



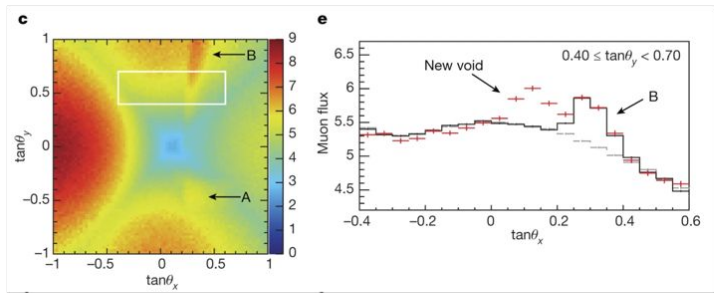
Automatic Differentiation in ROOT

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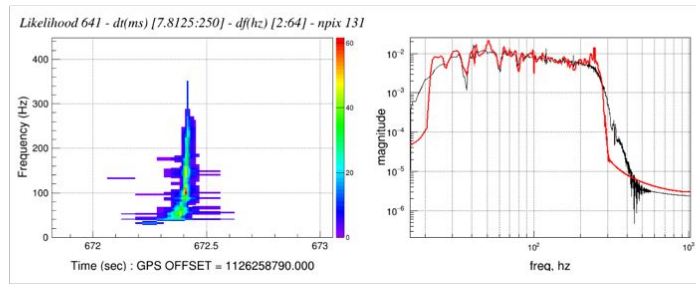
compiler-research.org

ROOT

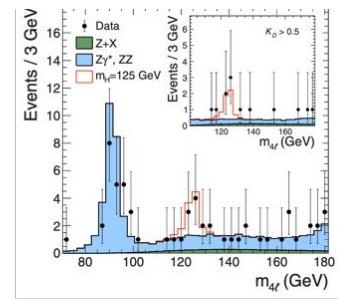
An Exabyte Data Analysis Framework



[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).

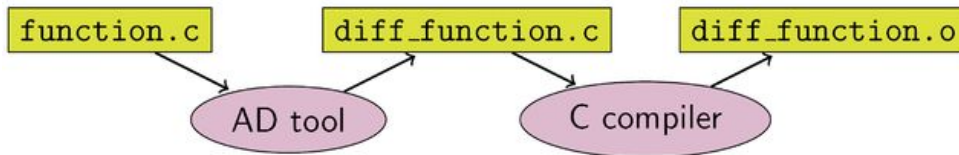
[2] B. P. Abbott, et al, Observation of Gravitational Waves from a Binary Black Hole Merger (2016)

[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

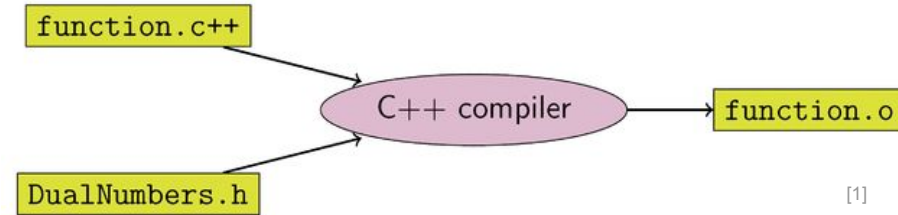


[1]

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

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

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.

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 generate 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](#)

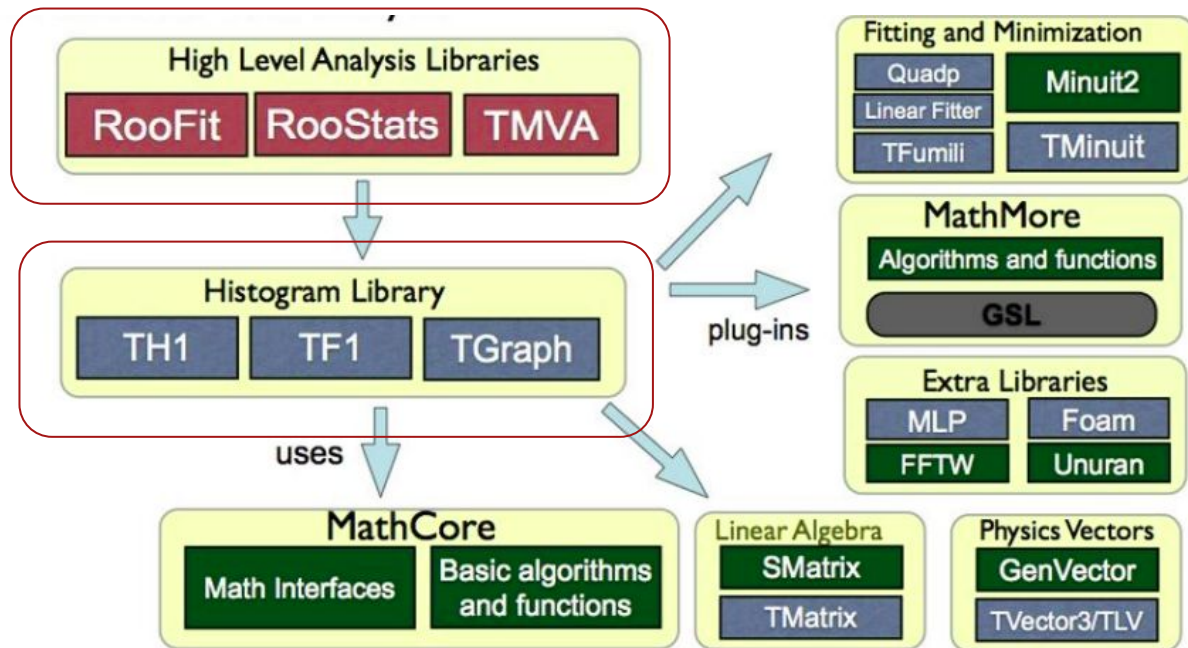
[3] :<https://github.com/root-project/cling>

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 define their formulae as strings which are then JIT compiled to functions that are used to fit and model data distributions

The following function is JIT compiled by Cling:

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



```
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, 0.00000000 }
root [9] std::cos(p[0])
(double) 0.86602540
```

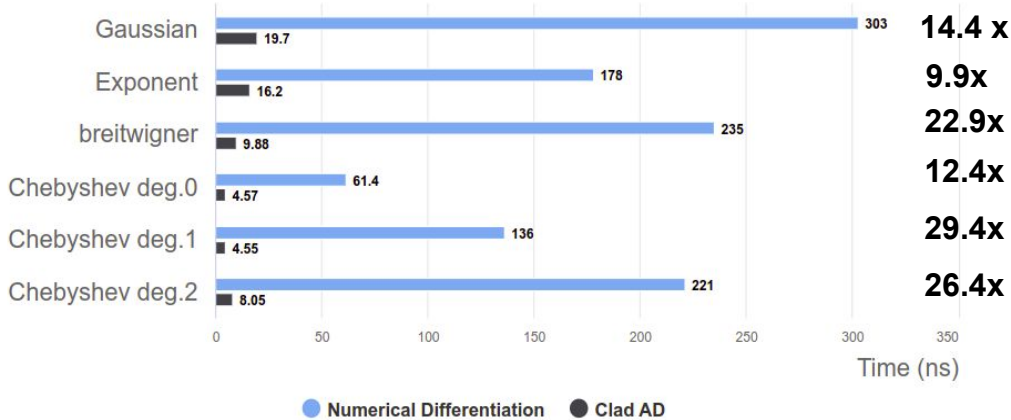
This will generate the gradient of the function with respect to the parameters `p`

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

Automatic Differentiation for TFormula

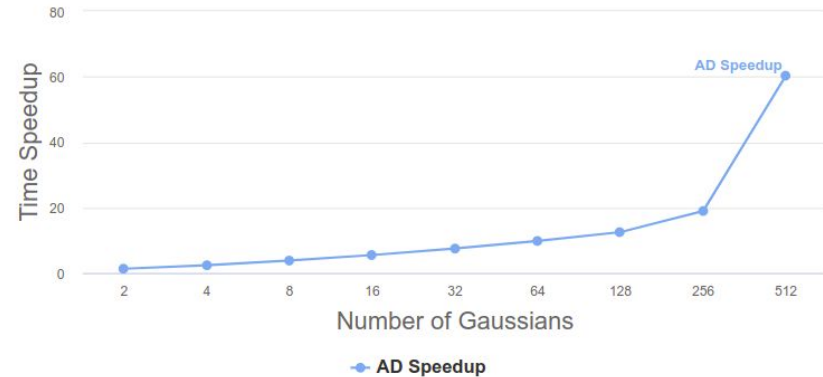
Benchmarks

Performance Comparision of Gradient Geneneration in TFormula



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

Performance Speedup of a Multi-Gaussian Fit (10000 bins)



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

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

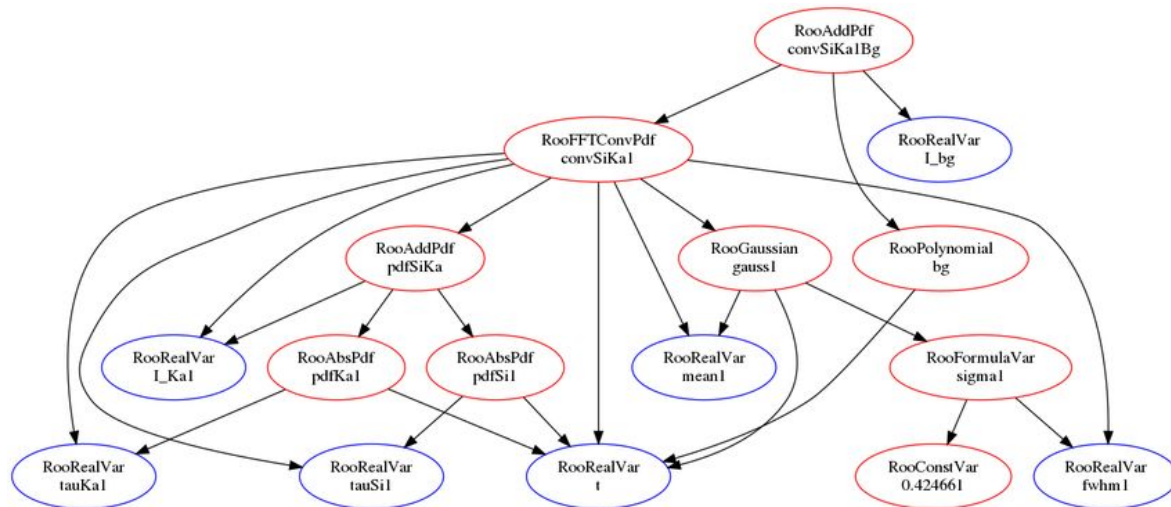
```
h1->Fit(f1, "S G Q N");
```



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.



How do we make RooFit more malleable to AD?

What that we want to differentiate

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	$\hat{x}_1, \hat{x}_1, \hat{x}_1, \dots$	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?

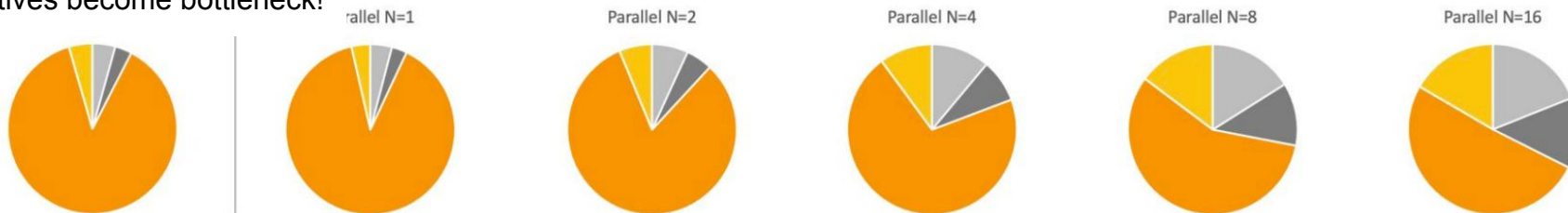
Automatic Differentiation in RooFit

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	setup_roofit	327	setup_roofit	315	setup_roofit	315	setup_roofit	312	setup_roofit	327
minuit_init	230	minuit_init	231	minuit_init	231	minuit_init	231	minuit_init	231	minuit_init	231
gradient_calc	6289	gradient_calc	7102	gradient_calc	3734	gradient_calc	1997	gradient_calc	1107	gradient_calc	879
line_search	323	line_search	287	line_search	287	line_search	287	line_search	287	line_search	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()`  `double RooGaussian::gauss(double x, double mu, double sig)`

– Caching & Bookkeeping

+ Normalization

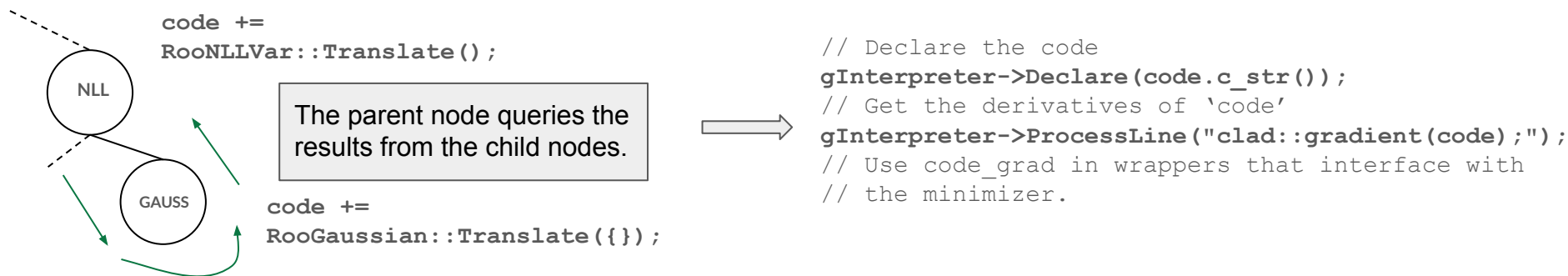
```
{  
    const double arg = x - mu;  
    double out = std::exp(-0.5 * arg * arg / (sig * sig));  
    return 1. / (std::sqrt(TMath::TwoPi()) * sigma) * out;  
}
```

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.



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 "";
}
```

`RooGaussian::evaluate()`

The RooFit call to evaluate a gaussian



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::gauss(x, mu, sig)`

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:

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

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

product of Poisson terms

constraints

$\vec{\eta}$: unconstrained parameters

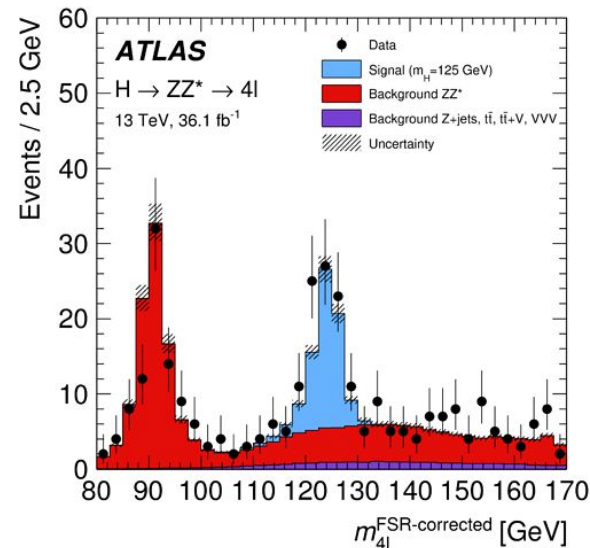
$\vec{\chi}$: constrained parameters

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

Good model class for showing AD in RooFit:

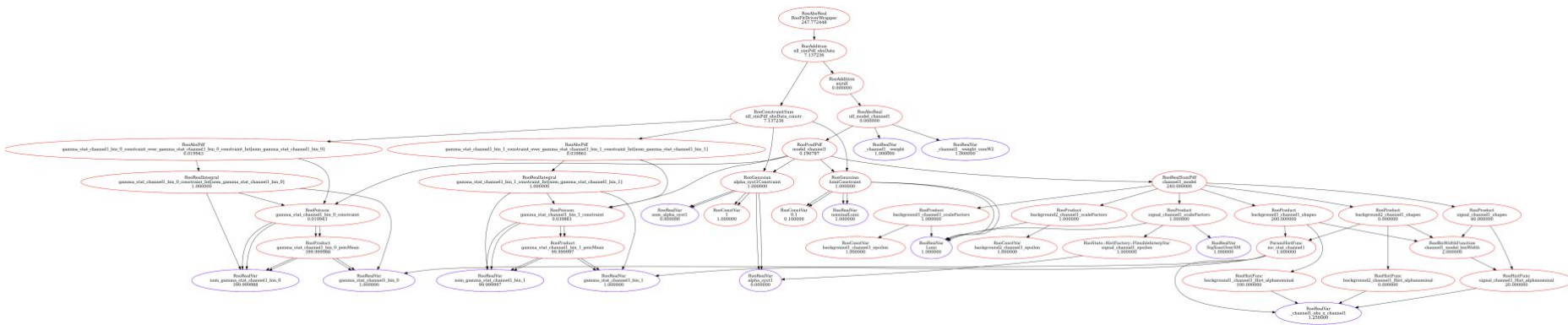
- many parameters
- rich computation graph
- few normalization integrals

Example binned likelihood with one channel: Higgs to 4 leptons



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.

Translated RooProducts.

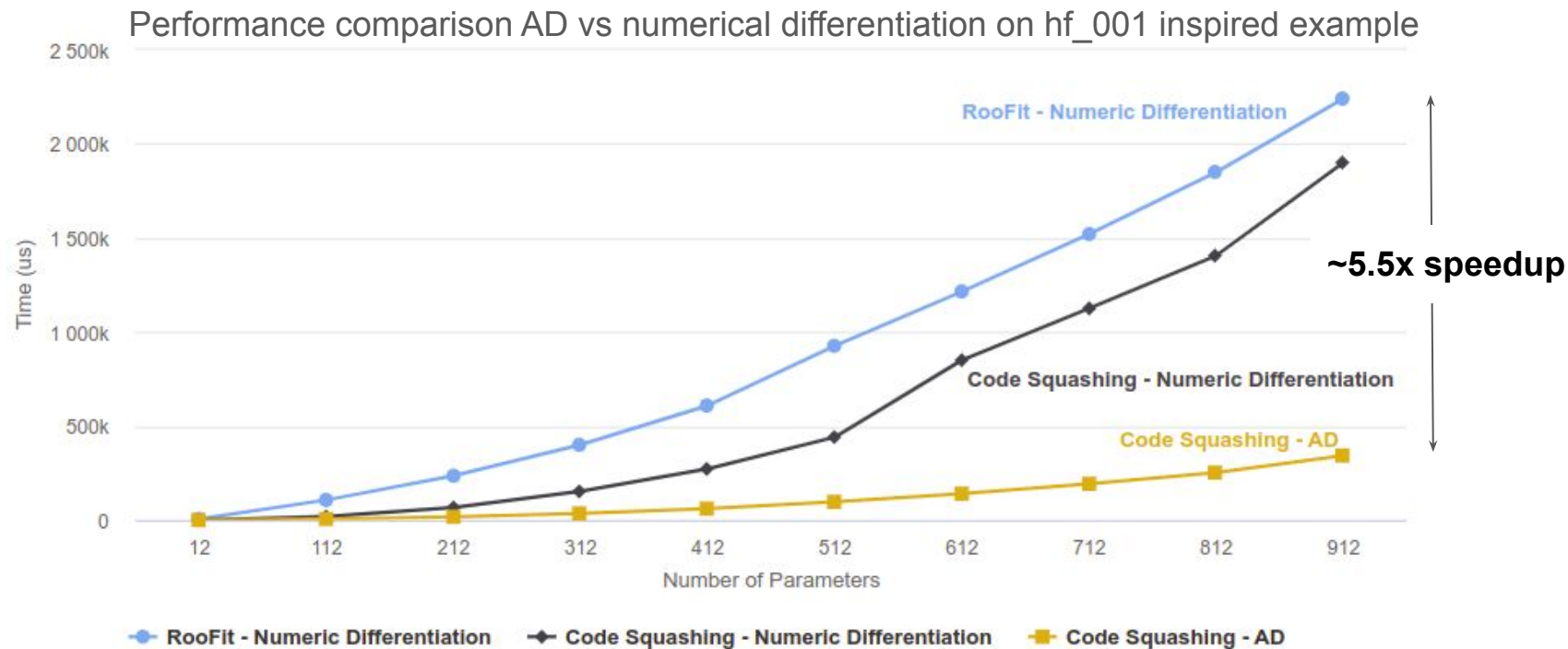
NLL

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;  
}
```

Automatic Differentiation in RooFit

Preliminary Results: HistFactory Minimization



Tested on ROOT v6.26.

Highcharts.com

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?



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<https://github.com/grimmmyshini>



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Backup