Automatic Differentiation in RooFit using Clad

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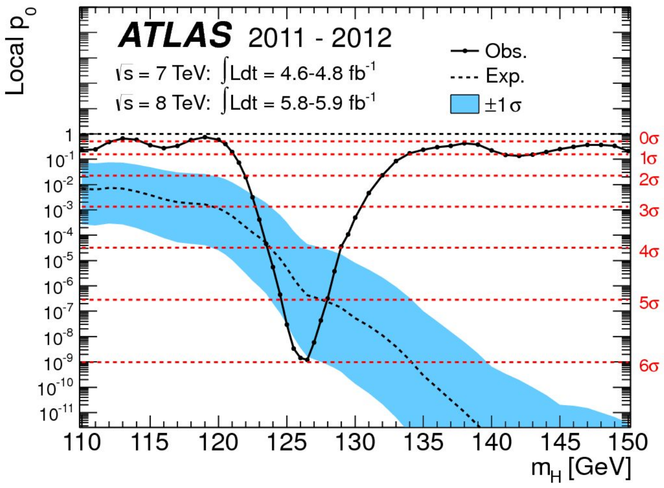
RooFit

RooFit: C++ library for statistical data analysis in ROOT.

- Used for modelling and normalization of probability density functions (p.d.f)

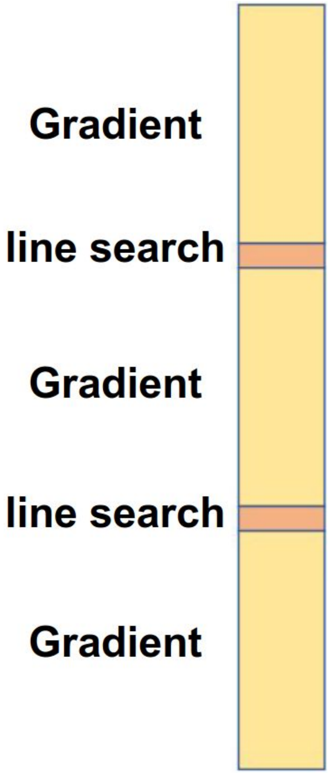
- Fitting likelihood models to the event data set.
  - Minimizing both binned and unbinned likelihoods

- Used most prominently by the LHC experiments, also for discovering the Higgs boson in 2012
  - Example of profile likelihood scan on the right



Minimization

- For optimizing parameters, we minimize the likelihood using **Minuit 2** (implements a minimization algo similar to BFGS)
- The minimization time for many-parameter models is dominated by gradient evaluation time
  (see also the ICHEP 2022 RooFit presentation)
- Our goal: make evaluating gradients cheap again with **Automatic differentiation (AD)** using **source code transformation**



Brief Intro of Automatic Differentiation

$$f(x) = e^{e^{e^{e^{e^x}}}}$$

Symbolic via Wolfram Alpha

$$\frac{d}{dx}\left(e^{e^{e^{e^{e^x}}}}\right) = e^{x+e^{e^{e^{e^x}}}+e^{e^{e^x}}+e^{e^x}+e^x}$$

Handcode

Figure out the analytical fn

```cpp
// f(x)=e^(e^(e^(e^(e^x))))
#include <cmath>
double f (double x, int N=5) {
  double result = x;
  for (unsigned i = 0; i < N; i++)
    result = std::exp(result);
  return result;
}
```

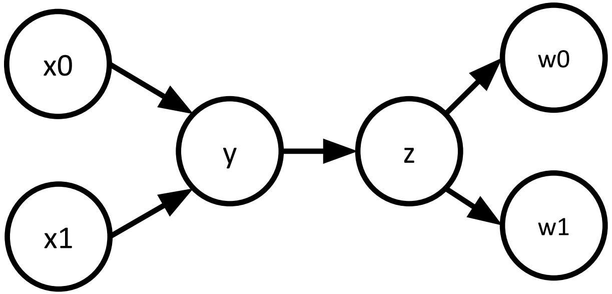
AD

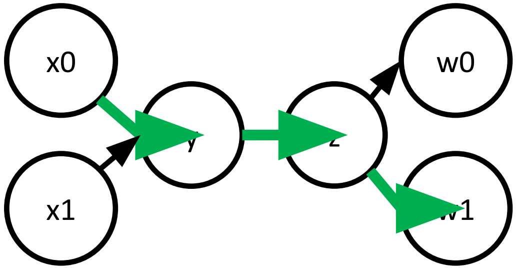
```cpp
double f_dx(double x, int N=5) {
  double result = x;
  double d_result = 1;
  for (unsigned i = 0; i < N; i++) {
     result = std::exp(result);
     d_result *= result;
  }
  return d_result;
}
```

Reference: *V. Vassilev – Accelerating Large Scientific Workflows Using Source Transformation Automatic Differentiation*

Crux of AD - Computational graph + Chain rule

```
y = f(x0, x1)
z = g(y)
w0, w1 = l(z)
```





$$\frac{\partial w1}{\partial x0} = \frac{\partial w1}{\partial z}\frac{\partial z}{\partial y}\frac{\partial y}{\partial x0}$$

Essentially, a generalization of backpropagation (from deep learning).

Clad

- ***Source transformation based AD tool for C++***
    - *Runs at compile time* - clad generates a readable (and easily debuggable) code for derivatives.
    - *Optimization capabilities of the Clang/LLVM Infrastructure enabled by default.*

- ***Support for control flow expression - not possible with operator overloading approaches.***
    - *Better handling of complex control flow logic handling compared to machine-learning frameworks like Tensorflow and Pytorch, hence more suitable for scientific computing scenarios.*

- ***Easy integration with ROOT infrastructure.***
    - *Clad's compiler research team has integration in High Energy Physics (HEP), and making significant improvements for RooFit use case.*

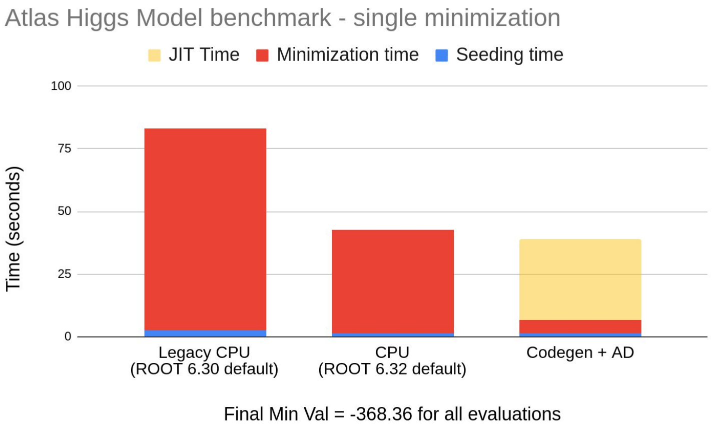
About Clad - usage example

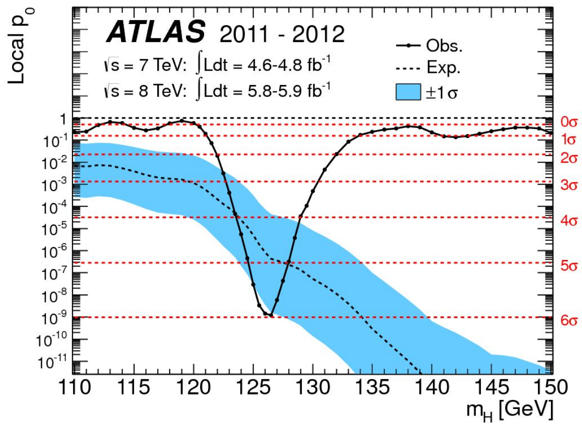
```cpp
// Source.cpp
#include "clad/Differentiator/Differentiator.h"
#include <iostream>

double f (double x, double y) {
  return x*y;
}

double main() {
  // Call clad to generate the derivative of f wrt x.
  auto f_dx = clad::differentiate(f, "x");

  // Execute the generated derivative function.
  std::cout << f_dx.execute(/*x=*/3, /*y=*/4) << std::endl;
  std::cout << f_dx.execute(/*x=*/9, /*y=*/6) << std::endl;

  // Dump the generated derivative code to stdout.
  f_dx.dump();
}
```

```
clang++ -I clad/include/ -fplugin=clad.so Source.cpp
```

```
4 // df/dx for (x,y) = (3, 4)
6 // df/dx for (x,y) = (9, 6)

double f_darg0 (double x, double y) {
  double _d_x = 1;
  double _d_y = 0;
  return _d_x * y + x * _d_y;
}
```

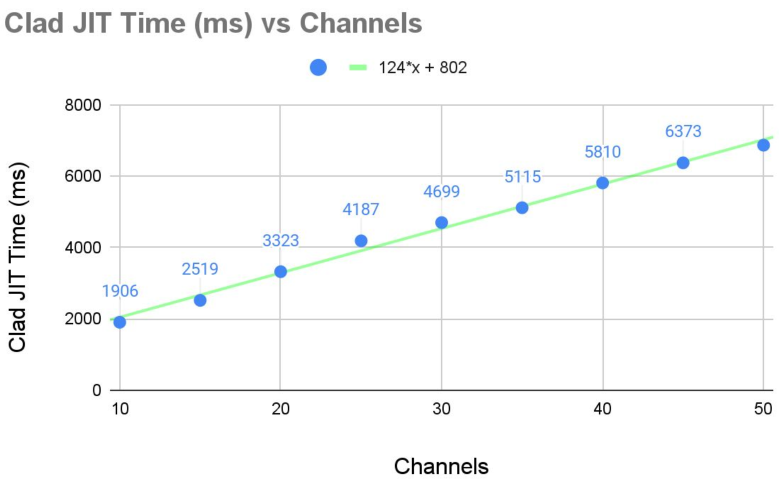
Experiments with Atlas Benchmark models

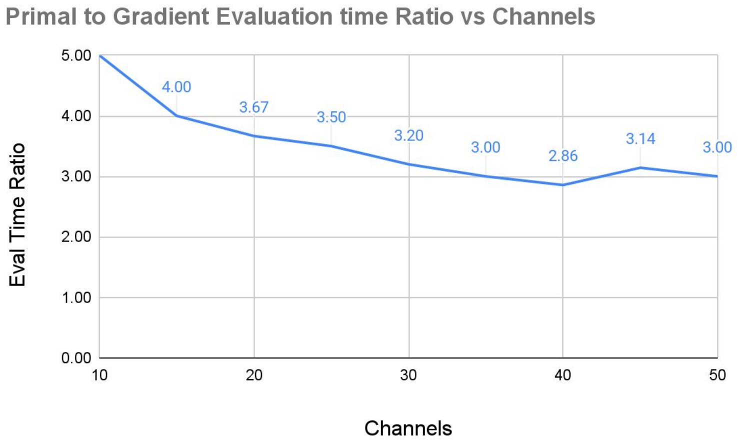




- For multiple minimizations w.r.t different constant parameters, the likelihood gradient can be reused.
    - Amortizing the JIT time across multiple minimizations.

Experiments with Atlas Benchmark models





- Memory consumption of gradient evaluation is very low compared to the python/ML based frameworks.
  - Constant factor of the consumption by primal function.

Further Improvements in Clad

- Using Automatic Differentiation for computing Hessians
  - Computing only the diagonal entries of Hessians.
- Further improvements in Clad to remove redundant computations for Gradients.
  - Advanced analysis for improving the efficiency of Gradient computations.
- Experimenting with make the gradient computation parallelizable.
  - Trying vector forward mode for Hessians.

Thank you

Questions or Comments ?