RooFit status and plans

Jonas Rembser for the RooFit team, presenting developments by Emmanouil Michalainas, Stephan Hageböck, Lorenzo Moneta, Jonas Rembser, Patrick Bos, Wouter Verkerke, Carsten Burgard, Harshal Shende, Rahul Balasubramanian

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Introduction

- **whoami**: Jonas Rembser, PhD student in CMS (2017-2020)
  - now in core ROOT team at CERN, responsible for RooFit support & development
- **RooFit**: C++ library for statistical data analysis in ROOT
  - provides tools for model building, fitting and statistical tests
- Recent development focused on:
  - **Performance** boost (preparing for larger datasets of **HL-LHC**)
  - More **user friendly** interfaces and high-level tools

In this presentation:

- Report on new **vectorized RooFit** interface with **GPU support** (aka **BatchMode**)
  - **CPU**: up to 10x speed up, **GPU**: up to 50x!
- Overview on other new RooFit features in the upcoming ROOT release **v6.26**
  - Highlight: **pythonizations**!
- Outlook on planned developments
- Some comments on RooFit & **CMS**
1. Faster vectorized RooFit: Now with GPU support
Current (scalar) RooFit computation:

1. Load a single data point into variables
2. Walk whole expression tree (minus cached branches)
3. Obtain one probability. Repeat at 1. with next data point.

This is problematic:

- Simple profiling: 50% L1/L2 cache misses
- No chance to vectorize computations

See RooFit presentation at ICHEP 2020
From scalar to vector computations

- **Evaluate** every RooFit object **once per** fitting **iteration**
  - Iterate over dataset entries in inner loop
- Better compiler optimizations, cache efficiency, **vectorization**, less virtual function calls
- For maximum efficiency:
  - Run multiple CUDA kernels, CPU and GPU computations **concurrently**
- To do this: **RooBatchCompute** library and **RooFitDriver** class explained next

Implementation of Gaussian in old RooFit code and new RooBatchCompute library compared:

```cpp
double RooGaussian::evaluate() const {
  double arg = x - mean;
  return std::exp(-0.5*arg*arg/(sigma*sigma));
}
```

```cpp
__global__ void computeGaussian(Batches batches) {
  auto x = batches[0], mean = batches[1], sigma = batches[2],
           normVal = batches[3];
  for (size_t i = BEGIN; i < batches.getNEvents(); i += STEP) {
    double arg = x[i] - mean[i];
    double halfBySigSq = -0.5 / (sigma[i] * sigma[i]);
    batches._output[i] = fast_exp(arg * arg * halfBySigSq / normVal[i]);
  }
}
```

---

#9004
The RooBatchCompute library

- A new ROOT library containing the code for the vector computations + some few extras
- Compiled multiple times for different target architectures (generic, SSE4.1, AVX, AVX2, AVX512 and CUDA)
  - We reuse code for CPU and CUDA implementations (modulo some #define)
  - Uses thrust, the CUDA C++ template library

- Automatic hardware inspection and loading of the right library at runtime
  - No need to recompile ROOT for your system!
- Handles broadcasting of scalar values to arrays with minimal overhead
- Also supports multithreading via ROOT::EnableImplicitMT()

- Try it out by passing “CPU” or “GPU” to the BatchMode() argument of fitTo():
  - pdf.fitTo(*data, RooFit::BatchMode(“GPU”));
The RooFitDriver approach

- Heterogeneous computing hard to implement with **recursive** interface (e.g. virtual calls to `RooAbsReal::getValV(const RooArgSet* normSet)`)
- We need logic to:
  - **analyze** the computation graph, figure out sizes of result arrays
  - handle **memory** both on the host and the CUDA device
  - choose correct instance of `RooBatchCompute` per call
  - **evaluate** RooFit objects in the correct order
  - manage CUDA streams, **synchronize** results, ...
- The new **RooFitDriver** class is responsible for all of that
- Improved **thread-safety** by bypassing result caching in RooFit objects

Game changer in RooFit implementation!
Computation graph analyzed

- Not all RooFit classes support GPU evaluation
  - RooFitDriver manages **concurrent evaluation** on CPU and GPU
- Host \( \leftrightarrow \) device copying times and CPU/GPU evaluation times are measured
  - This can be done in the first two minimization iterations
  - Decide if an object should be evaluated on the GPU given the **copying overhead**
- Together with multithreading capabilities of RooBatchCompute:
  => we can can use all CPU cores and GPU device for RooFit evaluations!

*Measured run times using RooFitDriver:*

<table>
<thead>
<tr>
<th>Node</th>
<th>Device</th>
<th>Address</th>
<th>CPU time:</th>
<th>CUDA time:</th>
</tr>
</thead>
<tbody>
<tr>
<td>nll</td>
<td>CUDA</td>
<td>0x5575eabb0600</td>
<td>3123 us</td>
<td>355 us</td>
</tr>
<tr>
<td>mean</td>
<td>CPU</td>
<td>0x5575eacc4090</td>
<td>0 us (param.)</td>
<td>nan</td>
</tr>
<tr>
<td>gauss</td>
<td>CUDA</td>
<td>0x5575eacef950</td>
<td>5560 us</td>
<td>376 us</td>
</tr>
<tr>
<td>sigma</td>
<td>CPU</td>
<td>0x5575e8f94e90</td>
<td>0 us (param.)</td>
<td>nan</td>
</tr>
</tbody>
</table>
Benchmark setup

- **CPU**: AMD Ryzen 9 3900 12-Core Processor (24 Threads)
- **GPU**: NVIDIA GeForce RTX 2070 SUPER
  - Note: **gaming GPU** not optimized for double precision (single precision to double precision register ratio 32:1)
  - Much better results expected in a data-center/scientific GPU
- Set up: Perform a full fit
  - Not easy to get benchmarks that represent vast variety of models in the wild
- Multithread results generated using all 24 threads

Some **caveats**:

- **Kahan summation** of log-likelihoods switched off (not implemented on GPU yet)
- **Recovery from invalid parameters** switched off ($\text{RecoverFromUndefinedRegions}(0.0)$)
# Benchmark results

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>Scalar time</th>
<th>Vector-ST (Speedup vs scalar)</th>
<th>Vector-MT (Speedup vs scalar)</th>
<th>CUDA (Speedup vs scalar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 million events</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Gaussian with one observable</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><code>gauss(x)</code></td>
<td>2632 ms</td>
<td>234 ms (11x)</td>
<td>82 ms (32x)</td>
<td>109 ms (24x)</td>
</tr>
<tr>
<td><strong>Gaussian with two observables</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><code>gauss(x,s)</code></td>
<td>1069 ms</td>
<td>116 ms (9x)</td>
<td>39 ms (27x)</td>
<td>63 ms (17x)</td>
</tr>
<tr>
<td><strong>Gaussian plus exponential</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><code>f * gauss(x) + (1-f) * exp(x, c1)</code></td>
<td>9784 ms</td>
<td>908 ms (11x)</td>
<td>238 ms (41x)</td>
<td>197 ms (50x)</td>
</tr>
<tr>
<td><strong>Addition benchmark 1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| `(fx * gauss(x) + (1-fx) * gauss(x)) *  
  (fy * gauss(y) + (1-fy) * poly(y)) * gamma(z)` | 112 s       | 12 s (9x)                     | 3.35 s (33x)               | 2.28 s (49x)            |
| **Addition benchmark 2**                      |             |                               |                               |                          |
| `ns1 * gamma(x) + ns2 * gamma(x) + ng2 *  
  gauss(x) + ng3 * gauss(x) + npol * poly(x)` | 93 s        | 15 s (6x)                     | 4.80 s (19x)               | 3.55 s (26x)            |

*ST = single thread, MT = multithreading*
2. Other new RooFit features
RooFit pythonizations

- PyROOT bindings **more pythonic** in v6.26
- Now you can for example:
  - use **Python keyword arguments** instead of RooFit command arguments
  - pass around **Python sets or lists** instead of RooArgSet or RooArgList
  - pass **Python dictionaries** to functions that take `std::map<>`
  - implicitly convert floats to `RooConstVar` in `RooArgList/Set` constructors
- All pythonizations are documented in the [reference guide](#)
- See also this [ROOT meeting presentation](#)

**Example code from the rf316_llratioplot.py tutorial showcasing the pythonizations:**

```python
# Create background pdf poly(x)*poly(y)*poly(z)
px = ROOT.RooPolynomial("px", "px", x, [-0.1, 0.004])
py = ROOT.RooPolynomial("py", "py", y, [0.1, -0.004])
pz = ROOT.RooPolynomial("pz", "pz", z)
bkg = ROOT.RooProdPdf("bkg", "bkg", [px, py, pz])

# Create composite pdf sig+bkg
fsig = ROOT.RooRealVar("fsig", "signal fraction", 0.1, 0., 1.)
model = ROOT.RooAddPdf("model", "model", [sig, bkg], [fsig])

data = model.generate((x, y, z), 20000)

# Make plain projection of data and pdf on x observable
frame = x.frame(Title="Projection on X", Bins=40)
data.plotOn(frame)
```
Interoperability with NumPy/Pandas

- **ROOT v6.26 new converters** between NumPy arrays/Pandas dataframes and RooDataSet/RooDataHist:
  - RooDataSet.from_numpy()
  - RooDataSet.to_numpy()
  - RooDataSet.from_pandas()
  - RooDataSet.to_pandas()
  - RooDataHist.from_numpy()
  - RooDataHist.to_numpy()

- No translation from RooDataHist to dataframe because histograms are in general multi-dimensional

- New **RooRealVar.bins()** function to get RooFit **bin boundaries** as NumPy array

**Example of exporting RooDataSet to Pandas:**

```python
from ROOT import RooRealVar, RooCategory, RooGaussian

x = RooRealVar("x", "x", 0, 10)
cat = RooCategory("cat", "cat",
                   \{"minus": -1, "plus": +1\})

mean = RooRealVar("mean", "mean", 5, 0, 10)
sigma = RooRealVar("sigma", "sigma", 2, 0.1, 10)

gauss = RooGaussian("gauss", "gauss", x, mean, sigma)

data = gauss.generate((x, cat), 100)
df = data.to_pandas()
```

```
x cat
0   6.997005  -1
1   7.211106  -1
2   3.196248   1
3   5.015624   1
4   7.782308   1
... ... ...
95  6.878027  -1
96  0.475900   1
97  4.451101  -1
98  3.481015  -1
99  4.010105  -1
```

100 rows x 2 columns
For many parameters, most fitting time is spent for the **numeric gradient computation** (re-evaluating after varying each parameter one at a time).

Distributing the **gradient calculation over multiple processes** is a very general way to speed up fitting (see [ACAT 2019 presentation](http://example.com)).

The gradient parallelization will be part of ROOT v6.26 (PR list, last PR #9349).

It comes together with **new likelihood classes** with improved performance for parallelization over entries.

Next year: work on faster gradient calculation with **automatic differentiation (AD)**.

Figure from the ACAT 2019 presentation showcasing the scaling of the gradient parallelization for an ATLAS Higgs combination fit.
There are higher-level tools to build RooFit models in RooWorkspaces (e.g. HistFactory or CMS Higgs combination tool)
  ○ require descriptive languages to define the model (like XML for HistFactory)
  ○ JSON or YAML is more readable and more standard nowadays

The new RooFit (v6.26) includes a new RooJSONFactoryWSTool to import/export RooWorkspaces to JSON or YAML
This can ease interoperability also with other statistics frameworks such as pyhf an zfit

Example on the right: JSON for Gaussian signal with RooArgusBG background
Other new features for v6.26

- **Creating RooFit datasets from RDataFrame** #7317
  - Works for both RooDataSet and RooDataHist
  - Weighted filling still needs to be implemented
  - Tutorial in C++ and Python

- **Global observables in RooFit datasets** #8788
  - Convenient way to store global observable values in RooDataSet/RooDataHist

- **Bin integration for simultaneous fits** #9358
  - v6.24 introduced bin integration option to avoid biases in binned fits
  - v6.26: set bin integration parameter separately for each pdf in RooSimultaneous

Last two features requested by ATLAS! #8788  #7317  #9358
3. RooFit & CMS
● RooFit’s high-level interface for binned fits: **HistFactory**
  ○ Some feature overlap with **CMS Higgs combine tool**...
  ○ ...but RooFit doesn’t have a command line interface
  ○ Higgs combine has yet another declarative language (**“data cards”**)
● For v6.26, targeted **changes to speed up** HistFactory / Higgs combine fits:
  ○ Motivated by [CMS analysis school example](#7907)
  ○ I want to **monitor** more **complex CMS workflows** for speedup ideas
● Potential synergies between RooFit and Higgs combine:
  ○ Identifying speedup possibilities on both sides
  ○ Improving Higgs combine with new RooFit features
  ○ Integrating pdfs from CMS into upstream ROOT
  ○ Common declarative language, also with other fitting frameworks
  ○ **In general:** **avoid duplicate work**
Idea: obfuscated models for validation

- My “dream”: having a **benchmark suite of cutting-edge LHC experiment workflows** to validate RooFit, get ideas for speedups and improvements, and ensure that experiment code still compiles with new releases.

- As RooFit developers, we don’t have the models that are actually used by experiments:
  - Big **hurdle** to realistic RooFit **benchmarking** and **validation**
  - ROOT development and **benchmarking** is public on GitHub, and **RooWorkspaces** by experiments are usually not public.

- Can we improve this situation by **obfuscation**, i.e. `RooWorkspace::obfuscate()`?
  - **Names** of all RooFit objects get obfuscated.
  - **Variable**, **dataset** and **histogram values** would be slightly kicked.

Just an idea so far, your input is welcome.
3. Outlook and summary
Outlook on planned developments

- Continue development on **faster** vectorized **RooFit**
  - Implement more RooFit operations on the **GPU** (e.g. analytic integrals, convolutions)
  - **Concurrent evaluation** of RooFit objects as alternative to parallelizing over entries

- Improve higher-level RooFit tools like **HistFactory**
  - Targeted **performance improvement** for binned fits
  - Make it easier to use and more stable

- Speed up gradient computation with **automatic differentiation**

- Continue to improve **Python** bindings
  - Solve object ownership issues

- **Your idea** here!
Talk summary

- RooFit is **evolving** steadily
  - Support and development from **ROOT team** at CERN
  - Many new features developed by **external contributors**

- Updated **vectorized** RooFit interface (**BatchMode()**) in v6.26
  - New computation library for multiple architectures
  - Significant refactor of RooFit computation graph
  - Up to 10x faster on a single **CPU** thread
  - Up to 50x faster on a gaming **GPU**

- New **pythonizations** and exclusive functions for Python interface, other new features

- more interaction between CMS and RooFit would be beneficial for **both sides**
Useful Links
Useful Links

- **RooFit tutorials** (Recommended! There are notebooks!)
- **RooFit documentation**
- **Release notes** (yet to come for ROOT v6.26)
- Test the faster batch mode:
  - `auto result = pdf.fitTo(*data, RooFit::BatchMode(“GPU”), RooFit::Save());`
  - Note: old scalar computation is the default
- Feature request or bug report? [https://github.com/root-project/root/issues](https://github.com/root-project/root/issues)
  - A new PDF that should go into RooFit?
  - Ideas for Python interfaces?
- Think that a certain workflow should be part of ROOT's tests?
  - [jonas.rembser@cern.ch](mailto:jonas.rembser@cern.ch)