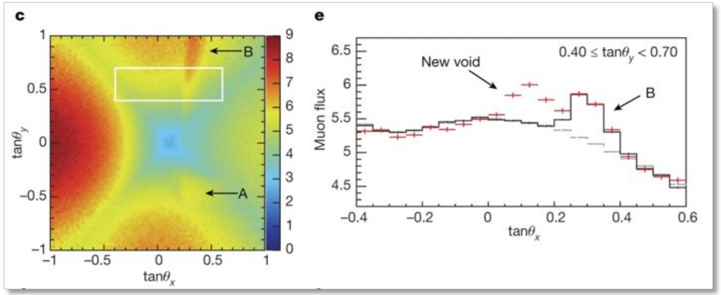
Automatic Differentiation in ROOT

Garima Singh (Princeton University), Jonas Rembser (CERN), Lorenzo Moneta (CERN), Vassil Vassilev (Princeton University)

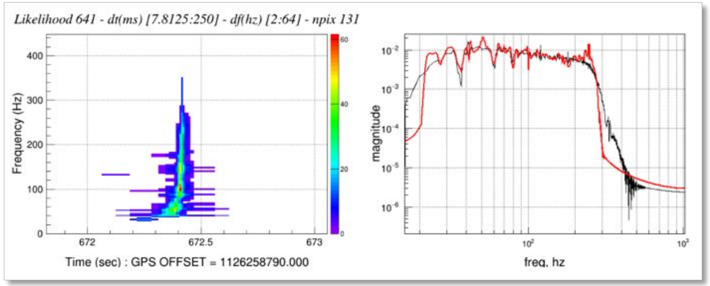
compiler-research.org

ROOT

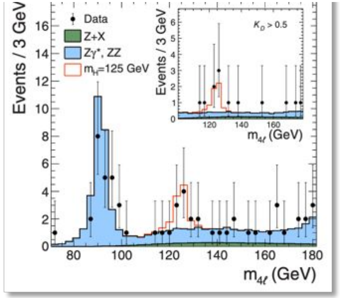
An Exabyte Data Analysis Framework



[1]



[2]



[3]

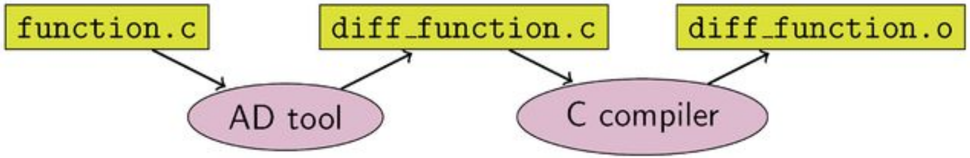
Scientific breakthrough such as the discovery of the big void in the Khufu's Pyramid, the gravitational waves and the Higgs boson heavily rely on the ROOT software package.

[1] Morishima, K., Kuno, M., Nishio, A. *et al.* Discovery of a big void in Khufu's Pyramid by observation of cosmic-ray muons. *Nature* 552, 386–390 (2017).
[2] B. P. Abbott, et al, Observation of Gravitational Waves from a Binary Black Hole Merger (2016)
[3] CMS Collaboration, Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC (2012)

Methods of Automatic Differentiation

The Two Techniques

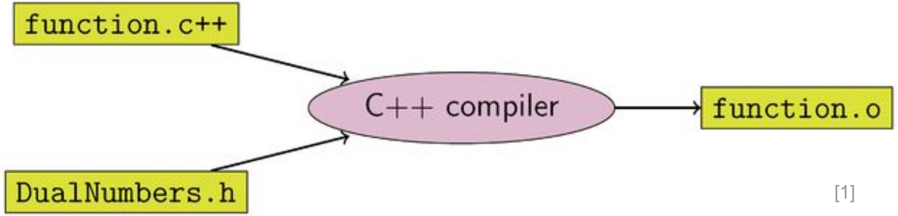
Source Code Transformation AD



[1]

- Synthesize derivative code from the input program *automatically*.
- **Faster** - allows for easier compiler optimization.
- Eg. Tapenade, Enzyme, **Clad**

Operator Overloading AD



[1]

- Use a new data type and operator overloading to keep track of derivatives as the original program executes.
- **Slower** and requires hand writing annotations and changing data types.
- Eg. PyTorch/TensorFlow, CoDiPack, etc.

[1] : https://en.wikipedia.org/wiki/Automatic_differentiation

An Efficient Method of Differentiation

Compiler-Based Source Transformation AD: Clad

Clad[2], a source code transformation AD tool, implemented as a plugin to the clang compiler. Clad inspects the internal compiler representation of the target function to generates its derivative.

```
double absFunc(double x) {
 if (x < 0) return -x;
 else return x;
}
```

`clad::differentiate(absFunc)` →

```
double absFunc_darg0(double x) {
   double _d_x = 1;
   if (x < 0) return -_d_x;
   else return _d_x;
}
```

- Proximity to compiler allows for more control over code generation.
- Support for a good subset of modern C++ constructs.

[2] : https://github.com/vgvassilev/clad

An Efficient Method of Differentiation

Compiler-Based Source Transformation AD: Clad

Clad also can be used within Cling[3], the C++ interpreter used with ROOT.

```
[2]: double fn(double x, double y) {
       return x*x*y + y*y;
     }

[3]: auto fn_dx = clad::differentiate(fn, "x");

[4]: fn_dx.execute(5, 3)

[4]: 30.000000
```

Binder Tutorial

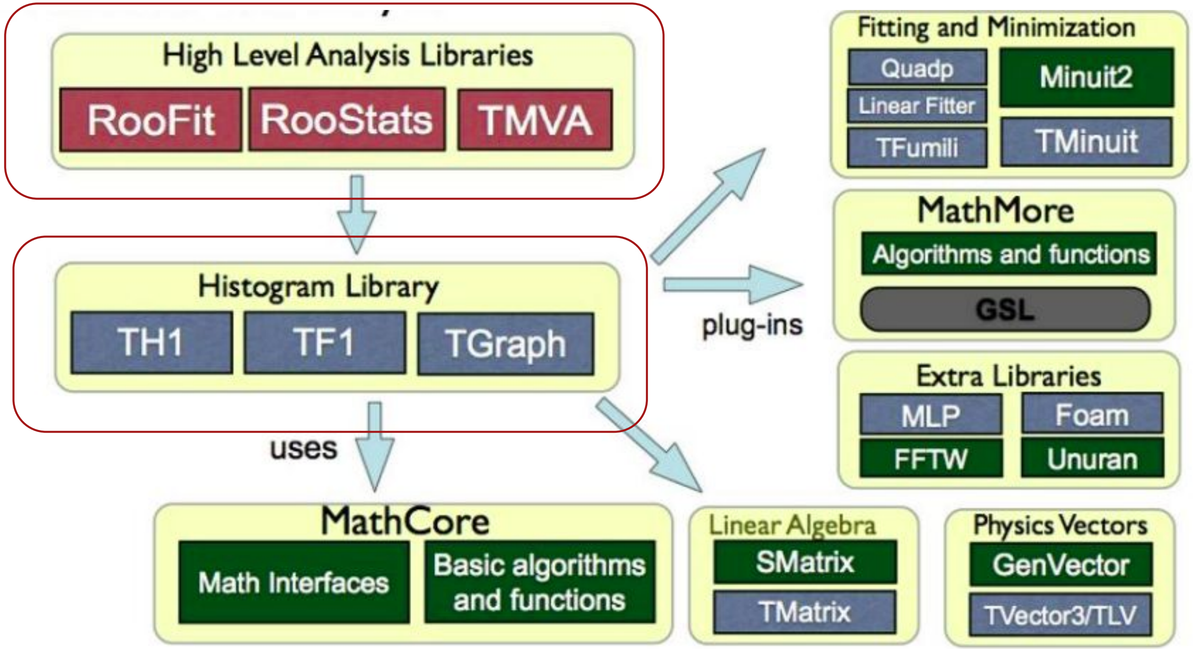
[3] :https://github.com/root-project/cling

AD in ROOT

ROOT's Math and Statistical Libraries

Then we demonstrate AD on one of the high-level analysis libraries - *RooFit*.

As a first, we demonstrate AD on one of the simpler *TFormula/TF1* class.



https://laconga.redclara.net/courses/modulo-datos/claseMD06/materialesMD06/ROOT_Introduction_CEVALE2VE_class_04_16_2016.pdf

Automatic Differentiation for TFormula

What is TFormula?

TFormula models formulae in ROOT by connecting compiled and interpreted code offering both performance and flexibility. It allows users to defined their formulae as strings which are then JIT compiled to functions that are used to fit and model data distributions

```
TFormula f("f", "x*std::sin([0]) -
                 y*std::cos([1])");
```

The following function is JIT compiled by Cling:

```
double f(double *x, double *p) {
  return x[0]*std::sin(p[0]) -
         x[1]*std::cos(p[1]);
}
```

This code can easily be differentiated by clad!

```
double p[2] = {TMath::Pi()/6, TMath::Pi()/3};
f.SetParameters(p);
f.Eval(1, 0);
```

This call internally calls : `f({1, 0}, p)`

Automatic Differentiation for TFormula

How to use AD in TFormula?

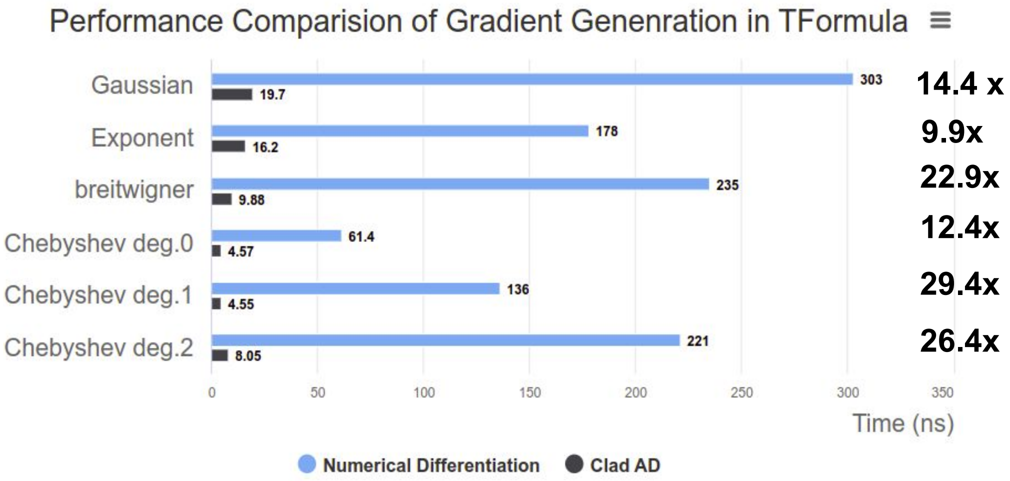
```
root [0] TFormula f("f", "x*std::sin([0]) - y*std::cos([1])");
root [1] double p[2] = {TMath::Pi()/6, TMath::Pi()/3};
root [2] f.SetParameters(p);
root [3] f.Eval(1, 0)
(double) 0.50000000
root [4] 1*std::sin(p[0])
(double) 0.50000000
root [5] TFormula::CladStorage result(2);
root [6] double in[2] = {1, 0};
root [7] f.GradientPar(in, result);
root [8] result
(TFormula::CladStorage &) { 0.86602540, 0.0000000 }
root [9] std::cos(p[0])
(double) 0.86602540
```

This will generate the gradient of the function with respect to the parameters `p`

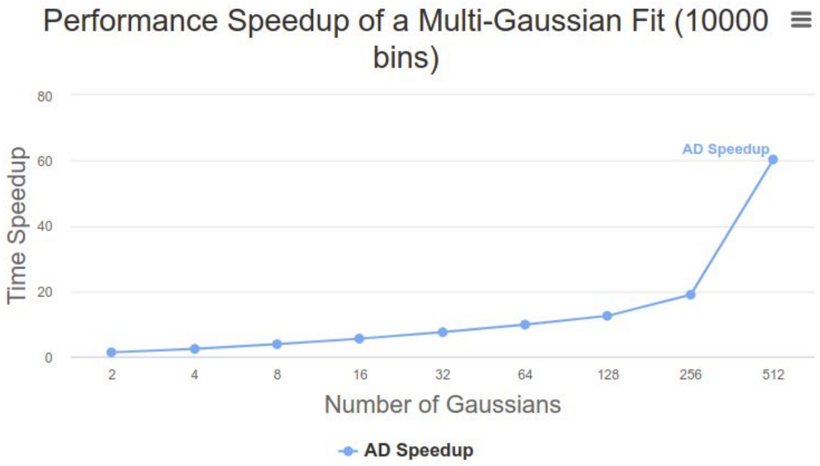
It is also possible to compute AD Hessians for TFormula through **`HessianPar`**.

Automatic Differentiation for TFormula

Benchmarks



TFormula benchmarks of gradient generation time from numerical differentiation and clad AD.



TF1 based benchmarks. TF1 is the TFormula fitting interface for fitting histograms.

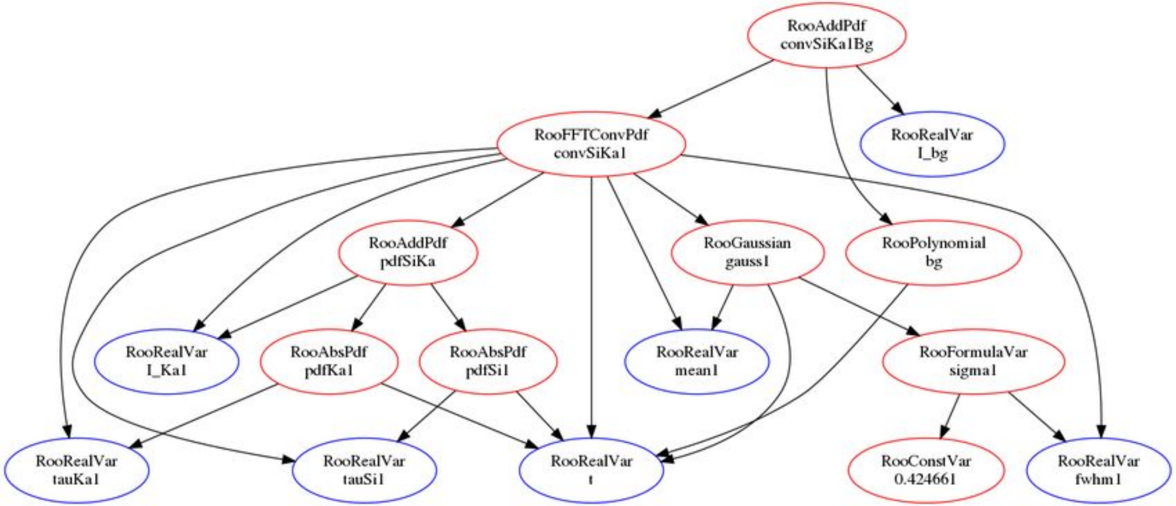
Clad can be used in TF1 through the "G" parameter to `Fit`.

```
h1->Fit(f1, "S G Q N");
```

Automatic Differentiation in RooFit

Overview

- A more complex application of AD, different from TF because it is hard to extract the code containing differentiable properties.



What that we want to differentiate

How do we make RooFit more malleable to AD?

Automatic Differentiation in RooFit

Challenges

RooFit represents all mathematical formulae as RooFit objects which are then brought, together into a compute graph. This compute graph makes up a model on which further data analysis is run.

Math Notations		RooFit Object
variable	x	RooRealVar
function	$f(x)$	RooAbsReal
PDF	$f(x)$	RooAbsPdf
space point	$\hat{x}$	RooArgSet
integral	$\int_a^b f(x)$	RooRealIntegral
list of space points	$\hat{x}_1, \hat{x}_1, \hat{x}_1 ...$	RooAbsData

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Gaussian Probability Distribution Function (pdf)

```
//Obj represents f(x) here
RooGaussian obj(x, mu, sigma);
```

Equivalent Code in C++ with RooFit

Programmers/users know this relationship. But how do we connect these two together when a connection is not obvious programmatically?

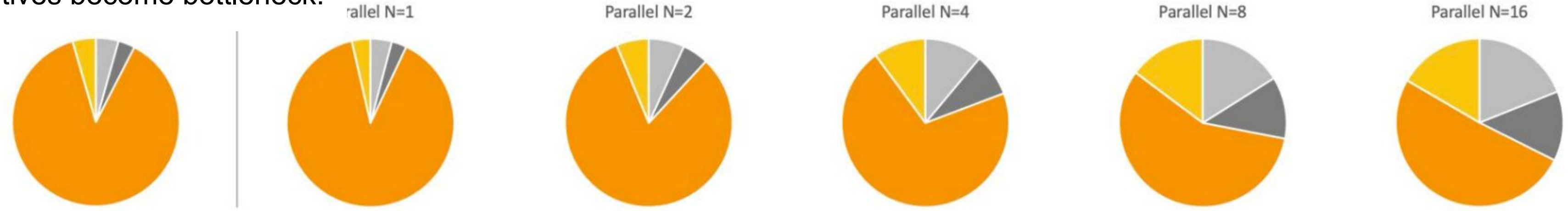
Automatic Differentiation in RooFit

Why AD?

- One goal - Make RooFit Faster. Results from a Higgs-combination fit:

	serial old	parallel N=1	parallel N=2	parallel N=4	parallel N=8	parallel N=16
setup_roofit	313	327	315	315	312	327
minuit_init	230	231	231	231	231	231
gradient_calc	6289	7102	3734	1997	1107	879
line_search	323	287	287	287	287	287

Derivatives become bottleneck!



ICHEP 2022 - Zeff Wolffs - https://agenda.infn.it/event/28874/contributions/169205/attachments/93887/129094/ICHEP_RooFit_ZefWolffs.pdf

- Good results, but still use numerical differentiation.
- Potential next step – use AD to compute the gradients.

Automatic Differentiation in RooFit

Making RooFit classes differentiable

A way of having some context for AD is to introduce a function for each of the RooFit nodes that would represent the underlying mathematical notation as code.

`RooGaussian::evaluate()` → *– Caching & Bookkeeping* / *+ Normalization*

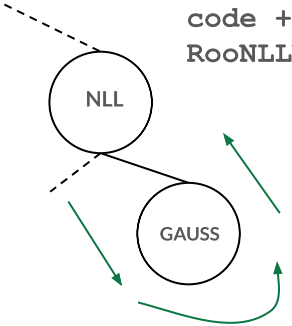
```
double RooGaussian::gauss(double x, double mu, double sig)
{
 const double arg = x - mu;
 double out = std::exp(-0.5 * arg * arg / (sig * sig));
 return 1. / (std::sqrt(TMath::TwoPi()) * sigma) * out;
}
```

This would allow us to calculate the derivatives of a RooGaussian just by differentiating just this function. However, how do we chain these individual functions to create code that represents a given RooFit model?

Automatic Differentiation in RooFit

Code Squashing : translating RooFit models

One way to do this is by defining a ‘translate’ function that returns an **`std::string`** representing the underlying mathematical notation of the class as code. This string can then be connected together to form a function.




```
code +=
RooNLLVar::Translate();
```

The parent node queries the results from the child nodes.

```
code +=
RooGaussian::Translate({});
```

```
// Declare the code
gInterpreter->Declare(code.c_str());
// Get the derivatives of ‘code’
gInterpreter->ProcessLine("clad::gradient(code);");
// Use code_grad in wrappers that interface with
// the minimizer.
```

Automatic Differentiation in RooFit

Code Squashing : translating RooFit models

The “glue” function enabling code squashing.

```
std::string
RooGaussian::translate(...) override {
 result = "RooGaussian::gauss(" +
                       _x->getResult() +
                       " ," + _mu->getResult() +
                       " ," + _sigma->getResult() +
                     ")";
 return "";
}
```

Stateless function enabling differentiation of each class.

```
static double RooGaussian::gauss(double x, double mean,
double sigma) {
 const double arg = x - mean;
 const double sig = sigma;
 double out = std::exp(-0.5 * arg * arg / (sig * sig));
 return 1. / (std::sqrt(TMath::TwoPi()) * sigma) * out;
}
```

`RooGaussian::evaluate()` ⇨ `RooGaussian::gauss(x, mu, sig)`

The RooFit call to evaluate a gaussian

The equivalent code generated

AD for binned likelihoods from HistFactory

A first application of AD for RooFit models

Many binned likelihoods follow a similar pattern:

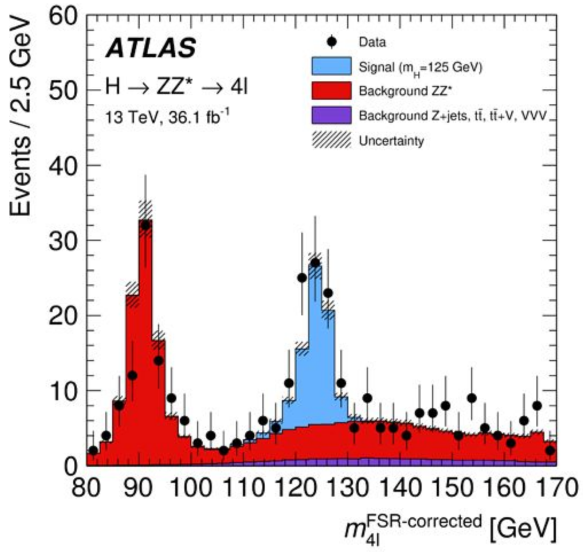
$$L(\vec{n}, \vec{a} \mid \vec{\eta}, \vec{\chi}) = \underbrace{\prod_{c \in \text{ channels}} \prod_{b \in \text{ bins}} \text{Pois}(n_{cb} \mid \nu_{cb}(\vec{\eta}, \vec{\chi}))}_{\text{product of Poisson terms}} \underbrace{\prod_{\chi \in \vec{\chi}} c_\chi(a_\chi \mid \chi)}_{\text{constraints}}$$

$\vec{n}$: data, $\vec{a}$: auxiliary data

$\vec{\eta}$: unconstrained parameters

$\vec{\chi}$: constrained parameters

Example binned likelihood with one channel: Higgs to 4 leptons



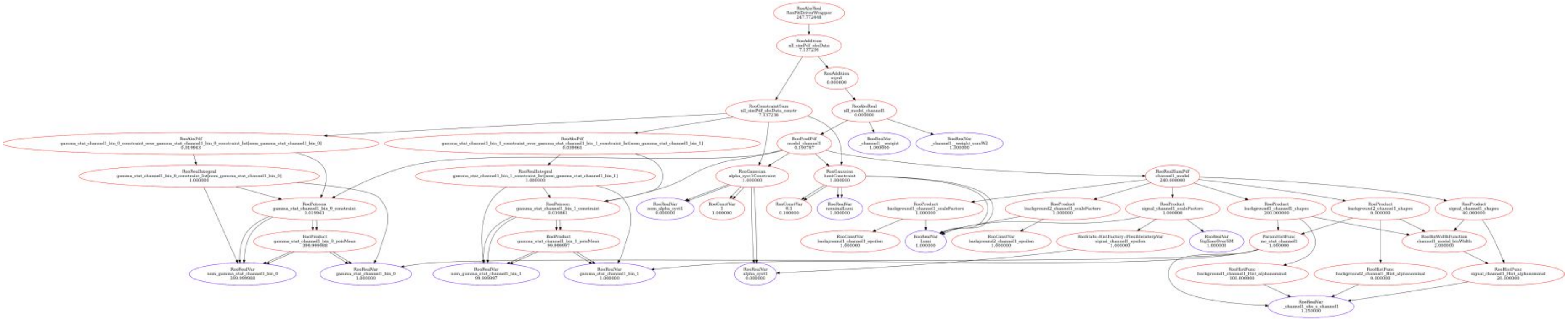
HistFactory is a higher-level tool to build such likelihoods in RooFit.

Good model class for showing AD in RooFit:

- many parameters
- rich computation graph
- few normalization integrals

Preliminary Results

Explicit Computation Graphs: An Example HistFactory Model



An example histogram fitting model with 2 bins and 2 channels, with 3 samples per channel. Based on the hf_001 example.

Preliminary Results

Explicit Computation Graphs: An Example HistFactory Model

```
double nll(double *in)
{
  double nomGammaB1 = 400;
  double nomGammaB2 = 100;
  double nominalLumi = 1;
  double constraint[3]{ExRooPoisson::poisson(nomGammaB1, (nomGammaB1 * in[0])),
                     ExRooPoisson::poisson(nomGammaB2, (nomGammaB2 * in[1])),
                     ExRooGaussian::gauss(in[2], nominalLumi, 0.100000)};
  double cnstSum = 0;
  double x[2]{1.25, 1.75};
  double sig[2]{20, 10};
  double binBoundaries1[3]{1, 1.5, 2};
  double bgk1[2]{100, 0};
  double binBoundaries2[3]{1, 1.5, 2};
  double histVals[2]{in[0], in[1]};
  double bgk2[2]{0, 100};
  double binBoundaries3[3]{1, 1.5, 2};
  double weights[2]{122.000000, 112.000000};
  for (int i = 0; i < 3; i++) {
     cnstSum -= std::log(constraint[i]);
  }
// cont…
```

Constraints defined as calls to their respective 'evaluate's.

Constraint sum.

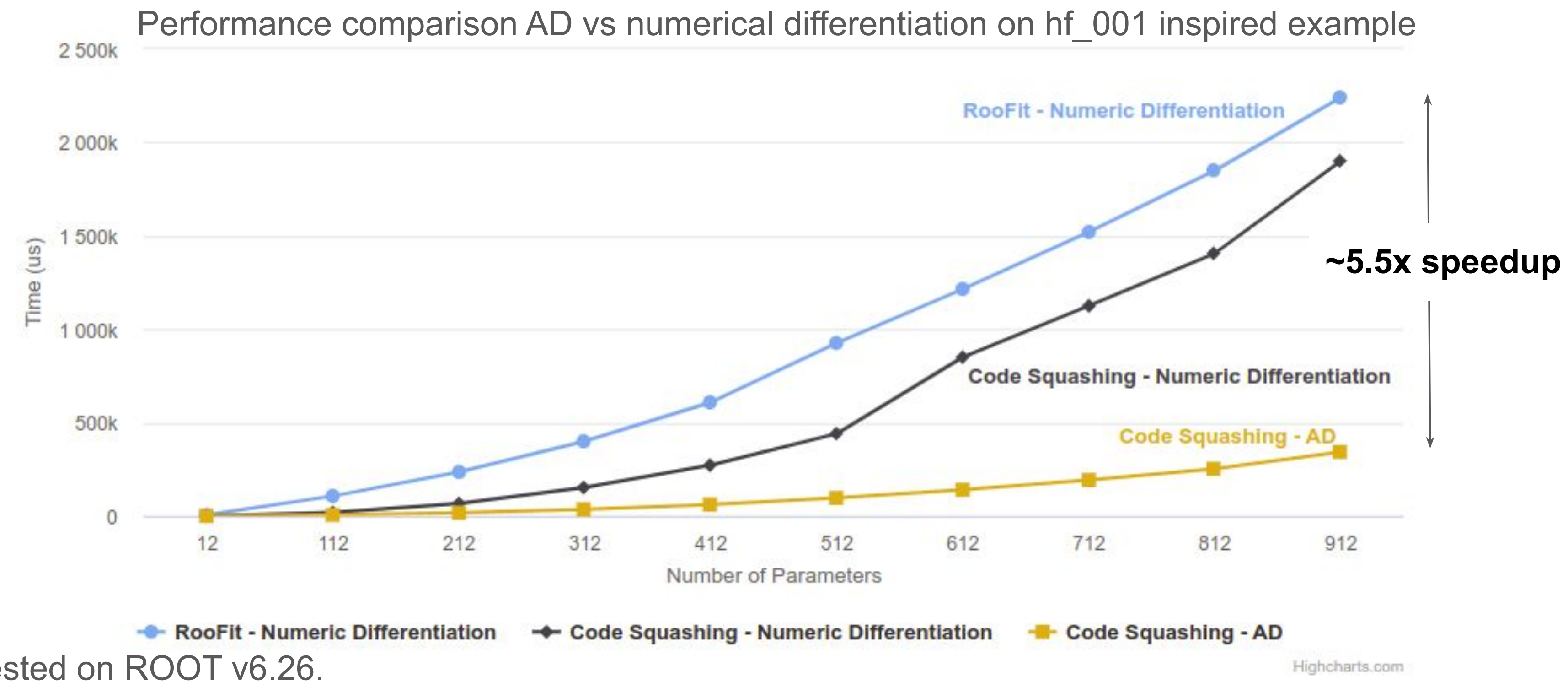
```
// cont..
  double mu = 0;
  double temp;
  double nllSum = 0;
  unsigned int b1, b2, b3;
  for (int iB = 0; iB < 2; iB++) {
     b1 = ExRooHistFunc::getBin(binBoundaries1, x[iB]);
     b2 = ExRooHistFunc::getBin(binBoundaries2, x[iB]);
     b3 = ExRooHistFunc::getBin(binBoundaries3, x[iB]);
     mu = 0;
     mu += sig[b1] * (in[3] * in[2]);
     mu += (bgk1[b2] * histVals[iB]) * (in[2] * 1.000000);
     mu += (bgk2[b3] * histVals[iB]) * (in[2] * 1.000000);
     temp = std::log((mu));
     nllSum -= -(mu) + weights[iB] * temp;
  }
  return cnstSum + nllSum;
}
```

Translated RooProducts.

NLL

Automatic Differentiation in RooFit

Preliminary Results: HistFactory Minimization



Tested on ROOT v6.26.

Automatic Differentiation in RooFit

Next Steps

- Adding externally provided Hessian support to MINUIT.
- Investigating applicability of AD to the rest of the HistFactory workflow - such as integrating AD based derivatives in profile likelihood calculations etc.
- Improving the external gradient interface in the RooFit minimizer wrappers
- Explore differentiating numerically computed integrals with AD.

Summary

- We present a compiler based AD tool - Clad, that is available as a plugin to the C++ compiler Clang.
- We showcase the addition of AD to ROOT’s TFormula class and present relevant results from the same.
- We demonstrate our current progress with adding AD to RooFit, more specifically HistFactory. We present promising results for incorporating AD to a complex math library such as RooFit.
- We also discuss future plans towards making RooFit more AD aware.

The End!

Questions?

https://www.linkedin.com/in/garimasingh28/

https://github.com/grimmmyshini

garima.singh@cern.ch

Backup