Accelerating RooFit with GPUs …and other RooFit news

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Introduction

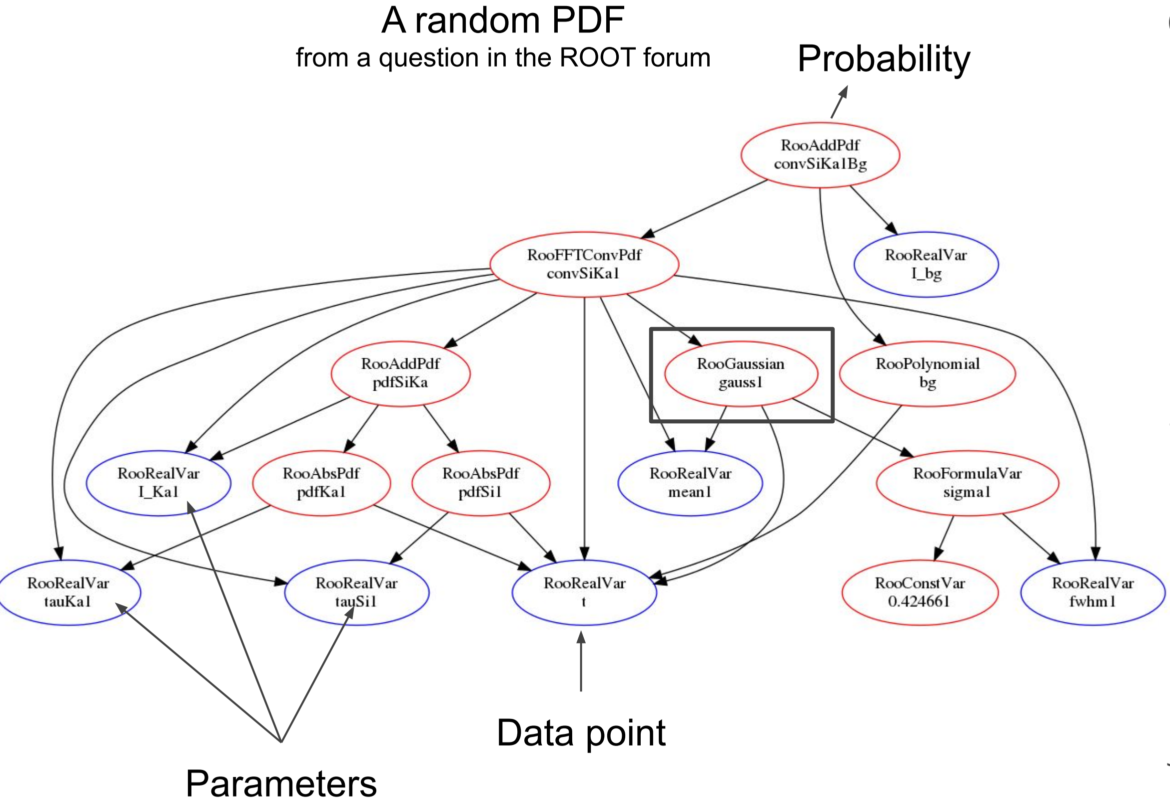
- **RooFit**: C++ library for statistical data analysis in ROOT
  - provides tools for model building, fitting and statistical tests
- Recent development focused on:
  - **Performance** boost (preparing for larger datasets of **HL-LHC**)
  - More **user friendly** interfaces and high-level tools

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

1. Faster vectorized RooFit: Now with GPU support

Why vectorizing RooFit



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

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

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

```
__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];
  }
}
```

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 ⇄ 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`*:*

```
------Copying times------
h2dTime=618us   d2hTime=597us
------Nodes------                        CPU time:          CUDA time:
nll        CUDA      0x5575eabb0600      3123 us            355 us
mean       CPU       0x5575eacc4090      0 us (param.)      nan
gauss      CUDA      0x5575eacef950      5560 us            376 us
sigma      CPU       0x5575e8f94e90      0 us (param.)      nan
```

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 (`RecoverFromUndefinedRegions(0.0)`)

Benchmark results

Benchmark 1 million events	**Scalar time**	**Vector-ST** (Speedup vs scalar)	**Vector-MT** (Speedup vs scalar)	**CUDA** (Speedup vs scalar)
Gaussian with one observable `gauss(x)`	2632 ms	234 ms (11x)	82 ms (32x)	109 ms (24x)
Gaussian with two observables `gauss(x,s)`	1069 ms	116 ms (9x)	39 ms (27x)	63 ms (17x)
Gaussian plus exponential `f × gauss(x) + (1-f) × exp(x, c1)`	9784 ms	908 ms (11x)	238 ms (41x)	197 ms (50x)
Addition benchmark 1 `(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]*

PR list

Example code from the [rf316_llratioplot.py] tutorial showcasing the pythonizations:

```
# 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()`

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- 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:

```
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	6.997865	-1
1	7.211196	-1
2	3.198248	1
3	5.015824	1
4	7.782388	1
...	...	...
95	6.878027	-1
96	0.475900	1
97	4.451101	-1
98	3.481015	-1
99	4.010105	-1

100 rows × 2 columns

Parallelized gradient calculation

- For many parameters, most fitting time is spent for the **numeric gradient computation** (re-evaluatoin 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)
- 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)**

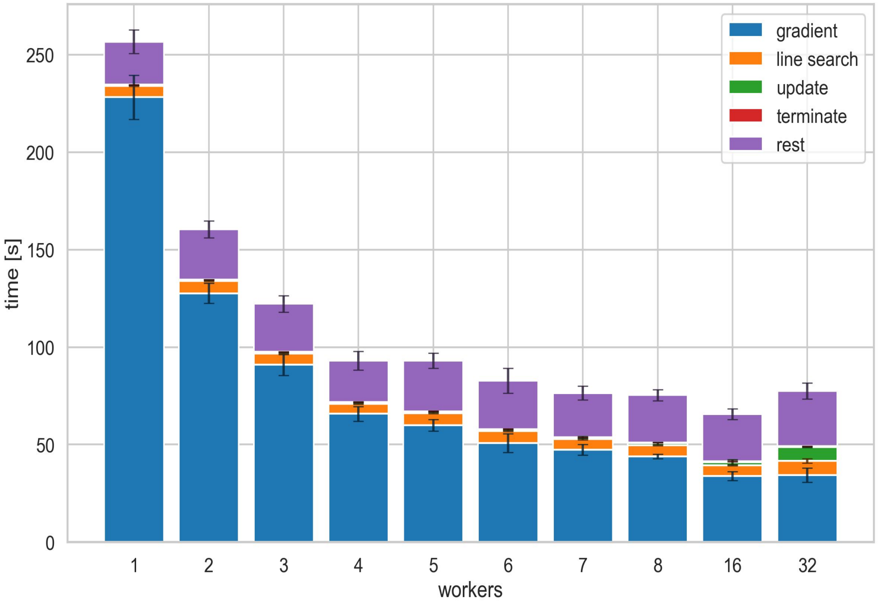

Figure from the ACAT 2019 presentation showcasing the scaling of the gradient parallelization for an ATLAS Higgs combination fit

RooWorkspace ⇄ JSON/YAML

- 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*

```
"pdfs": {
        "signal": {
            "type": "Gaussian",
            "x": "mes", "mean": "sigmean", "sigma": "sigwidth"
        },
        "background": {
            "type": "ARGUS",
            "mass": "mes", "resonance": 5.291,
            "slope": "argpar", "power": 0.5
        },
        "model": {
            "type": "pdfsum",
            "summands": [
                "signal",
                "background"
            ],
            "coefficients": [
                "nsig",
                "nbkg"
            ],
            "tags": [
                "toplevel"
            ]
        }
},
"variables": {
        "mes": { "value": 5.25, "min": 5.2, "max": 5.3 },
        "sigmean": { "value": -5.28, "min": 5.2, "max": 5.3 },
        "nsig": { "value": 200, "min": 0, "max": 10000 },
        "argpar": { "value": -20, "min": -100, "max": -1 },
        "nbkg": { "value": 800, "min": 0, "max": 10000 }
}
```

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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

Last two features requested by **ATLAS!**

- **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
  - ATLAS Higgs combination effort wanted to set the bin integration parameter
  - *v6.26*: set bin integration parameter **separately** for **each pdf** in **`RooSimultaneous`**

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

Please try it out and get in touch with us!

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
    - A new PDF that should go into RooFit?
    - Ideas for Python interfaces?
- Tricky problems? https://root-forum.cern.ch/c/roofit-and-roostats
- Think that a certain workflow should be part of ROOT's tests? jonas.rembser@cern.ch