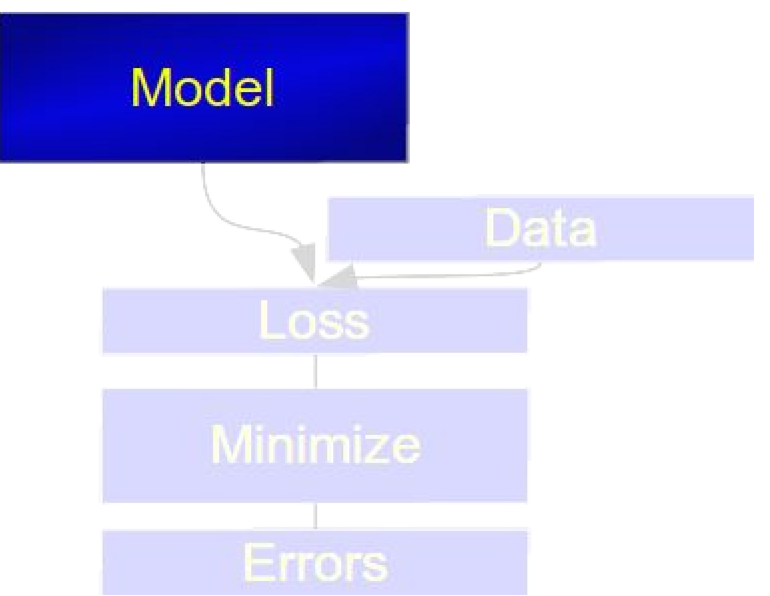


Custom PDF

```python
from zfit import ztf


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

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

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

Example of Base Classes *in general* inside zfit

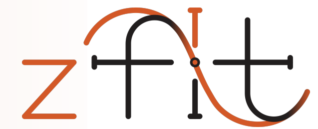
```python
custom_pdf = CustomPDF(obs=obs, alpha=0.2)

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

} use functionality of model

LHCb Angular Analysis

```
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_k, costheta_l, 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
```

Complete fit: Data



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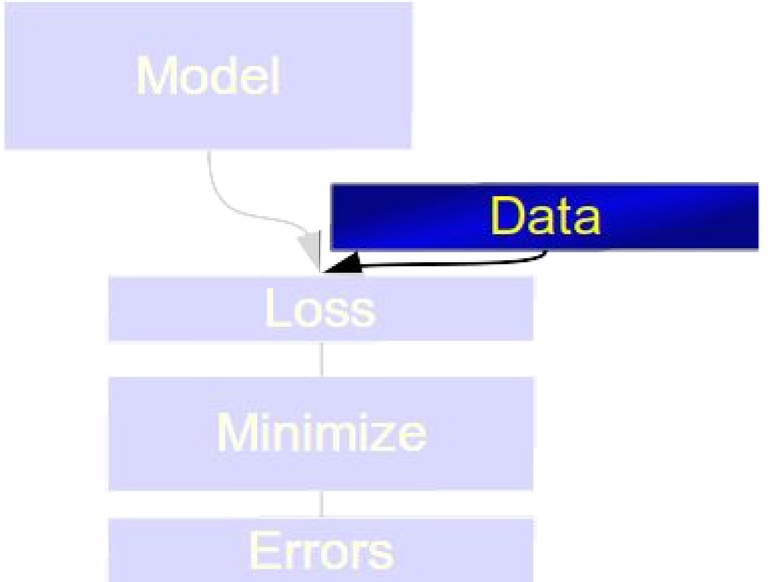
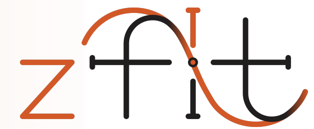


Complete fit: Loss

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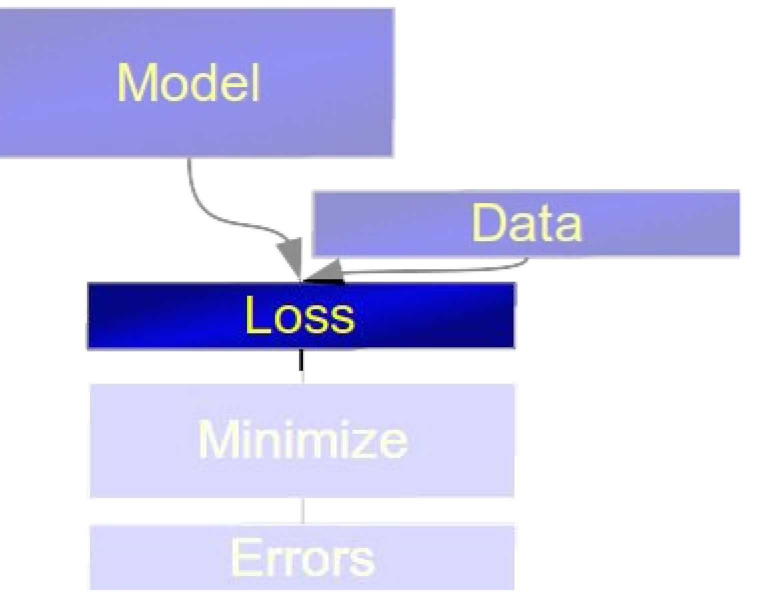
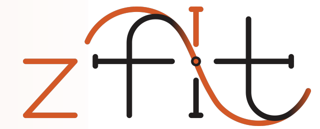


Complete fit: Minimization

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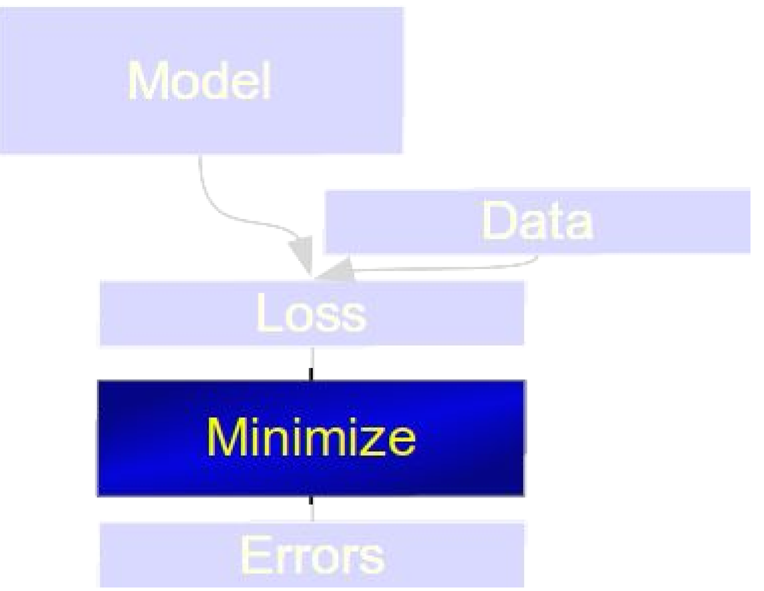
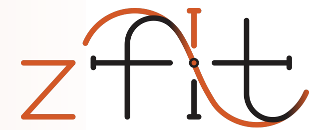


Complete fit: Result

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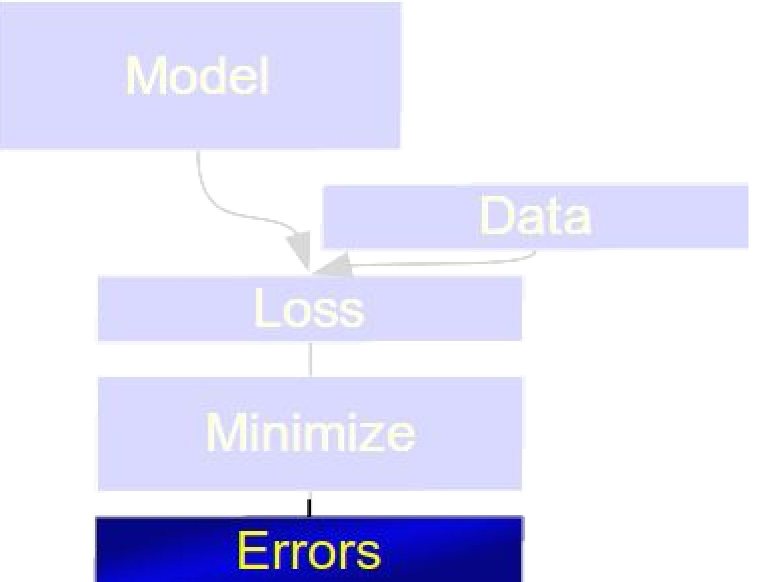
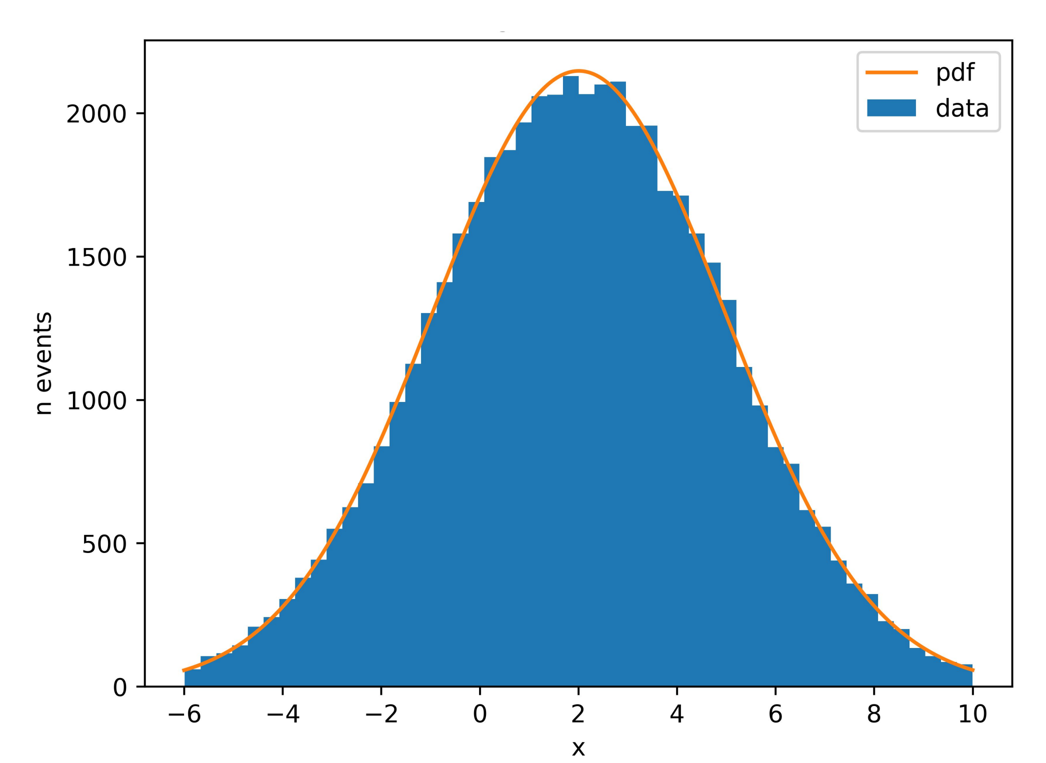
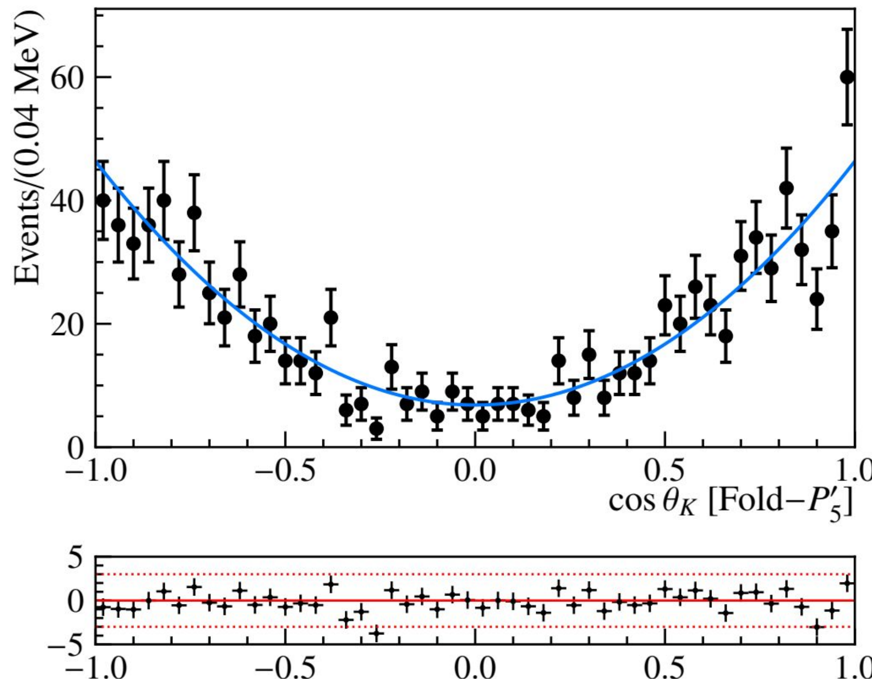


Complete fit: plots

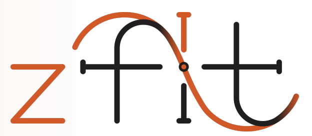
Gaussian example



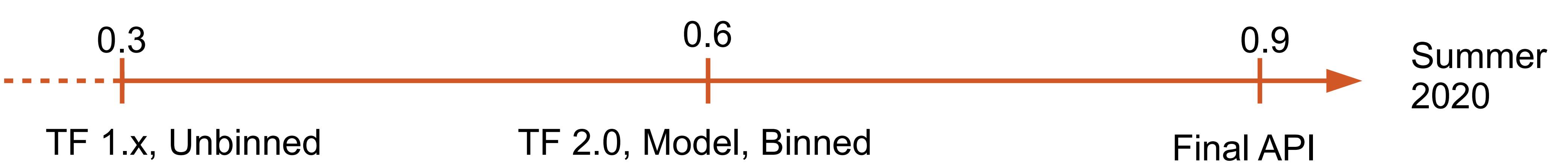
Angular Analysis



zfit: status



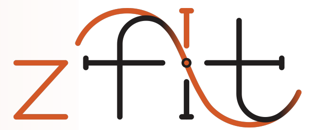
Public beta stage *(pip/conda install zfit)*



Focus on
- stable API & workflow
- core implementations
- interface & base classes

Not on content

Community involvement



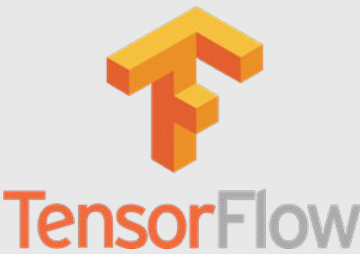
Who

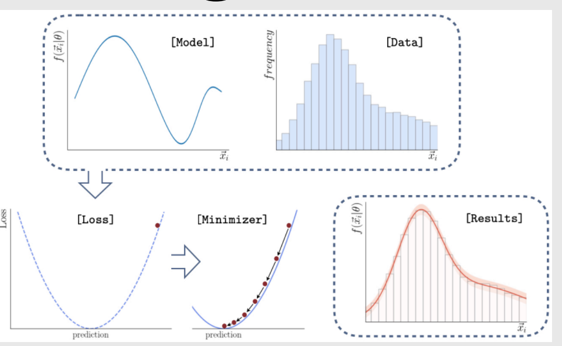
Everyone who does likelihood fits

What

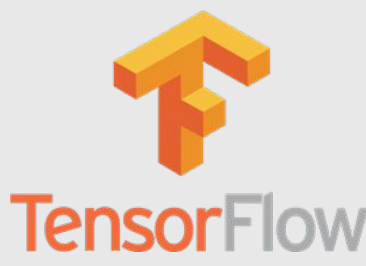
- Discussions (API, features, …): zfit-development
  - Usecases
  - Ideas
  - Experience
  - Doubts
- Use it; ask; wish; criticize

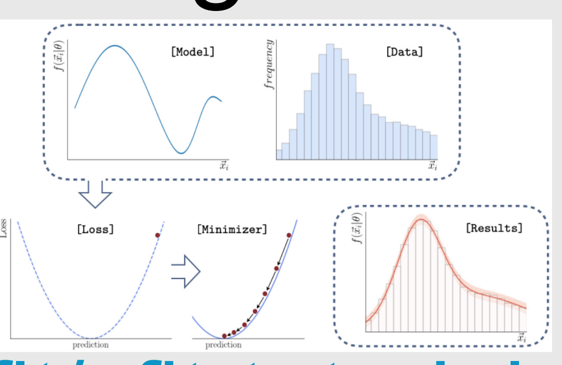
scalable pythonic





scalable pythonic fitting





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

Backup Slides

https://zfit.github.io/zfit/

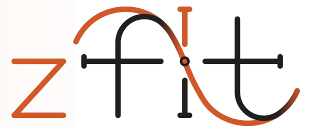
zfit@GitHub

Gitter channel

zfit@physik.uzh.ch

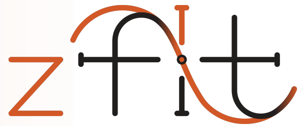
Join the discussion!

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,…)

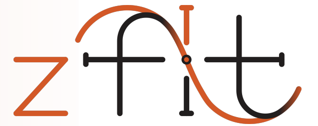
RooFit



- *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*

HEP Python projects



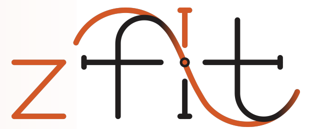
Probfit, TensorProb,…

- Lack generality and extendibility
- “experimental”, but great proof of concept

} General impression in comparison with other HEP packages

  - API and Python in general
  - Computational backends (e.g. Cython, TensorFlow)
  - Building an ecosystem (iminuit,…)

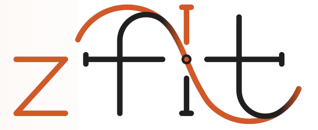
Non-HEP



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, …

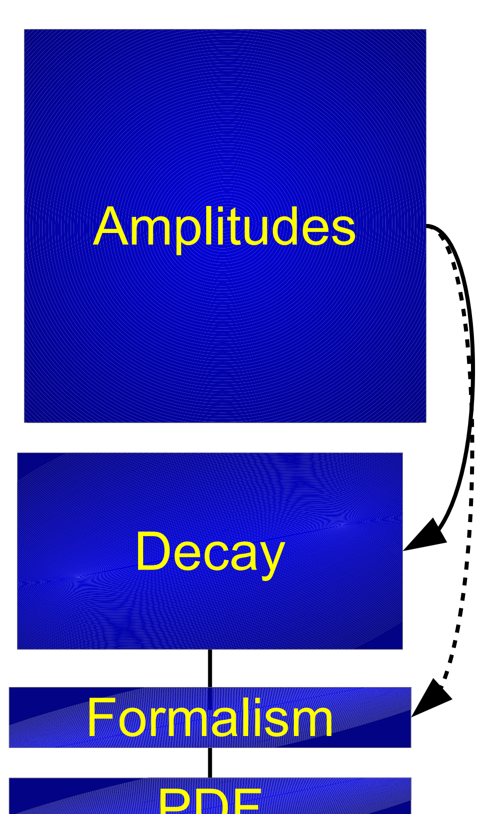
TFA: approach & differences



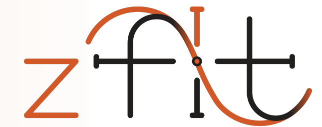
- Build «optimized» TensorFlow
  - accept-reject as tf.while_loop, Dataset input,...
- ...and hide the tedious, unambiguous parts
  - automatic normalization, Tensor cache, ...
- Well defined structures, e.g.
  - String name order (like columns) in PDFs, data, limits,...
    - pdf(„x“) * pdf(„y“) =>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

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)
```

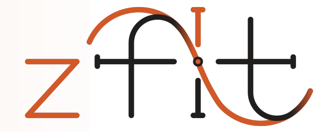


zfit project



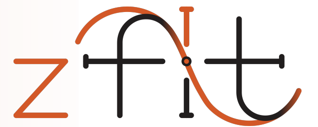
- zfit: stable core
  - Unbinned fits, binned WIP
  - n-dim models with integral, pdf, sample
- zfit-physics: HEP specific content
  - BreitWigner, DoubleCB,…
  - Faster development, more content
  - Ideal for contributions
    - Auto testing of new pdfs/func
    - Contribution guidelines

Pythonic



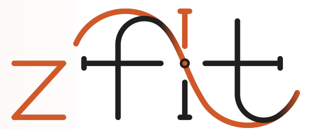
- Pure Python («pip install zfit»)
- Integrated into python ecosystem
  - Load ROOT files (uproot,no ROOT dependence!)
  - Use Minuit for minimization (iminuit)
  - Data preprocessing with Pandas DataFrame
  - Plotting with matplotlib
  - High level statistics (lauztat, more WIP)
- Extendable classes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

Scalable

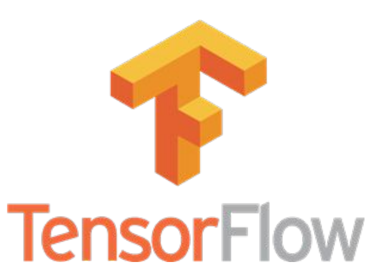


- TensorFlow **hidden** backend, uses graphs
  - numpy-like syntax
  - parallelization on CPU/GPU, analytic gradient,...
- Writing functions simple for users *and* developers
  - No Cython, MPI, CUDA,... for *state-of-the-art performance*
  - No low-level maintenance required!
- Used in multiple physics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

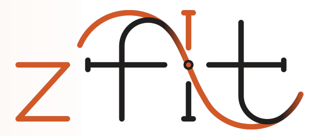
Scalable: TensorFlow



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

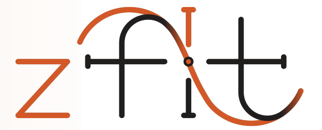


Graph elements



… do not have to be constant!

Graph elements

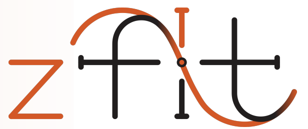


… do not have to be constant!

Parameters

Can change their value

Graph elements



… do not have to be constant!

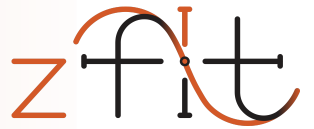
Parameters

Can change their value

Random numbers

Generate newly on every graph execution: MC integration,…

Graph elements



… do not have to be constant!

Parameters

Can change their value

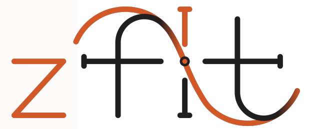
Random numbers

Generate newly on every graph execution: MC integration,…

Control flow (if, while)

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

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)

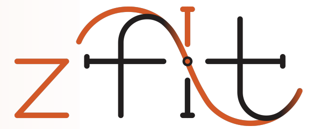
Steer the execution: Accept-reject sampling (while), etc.

Static, not constant

Can we express model fitting as static graphs?

Yes!

HPC perspective



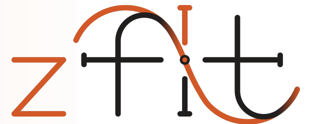
1) Definition of computation, shape etc. (add static knowledge)
2) Compilation of the graph
3) Execution of computation (re-use optimized graph)

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

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)
```

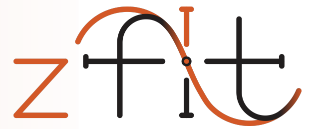
simultaneous loss

```
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)
```

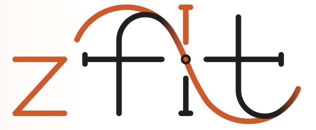
Custom Loss

```
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)
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

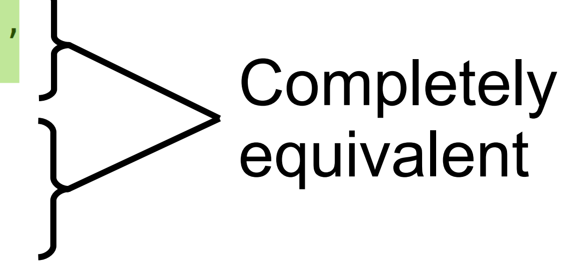
} models

Simultaneous fit

```
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