Data analysis tools from within particle physics and from industry

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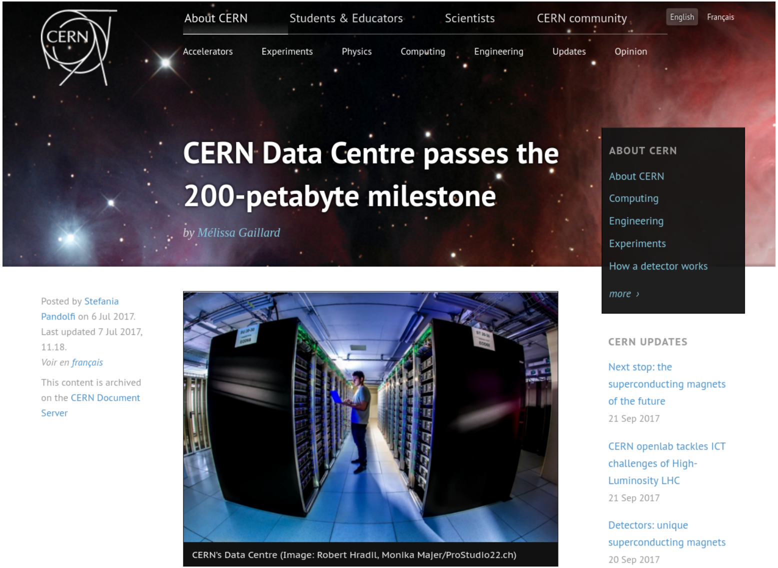
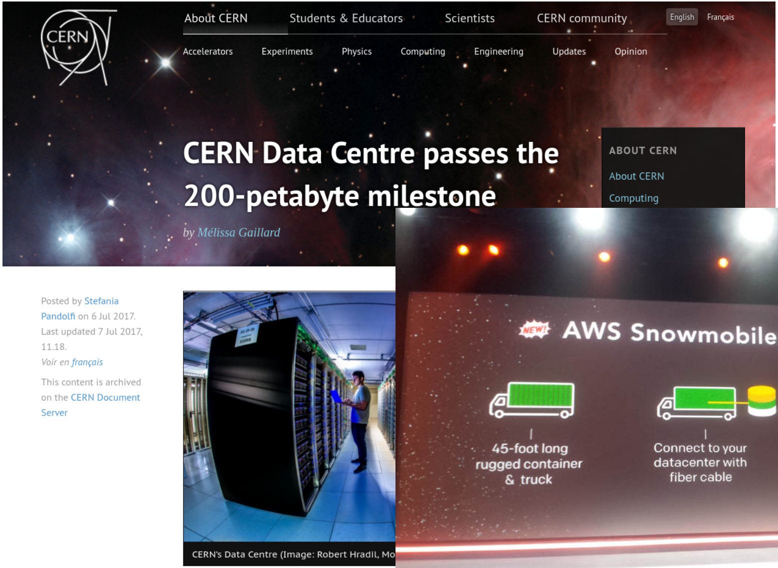
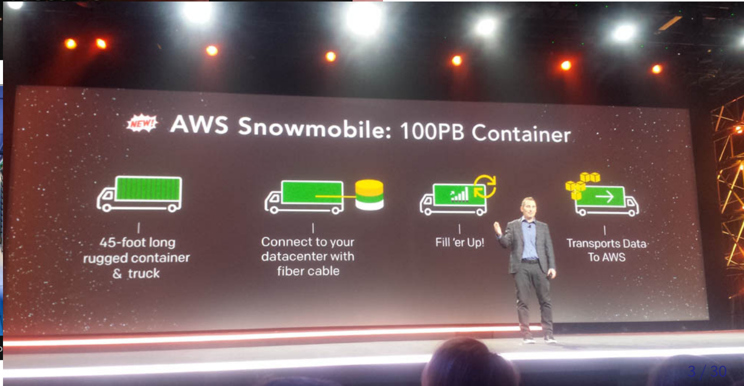
In short, we should become like other sciences, such as astronomy or biology: common libraries for common stuff and our own libraries for domain-specific stuff.

We measure globally distributed data in hundreds of PB

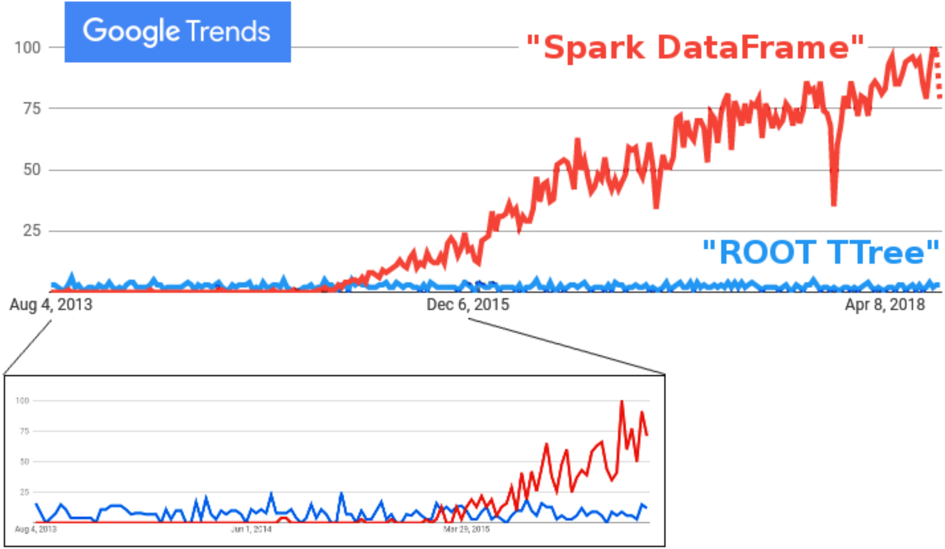


But for web scale companies, 100 PB = 1 truck





Number of people (users and developers) also dwarf our field



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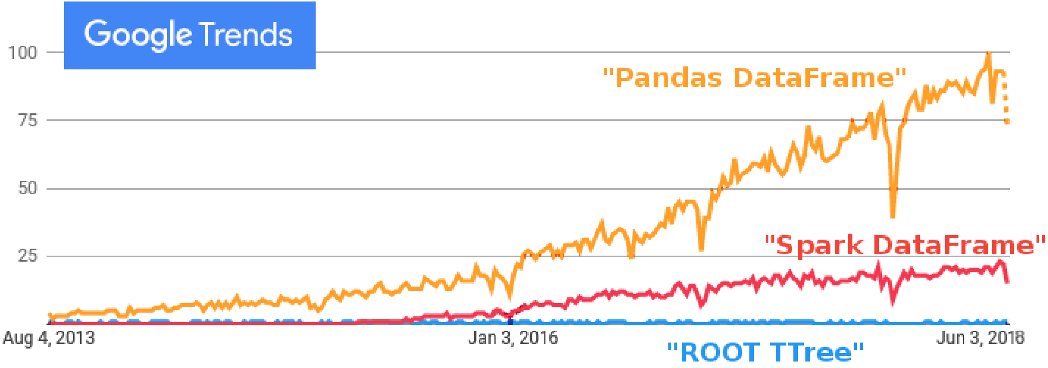

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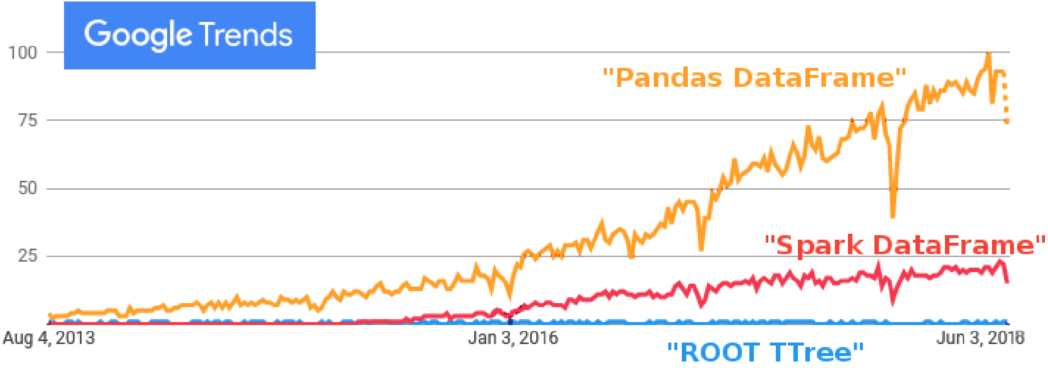

More users means more bug reports, more online help, more how-to blogs. . .

More developers means more bug-fixes, more features, more connectors. . .

Another important metric: experience!

- Physicists have been performing big data analytics (reducing large datasets to statistical inferences) for about 50 years.
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The simple prescription of "just use Spark" would leave analyzers without some necessary tools.

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Continue developing our own everything.

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#3 is my opinion, but what's domain-specific and what's not?

Three examples each:

What web scale software's got

1. Distributed DAG processing
2. Indexed analysis
3. Machine learning

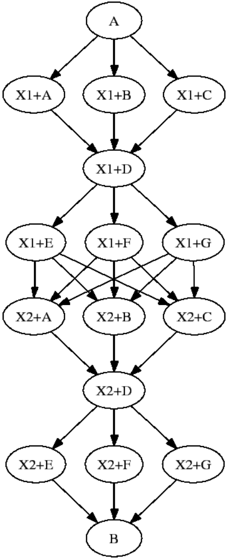
What we need that it hasn't got

1. Nested data structures
2. Advanced histogramming
3. Ansatz fitting

Distributed DAG processing

not physics-specific

Distributed DAG processing



DAG: Directed Acyclic Graph of dependencies between subtasks.
Some would say this is what big data processing *is*.

Many frameworks distribute work this way:

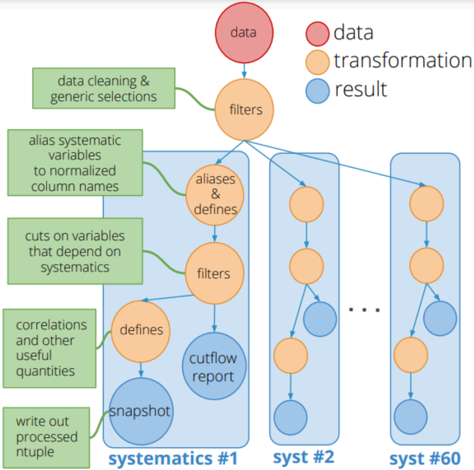
Spark (JVM), Dask, Joblib, Parsl (Python), Storm (continuous), Thrill (C++), DAGMan (HTCondor), TensorFlow (fitting)...

Physics software is embracing this approach:

- RDataFrame in ROOT
- Dozens of other examples at CHEP

RDataFrame from the ROOT Workshop (last week)

Case study: ATLAS SUSY ntuple → ntuple



E. Guiraud, "RDataFrame", ROOT users' workshop 2018

Local ntuple → ntuple processing
MC data is processed to add quantities that are relevant for publication

- ➔ program's **main** reads similarly to this graph
- ➔ the large blue boxes represent one single function that applies the same operations to an RDF variable and is re-used for all different systematics
- ➔ cuts, calculations and writing of the 60 output trees all happen in the same multi-thread event loop

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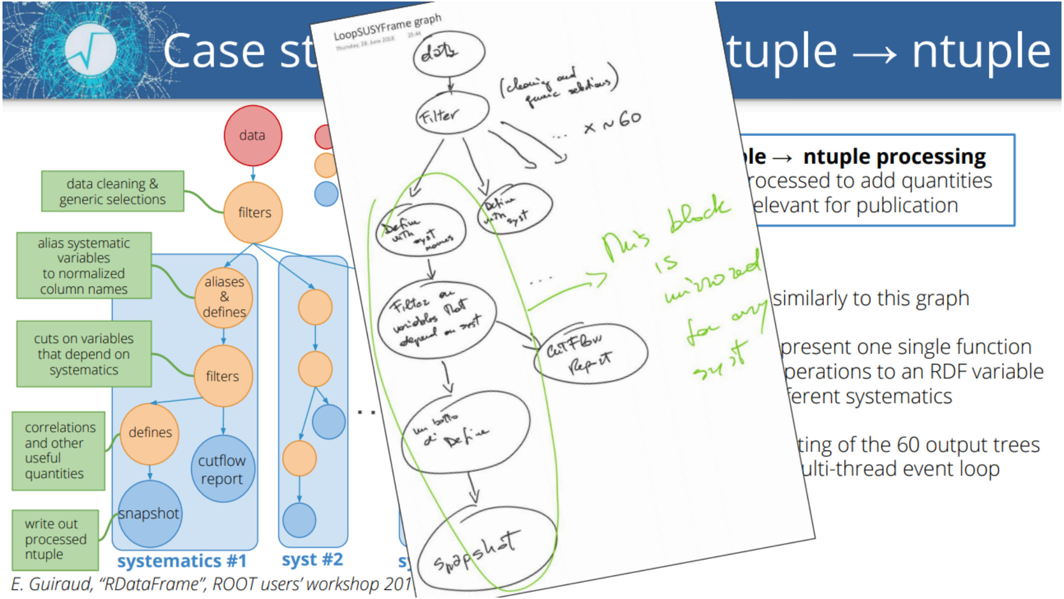

But how will it develop?

Will RDataFrame be a *programming model* that *interfaces* with distributed processing systems such as Spark?

Or will it be *part* of a ROOT *implementation* of distributed DAG processing? A new PROOF, for instance?

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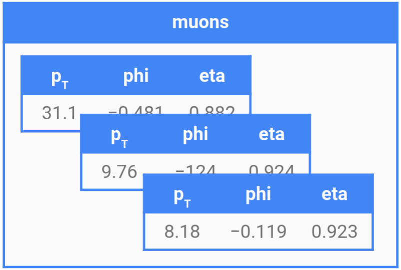
Or will it be *part* of a ROOT *implementation* of distributed DAG processing? A new PROOF, for instance?

Distributing computational tasks with dependencies is a good example of a non-domain-specific problem.

Nested data structures

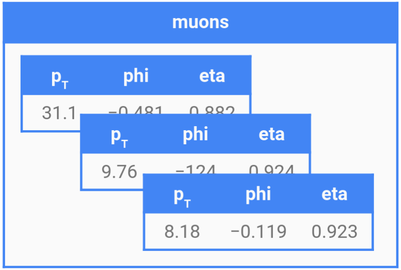
strangely physics-specific, but shouldn't be

Nested data structures



mu1 p_T	mu1 phi	mu1 eta	mu2 p_T	mu2 phi	mu2 eta
31.1	−0.481	0.882	9.76	−0.124	0.924
5.27	1.246	−0.991	n/a	n/a	n/a
4.72	−0.207	0.953	n/a	n/a	n/a
8.59	−1.754	−0.264	8.714	0.185	0.629

Nested data structures



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Objects are essential in physics analysis.

Many physicists consider TTrees with `std::vector<float>` branches to be “minimal” or “flat.”

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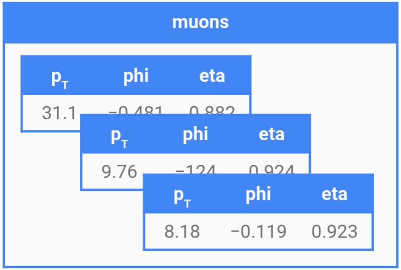

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Most data analysis tools have an SQL mindset, with rectangular data tables.

Objects → rectangular tables is lossy!

Performance claims often start the stopwatch after this “data cleaning.”

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Spark/Parquet/Arrow/HDF5/Pandas
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- HDF5 has lists of compounds, but they're rowwise ("unsplit").
- Pandas can put arbitrary Python objects in DataFrames, but most operations only apply to numbers.

Nested data structures

```
>>> import uproot
>>> t = uproot.open("tests/samples/HZZ.root")["events"]
>>> t.pandas.df(["MET_px", "Muon_Px", "Electron_Px"], entrystart=-20, flatten=False)

         MET_px                 Muon_Px              Electron_Px
2401   2.998099             [-1.492689]                       []
2402  27.944883             [-4.560287]                       []
2403   3.787466             [-9.715589]                       []
2404   9.378232            [-31.072098]                       []
2405 -17.310106   [47.484627, 4.6953125]                       []
2406 -81.965927   [74.75617, -20.911081]                       []
2407  -9.059591 [25.786427, -29.265024]                       []
2408  25.649775                      []                       []
2409  29.691553              [-24.7368]                       []
2410 -25.754967 [53.005814, -30.208649]  [-37.681973, 18.453588]
2411  -2.426847   [55.7203, -26.914448]                       []
2412 -15.611773             [14.896802]                       []
2413  18.921183            [-24.158083]                       []
2414 -11.730723             [-9.204197]                       []
2415 -10.648725  [34.506527, -31.56778]                       []
2416 -14.607650            [-39.285824]                       []
2417  22.208313             [35.067146]                       []
2418  18.101646            [-29.756786]                       []
2419  79.875191             [1.1418698]                       []
2420  19.713749             [23.913206]                       []
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In some cases, maybe we're using the wrong idiom: instead of working with structured values, Pandas prefers structured indexes.

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entry subentry
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2404  0            9.378232  -31.072098          NaN
2405  0          -17.310106   47.484627          NaN
      1                 NaN    4.695312          NaN
2406  0          -81.965927   74.756172          NaN
      1                 NaN  -20.911081          NaN
2407  0           -9.059591   25.786427          NaN
      1                 NaN  -29.265024          NaN
2408  0           25.649775         NaN          NaN
2409  0           29.691553  -24.736799          NaN
2410  0          -25.754967   53.005814   -37.681973
      1                 NaN  -30.208649    18.453588
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2415  0          -10.648725   34.506527          NaN
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This is my main project now: fast manipulation of columnar data.

General programming model

```python
@numba.jit     # LLVM-compiled Python
def deltaphi(event):
    metphi = event.MET.phi
    for jet in event.jets:
        yield metphi - jet.phi
```

Numpy-like broadcasting

Awkward Array

```python
# one per event          one per particle
event["MET"]["phi"] - event["jet"]["phi"]
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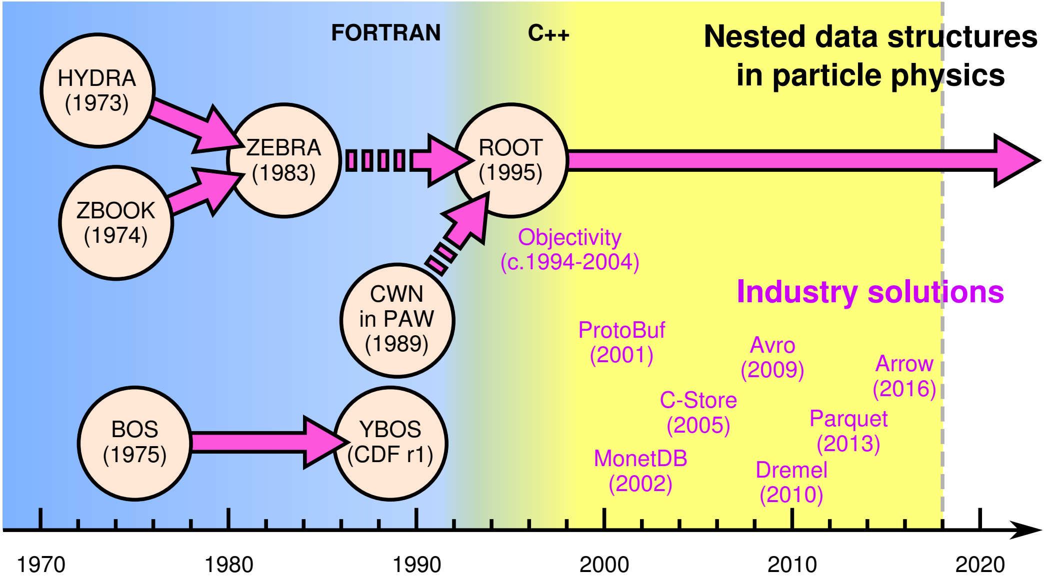
Also, this *should* be of wider interest than physics: developers of Arrow, Dask, and XND (∼Numpy 2.0) are curious about it.

Missed opportunity



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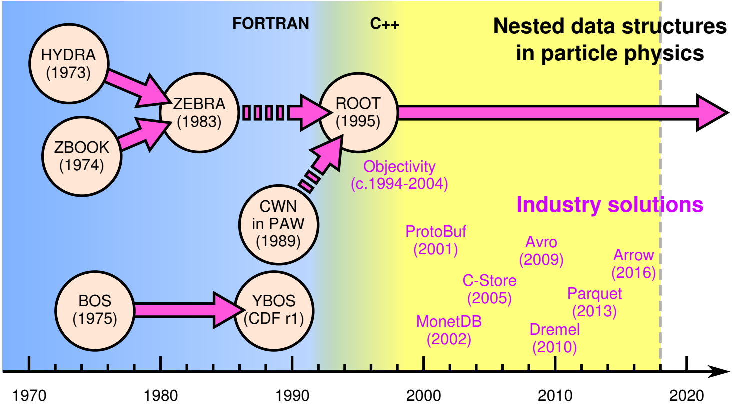
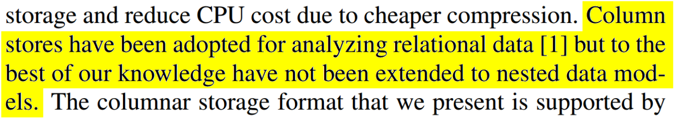


Google Dremel paper (2010):
(inspired Parquet)



storage and reduce CPU cost due to cheaper compression. Column stores have been adopted for analyzing relational data [1] but to the best of our knowledge have not been extended to nested data models. The columnar storage format that we present is supported by

Indexed analysis

not well-known in our field

What is indexing?

A way of organizing analysis:

- PAW/HBOOK histograms were indexed by *integer IDs*
- ROOT histograms are indexed by *string names*
- ROOT TTrees are indexed by *integer entry numbers*
- Excel spreadsheets are indexed by *integer row and letter column IDs*
- SQL tables are indexed by *unordered sets*
- Pandas DataFrames are indexed by *ordered, structured series*

Pandas is not a TTree replacement!

Most of Pandas's functionality is about manipulating data by index, and the whole DataFrame must fit in memory.

```python
result = left.join(right, how="inner")
```

left

	A	B
K0	A0	B0
K1	A1	B1
K2	A2	B2

right

		C	D
K0	Y0	C0	D0
K1	Y1	C1	D1
K2	Y2	C2	D2
K2	Y3	C3	D3

Result

		A	B	C	D
K0	Y0	A0	B0	C0	D0
K1	Y1	A1	B1	C1	D1
K2	Y2	A2	B2	C2	D2
K2	Y3	A2	B2	C3	D3

None (?) of TTree's functionality is about manipulating data by index, and it's focused on lazily loading large datasets.

Pandas DataFrames resemble histograms, not TTrees

Histograms are mappings from intervals to weighted counts and their errors.

Profiles are mappings from intervals to weighted means and standard deviations.

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(Stop making arrays and `std::maps` of TH3!)

Indexed analysis

```
>>> from histbook import *
>>> multihist = Hist(
...     bin("mass", 100, 0, 500), cut("q1*q2 < 0"),
...     split("mt1", [0.2, 0.5]), split("mt2", [0.2, 0.5]), fill=df)
>>> multihist.pandas()
                  MultiIndex key                         Columns
---------------------------------------------------+---------------------
                                                   | count() err(count())
mass           q1*q2 < 0 mt1         mt2           |
[-inf, 0.0)    fail      [-inf, 0.2) [-inf, 0.2)   |     0.0          0.0
                                     [0.2, 0.5)    |     0.0          0.0
                                     [0.5, inf)    |     0.0          0.0
                         [0.2, 0.5)  [-inf, 0.2)   |     0.0          0.0
                                     [0.2, 0.5)    |     0.0          0.0
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                                     [0.5, inf)    |     0.0          0.0
               pass      [-inf, 0.2) [-inf, 0.2)   |     0.0          0.0
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>>> multihist.step("mass")
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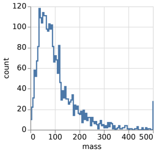

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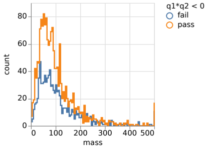
>>> multihist.overlay("q1*q2 < 0").step("mass")
```



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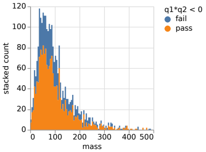
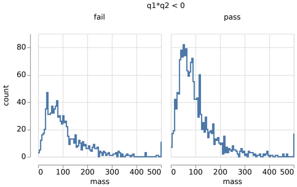
>>> multihist.stack("q1*q2 < 0").area("mass")
```



Indexed analysis

```
>>> from histbook import *
>>> multihist = Hist(
...         bin("mass", 100, 0, 500), cut("q1*q2 < 0"),
...         split("mt1", [0.2, 0.5]), split("mt2", [0.2, 0.5]), fill=df)
>>> multihist.beside("q1*q2 < 0").step("mass")
```



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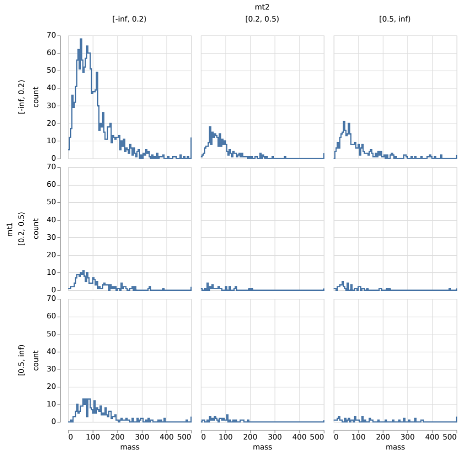
>>> multihist.below("mt1").beside("mt2").step("mass")
```



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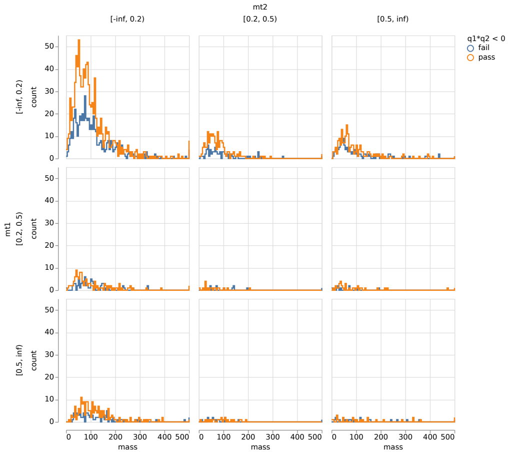
>>> multihist.below("mt1").beside("mt2").overlay("q1*q2 < 0").step("mass")
```



From “Pandas DataFrames for F.A.S.T. binned analysis at CMS”

			name	pass	total
component	depth	class			
data	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	16208	469384
		LambdaStr	ev: ev.triggerIsoMu24[0]	16208	16208
		LambdaStr	ev: ev.Muon_Pt[0] > 25	15995	16208
dy	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	37559	77729
		LambdaStr	ev: ev.triggerIsoMu24[0]	37559	37559
		LambdaStr	ev: ev.Muon_Pt[0] > 25	37263	37559
qcd	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	0	142
		LambdaStr	ev: ev.triggerIsoMu24[0]	0	0
		LambdaStr	ev: ev.Muon_Pt[0] > 25	0	0
single_top	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	111	5684
		LambdaStr	ev: ev.triggerIsoMu24[0]	111	111
		LambdaStr	ev: ev.Muon_Pt[0] > 25	110	111
ttbar	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
wjets	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
ww	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
wz	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
zz	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev: ev.triggerIsoMu24[0]	1235	1235
		LambdaStr	ev: ev.Muon_Pt[0] > 25	1232	1235

Example Cut-flow Dataframe

```
# Apply an event selection
Selection:
    Selection:
        All:
            - len(ev.Muon_Iso_Idx) >= 2
            - ev.triggerIsoMu24[0]
            - ev.Muon_Pt[0] > 25
```

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10 July 2018, b.krikler@cern.ch 13 FAST: Pandas-based binned analysis

Pandas DataFrames filled by AlphaTwirl, analyzed by F.A.S.T.

From "Pandas DataFrames for F.A.S.T. binned analysis at CMS"

Manipulating DFs: Long to wide form

```python
# Convert variance --> error
df["err"] = np.sqrt(df.nvar)

# Switch to long-form
df2 = df.pivot_table(index="dimu_mass", columns="component", values=["n", "err"])
df2 = df2.sort_index(axis=1, ascending=False)

# Sort components to match tutorial
order = ["data", "ttbar", "wjets", "dy", "ww", "wz", "zz", "qcd", "single_top"]
df2 = df2.reindex(order, axis=1, level="component")

# Show first 10 rows
df2.head(10)
```

	n								err		
component	**data**	**ttbar**	**wjets**	**dy**	**ww**	**wz**	**zz**	**single_top**	**data**	**ttbar**	**wjets**
dimu_mass											
-inf	993.0	11.392980	0.311917	655.570771	3.600221	0.320914	0.360053	1.741041	31.511903	1.752727	0.311917
60.000000	38.0	0.840432	0.000000	23.963227	0.063284	0.053328	0.000000	0.065288	6.164414	0.486302	0.000000
61.000000	25.0	0.319709	NaN	25.572841	0.102053	0.000000	NaN	0.005831	5.000000	0.275655	NaN
62.000000	22.0	0.274432	NaN	29.271624	0.068484	0.038697	NaN	0.000000	4.690416	0.274432	NaN
63.000000	28.0	0.000000	NaN	22.941727	0.194258	0.000000	0.009475	NaN	5.291503	0.000000	NaN
64.000000	29.0	0.847224	NaN	20.534599	0.065338	0.081642	0.009540	NaN	5.385165	0.490427	NaN
65.000000	17.0	0.352667	NaN	29.464412	0.130224	0.000000	0.004153	0.093700	4.123106	0.282423	NaN
66.000000	37.0	0.570011	NaN	27.861013	0.128668	0.059988	0.015375	0.000000	6.082763	0.403615	NaN
67.000000	34.0	0.817704	NaN	34.173523	0.063818	0.000000	0.017707	0.000652	5.830952	0.475827	NaN
68.000000	31.0	0.753107	NaN	26.971645	0.024008	0.042326	0.000000	0.000000	5.567764	0.440761	NaN

Depending on task, "wide-form" tables can be easier to work with

Pandas DataFrames filled by AlphaTwirl, analyzed by F.A.S.T.

Advanced histogramming

very physics-specific

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The histograms themselves, however, are more sophisticated in particle physics software than elsewhere.

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These features are our responsibility.

Machine learning versus ansatz fitting

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We can look to industry for machine learning innovations, but the best ansatz fitters are in our field: RooFit, GooFit, HistFitter, HistFactory, Combiner, pyhf...

Areas of overlap

What they've got

1. Distributed DAG processing
2. Indexed analysis
3. Machine learning

What we'd need

1. Nested data structures
2. Advanced histogramming
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What we'd need

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Nearly all ML techniques require flattened or sequences of flattened data, but we have real problems that need nested data: e.g. classifying N_i jets per event (nested, unordered sets). RNNs and LSTMs (for non-nested, ordered sequences) are designed for a different data type!

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F.A.S.T. and histbook are incorporating Pandas indexing into advanced histogramming.

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As fits get bigger, they may need to be distributed, for instance with iterative map-reduce.

Conclusions

Data analysis tools outside of particle physics are mature but not a perfect fit to our needs.

- Some of what we need is available now: can we use it?
- Some exists only as physics software: can it interoperate?
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Data analysis tools outside of particle physics are mature but not a perfect fit to our needs.

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- Some of what's available is unlike anything we do now: an opportunity to do better physics?
- The door swings both ways: we have things to teach the world!