Making Likelihood Calculations Fast: Automatic Differentiation Applied to RooFit

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

compiler-research.org

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Introduction

Source Code Transformation Based Automatic Differentiation

Automatic Differentiation (AD) is a set of techniques to evaluate the exact derivative of a computer program.

- Faster than numerical differentiation - scales better for problems with large number of parameters.
- More accurate than numerical differentiation - fewer numerical errors!

Source code transformation based AD synthesizes derivative code from the internal representation of the target program.

\[\text{Clad}^{[1]}\], a compiler based source-code-transformation AD tool. Clad inspects the internal compiler representation of the target function to generate its derivative.

[1]: https://github.com/vgvassilev/clad
Motivation

Why AD?

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

<table>
<thead>
<tr>
<th>serial old</th>
<th>parallel N=1</th>
<th>parallel N=2</th>
<th>parallel N=4</th>
<th>parallel N=8</th>
<th>parallel N=16</th>
</tr>
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<tbody>
<tr>
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</tbody>
</table>

Derivatives become bottleneck!

- We have seen some promising results (in ROOT) already!

<table>
<thead>
<tr>
<th>Performance Comparison of Generation in TFormula</th>
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</thead>
<tbody>
<tr>
<td>Gaussian</td>
</tr>
<tr>
<td>Exponential</td>
</tr>
<tr>
<td>breitwigner</td>
</tr>
<tr>
<td>Chebyshev deg.0</td>
</tr>
<tr>
<td>Chebyshev deg.1</td>
</tr>
<tr>
<td>Chebyshev deg.2</td>
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</table>

<table>
<thead>
<tr>
<th>Performance Speedup of a Multi-Gaussian Fit (10000 bins)</th>
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</thead>
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<tr>
<td>Speedup of 60x!</td>
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</tbody>
</table>

TF1 based benchmarks. TF1 is the TFormula fitting interface for fitting histograms.
Motivation
Okay, but why AD in RooFit????

Performance comparison AD vs numerical differentiation on hf_001 inspired example

Great results on proof of concept! Next step: integrate this into RooFit

Automatic Differentiation in RooFit

How Does it work?

What we want to differentiate

A typical RooFit statistical model

Made up of various RooFit objects

Feed to AD tool

AD Tool
Automatic Differentiation in RooFit

How Does it work?

What that we want to differentiate

A typical RooFit statistical model

Made up of various RooFit objects

Some way to expose differentiable properties of the graph as code.

C++ code the AD tool can understand

AD Tool

RooFit has an object oriented model which deliberately hides the differential properties of the nodes in favor of ease of use.
Automatic Differentiation in RooFit

How Does it work?

What that we want to differentiate

C++ code the AD tool can understand

Define 2 Functions in RooFit

Stateless function enabling differentiation of each class.

double ADDetail::gauss(double x, double mean, double sigma) {
    const double arg = x - mean;
    const double sig = sigma;
    return std::exp(-0.5 * arg * arg / (sig * sig));
}

The “glue” function enabling graph squashing.

void RooGaussian::translate(...) override {
    result = "ADDetail::gauss(" +
                _x->getResult() +
                "," + _mu->getResult() +
                "," + _sigma->getResult() + ")";
}
Automatic Differentiation in RooFit

*How Does it work?*

What that we want to differentiate

C++ code the AD tool can understand

Define 2 Functions in RooFit

**RooGaussian::evaluate()**
*The RooFit call to evaluate a gaussian*

- **Bookkeeping**
  & **caching**

**ADDetail::gauss(x, mu, sig)**
*The equivalent code generated*

**ADDetail::gauss(x, mu, sig) / ADDetail::gaussIntegral(...)**
*The equivalent code generated (given the class supports analytical integrals)*
Automatic Differentiation in RooFit

The Big Picture

What that we want to differentiate

‘Squash’ the graph into code

Roo*::translate()

C++ code the AD tool can understand

C++ code the AD tool can understand

The AD tool

Derivative code of the model!

+ Clad

Current Status

What Can I Do Right Now?*

```cpp
root[0] RooWorkspace myWS;
root[1] myWS.factory("sum::mu_shifted(mu[0, -10, 10], shift[1.0, -10, 10])");
root[2] myWS.factory("prod::sigma_scaled(sigma[3.0, 0.01, 10], 1.5)");
root[3] myWS.factory("Gaussian::gauss(x[0, -10, 10], mu_shifted, sigma_scaled)");
root[4] RooAbsReal &x = *myWS.var("x");
root[6] RooArgSet normSet{x};
```

*In ROOT master as of May 2023.
Current Status

What Can I Do Right Now?*

```cpp
root[6] RooFuncWrapper gaussFunc("myGauss", "myGauss", pdf, normSet);

(double (*)(double *, const double *)) Function @0x7fcfbd2f6000
at input_line_19:1:

double myGauss(double *params, double const *obs)
{
    const double sigma_scaled = params[2] * 1.5;
    const double mu_shifted = params[0] + params[1];
    const double gauss_Int_x = ADDetail::gaussianIntegral(-10, 10, mu_shifted, sigma_scaled);
    const double gauss = ADDetail::gauss(params[3], mu_shifted, sigma_scaled);
    const double normGauss = gauss / gauss_Int_x;
    return normGauss;
}
```

*In ROOT master as of May 2023.

Current Status

What Can I Do Right Now?*

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root[6] RooFuncWrapper gaussFunc("myGauss", "myGauss", pdf, normSet);

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at input_line_19:1:
double myGauss(double *params, double const *obs)
{
    const double sigma_scaled = params[2] * 1.5;  // "prod::sigma_scaled(sigma[3.0, 0.01, 10], 1.5)"
    const double mu_shifted = params[0] + params[1];  // "sum::mu_shifted(mu[0, -10, 10], shift[1.0, -10, 10])"
    const double gauss_Int_x = ADDetail::gaussianIntegral(-10, 10, mu_shifted, sigma_scaled);
    const double gauss = ADDetail::gauss(params[3], mu_shifted, sigma_scaled);
    const double normGauss = gauss / gauss_Int_x;  // "Gaussian::gauss(x[0, -10, 10], mu_shifted, sigma_scaled)"
    return normGauss;
}
```

*In ROOT master as of May 2023.

Results

**Performance Comparison for Minimization Time**

*model used: gauss + gauss + expo*

Tested on ROOT master as of May 2023.

*Excludes the seed generation time, more info - [look here](#)*

RooFit has clear advantages over “hand-writing” models, but can be pushed more with AD!

18x Faster!

Tested on ROOT master as of May 2023.
*Excludes the seed generation time, more info - look here

## Results

### Why??

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## Results

### Why? Code-Squashing vs RooFit (Numerical)

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~3.5x Slower time/iteration.

**Why?** Even though both use num-diff, RooFit uses complex caching logic, making it faster!

Tested on ROOT master as of May 2023.
## Results

### Why? Code-Squashing AD vs RooFit Numerical

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## Results

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- **~8x Faster Derivatives**
  - **Why?** AD is faster than NumDiff, esp. For large number of params!

- **Faster (and better) Convergence** (for large fits)
  - **Why?** AD is more numerically stable than NumDiff. Less num error = faster convergence!

Tested on ROOT master as of May 2023.
Conclusion
Summary and Future Work

Our work presents an efficient way to translate complex models such that they can be differentiated using AD. We demonstrate that AD can be used to effectively lower the fitting time for non-trivial models.

- Completely avoid the use of numerical gradients in fits using MINUIT.
- Extend support to cover HistFactory and other parts of RooFit.
- Optimize Clad generated derivatives and further explore how they can be parallelized (OpenMP or CUDA).

Work with experiments to show similar speedups on their production workflows.
The End!

Questions?

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

https://github.com/grimmmyshini

garima.singh@cern.ch
Backup
Backup
Model From Benchmarks

A RooPlot of "x_1"

Plot for number of channels = 1
RooRealVar c("c", "c", -0.5, -0.8, 0.2);
RooExponential expo("expo", "expo", x, c);

// Create two Gaussian PDFs g1(x,mean1,sigma) anf g2(x,mean2,sigma) and their parameters
RooRealVar mean1("mean1", "mean of gaussians", 3, 0, 5);
RooRealVar sigma1("sigma1", "width of gaussians", 0.8, .01, 3.0);
RooRealVar mean2("mean2", "mean of gaussians", 6, 5, 10);
RooRealVar sigma2("sigma2", "width of gaussians", 1.0, .01, 3.0);
RooGaussian sig1("sig1", "Signal component 1", x, mean1, sigma1);
RooGaussian sig2("sig2", "Signal component 2", x, mean2, sigma2);

// Sum the signal components
RooRealVar sig1frac("sig1frac", "fraction of signal 1", 0.5, 0.0, 1.0);
RooAddPdf sig("sig", "g1+g2", {sig1, sig2}, {sig1frac});

// Sum the composite signal and background
RooRealVar sigfrac("sigfrac", "fraction of signal", 0.4, 0.0, 1.0);
RooAddPdf model("model"), "g1+g2+a", {sig, expo}, {sigfrac});
Backup

*Share of fitting time for 700 parameters*

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<tr>
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<th>Seeding Time</th>
<th>Minimization Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>RooFit Num-Diff</td>
<td>130 ms</td>
<td>11700 ms</td>
</tr>
<tr>
<td>Code Squashing Num-Diff</td>
<td>723 ms</td>
<td>51762 ms</td>
</tr>
<tr>
<td>Code Squashing AD</td>
<td></td>
<td>652 ms</td>
</tr>
</tbody>
</table>

Seeding uses numerical differentiation = Larger times for AD

Possible Fix? Use AD here too!

Seeding: initial parameter scale estimation to get the step size for the minimization.
Backup

How models are translated

The parent node queries the results from the child nodes.

```cpp
// 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.

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

code += RooNLLVar::Translate();
```
Clad, a compiler based source-code-transformation AD tool. 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;
}
```

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

Can be used within Cling\[^2\], the C++ interpreter used with ROOT.

Off the shelf JIT compiled Derivatives!

\[^2\]:https://github.com/root-project/cling
Large number of parameters usually causes numerical issues\(^3\) with minimizations, leading to fluctuation in step sizes and eventually leading to longer or no convergence.

\(^3\): https://root.cern.ch/root/htmldoc/guides/minuit2/Minuit2.html#convergence-in-mboxmigrad-and-positivedefiniteness
Future Work

Some Interesting Ideas: Partial Code Squashing

Classes supported by AD-Code Squashing

Only Squash classes we support = Can use AD with existing models without requirements!

Classes not supported by AD-Code Squashing
Future Work

Some Interesting Ideas: Partial Code Squashing

Squashed Sub-Graph

RooFit selects to get derivatives by AD here.

Everywhere else, RooFit uses numerical-diff.

Only squash classes we support = Can use AD with existing models without requirements!