

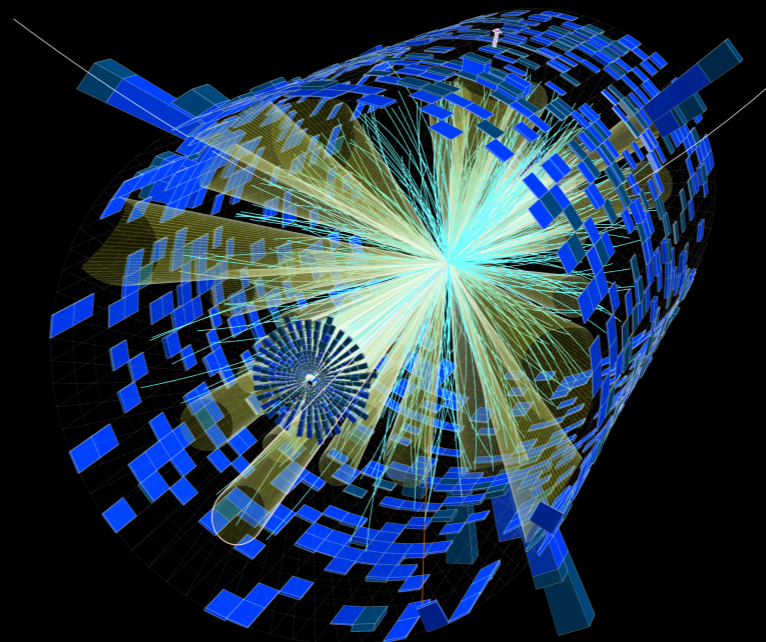


NYU CENTER
FOR DATA
SCIENCE

CENTER FOR
COSMOLOGY AND
PARTICLE PHYSICS



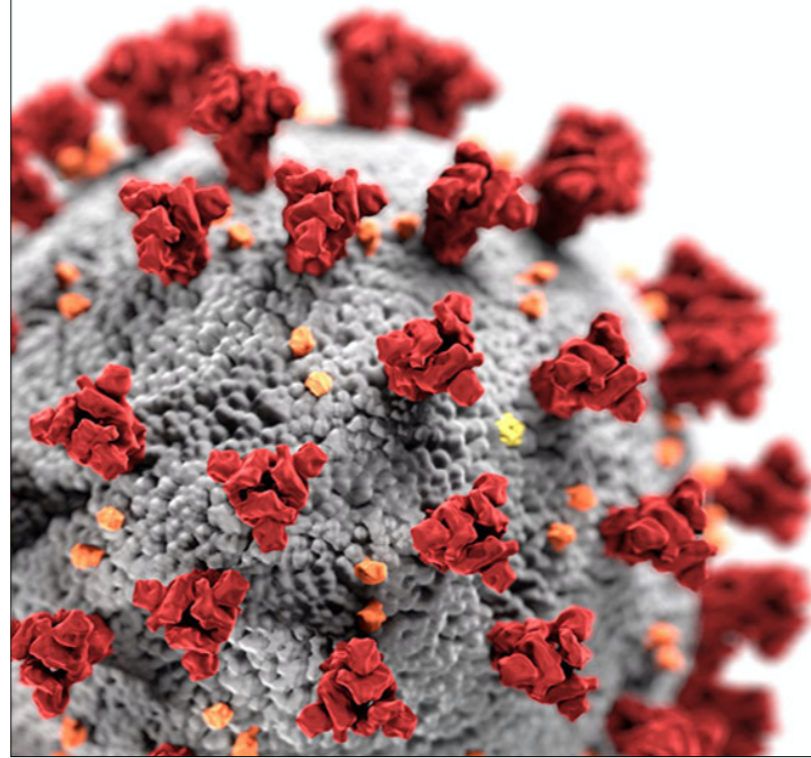
FUTURE ANALYSIS SYSTEMS



@KyleCranmer

New York University
Department of Physics
Center for Data Science
CILVR Lab

Sorry if this is a little disorganized, COVID has complicated work life



SUPPORT



The SCAILFIN Project
scailfin.github.io



ACKNOWLEDGEMENTS

EP-IT Data science seminars

HEP in the Cloud Computing and Open Science Era

by Lukas Alexander Heinrich (CERN)

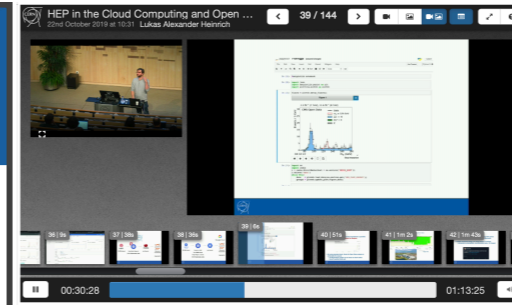
📅 Wednesday 23 Oct 2019, 11:00 → 12:00 Europe/Zurich
📍 500/1-001 - Main Auditorium (CERN) <https://indico.cern.ch/event/840837/>

Description As the LHC readies for Run-3 and its second decade of data-taking, the world around us is changing rapidly. Since the discovery of the Higgs boson in 2012 cloud computing has fundamentally changed the style and access of distributed computing, Deep Learning and Data Science have entered the public vocabulary and Open Science and Reproducibility has been grown in importance. The LHC experiment, with their vast amounts of data, unique dataset is necessarily find themselves at the forefront of these developments. In this talk, I will discuss about how these trends enable new research avenues and data analysis capabilities, such as a systematic reinterpretation program for Beyond the Standard Model search using cloud-native workflows and RECAST, "rediscovering" the Higgs boson in CERN Open Data within a few minutes on the cloud, to enabling third-party research through open access to high-fidelity data products of LHC searches the wider HEP community.

📎 DataScience23.10... 📎 data_science_semi... 📎 Recording

Organized by M. Girone, M. Elsing, L. Moneta, M. Pierini..... **Coffee will be served at 10h30**

Webcast 📺 There is a live webcast for this event [Watch](#)



 **Scalable cyberinfrastructure applications**
Team: J. Brehmer^{1,2}, K. Cranmer^{1,2}, Irina Espejo^{1,2}, S. Macaluso^{1,2} and H. Müller²
Institutions: ¹Center for Data Science, New York University ²Department of Physics, New York University  The SCAILFIN Project

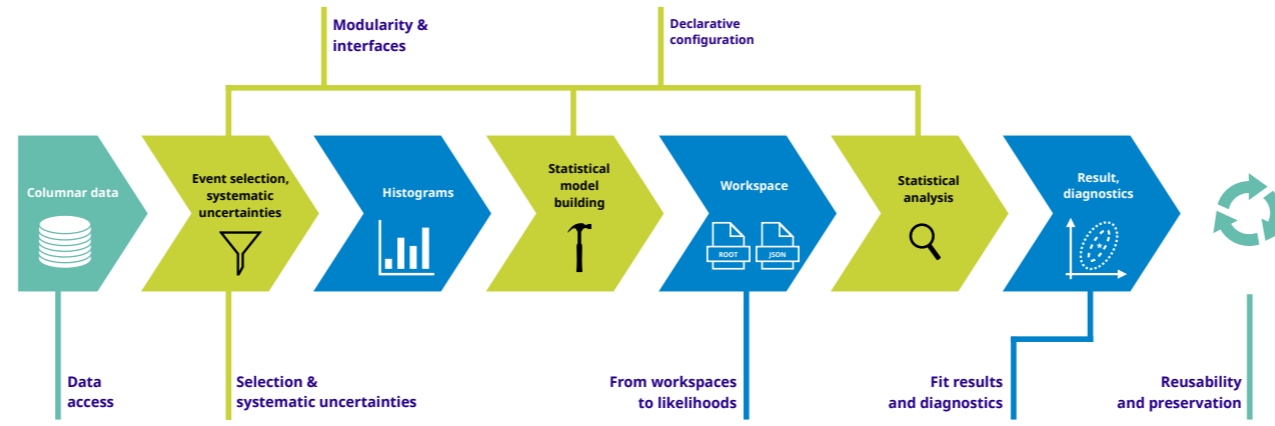


 **Matthew Feickert**
@HEPfeickert

Thanks to everyone at #SciPy2019 who came and asked me great questions about pyhf!



ANALYSIS SYSTEMS



TOPICS

Accelerating analysis design

- more powerful observables
- end-to-end optimization
- benchmarking of algorithms

Accelerating fitting

- pyhf and a fitting service

More efficient simulation

- excursion
- Probabilistic programming

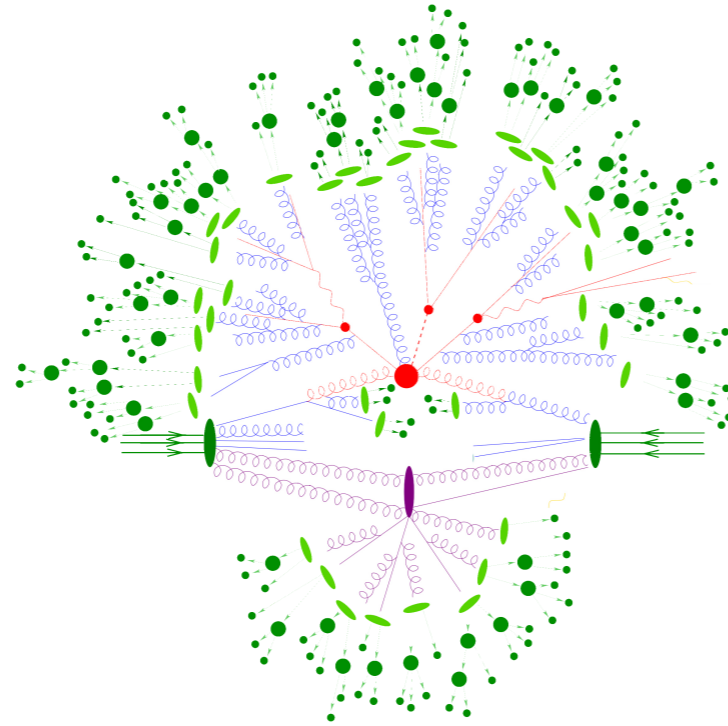
Extending impact of results

- RECAST

Core technologies:

- automatic differentiation
- GPUs & TPUs
- Cloud-native : docker, kubernetes
- Workflows & REANA
- Functions as a service Accelerating analysis design

PREDICTIONS IN PARTICLE PHYSICS



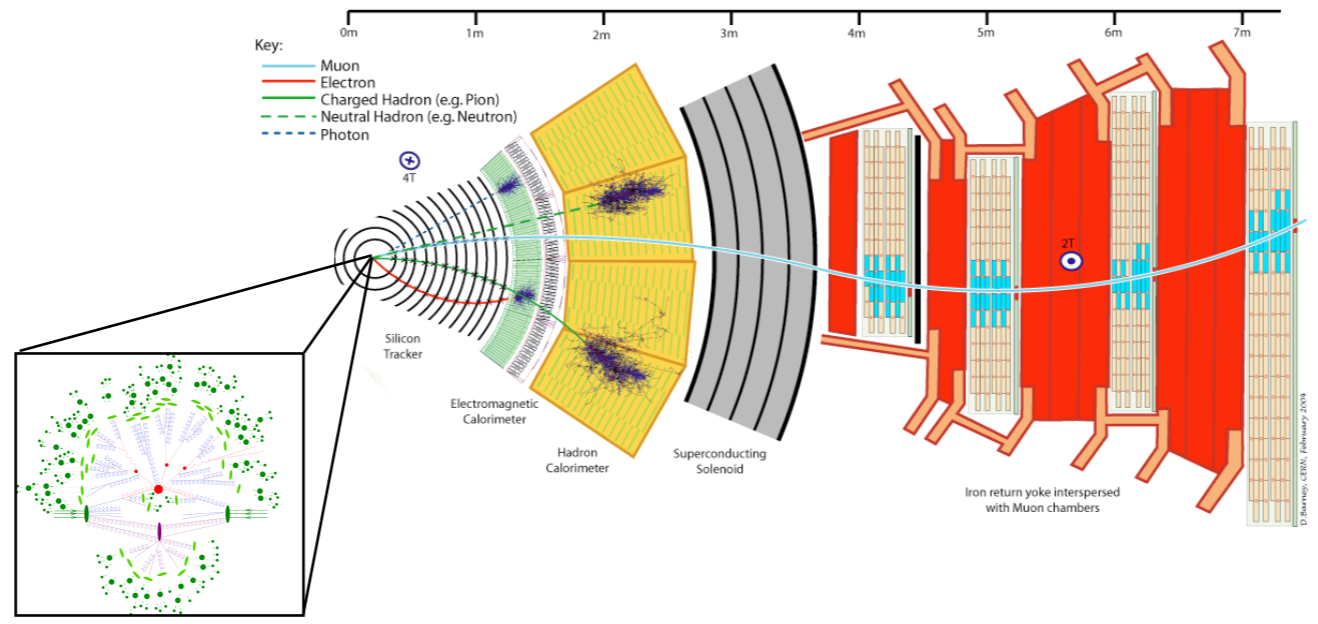
$$\begin{aligned}
 \mathcal{L}_{SM} = & \underbrace{\frac{1}{4} \mathbf{W}_{\mu\nu} \cdot \mathbf{W}^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} G_{\mu\nu}^a G^{a\mu\nu}}_{\text{kinetic energies and self-interactions of the gauge bosons}} \\
 & + \underbrace{\bar{L} \gamma^\mu (i\partial_\mu - \frac{1}{2} g \boldsymbol{\tau} \cdot \mathbf{W}_\mu - \frac{1}{2} g' Y B_\mu) L + \bar{R} \gamma^\mu (i\partial_\mu - \frac{1}{2} g' Y B_\mu) R}_{\text{kinetic energies and electroweak interactions of fermions}} \\
 & + \underbrace{\frac{1}{2} |(i\partial_\mu - \frac{1}{2} g \boldsymbol{\tau} \cdot \mathbf{W}_\mu - \frac{1}{2} g' Y B_\mu) \phi|^2 - V(\phi)}_{W^\pm, Z, \gamma, \text{ and Higgs masses and couplings}} \\
 & + \underbrace{g'' (\bar{q} \gamma^\mu T_a q) G_\mu^a}_{\text{interactions between quarks and gluons}} + \underbrace{(G_1 \bar{L} \phi R + G_2 \bar{L} \phi_e R + h.c.)}_{\text{fermion masses and couplings to Higgs}}
 \end{aligned}$$

DETECTOR SIMULATION

Conceptually: $\text{Prob}(\text{detector response} \mid \text{particles})$

Implementation: Monte Carlo integration over micro-physics

Consequence: evaluation of the likelihood is intractable

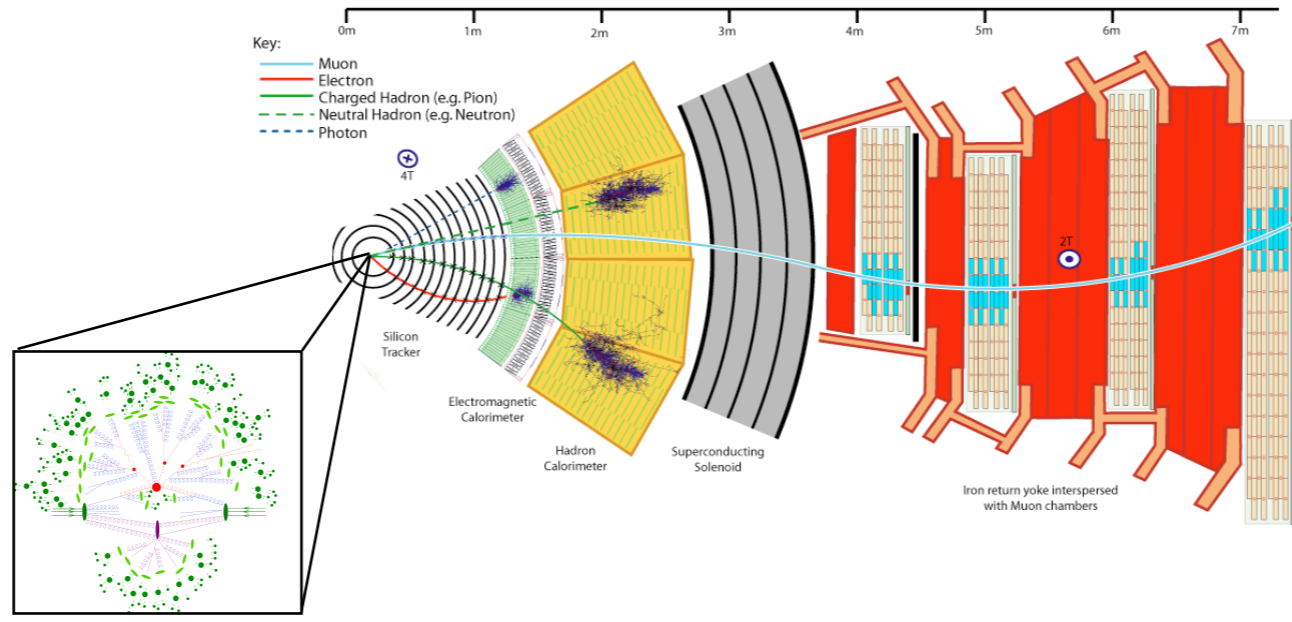


THE CAUSAL, GENERATIVE MODEL

Observables Detector interactions Shower splittings Parton-level momenta Theory parameters

$x \longleftarrow z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$

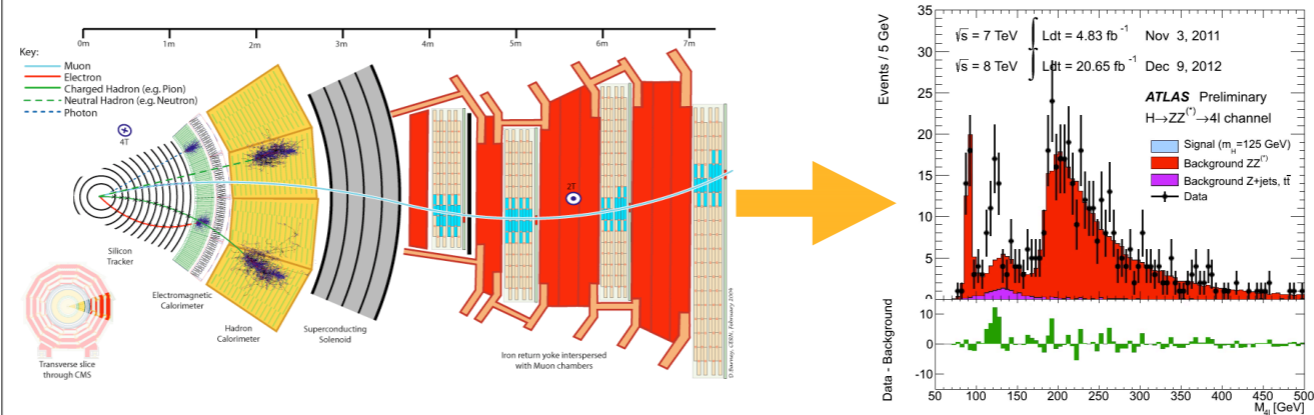
$$p(x|\theta) = \int dz_d \int dz_s \int dz_p p(x|z_d) p(z_d|z_s) p(z_s|z_p) p(z_p|\theta)$$



10^8 SENSORS \rightarrow 1 REAL-VALUED QUANTITY

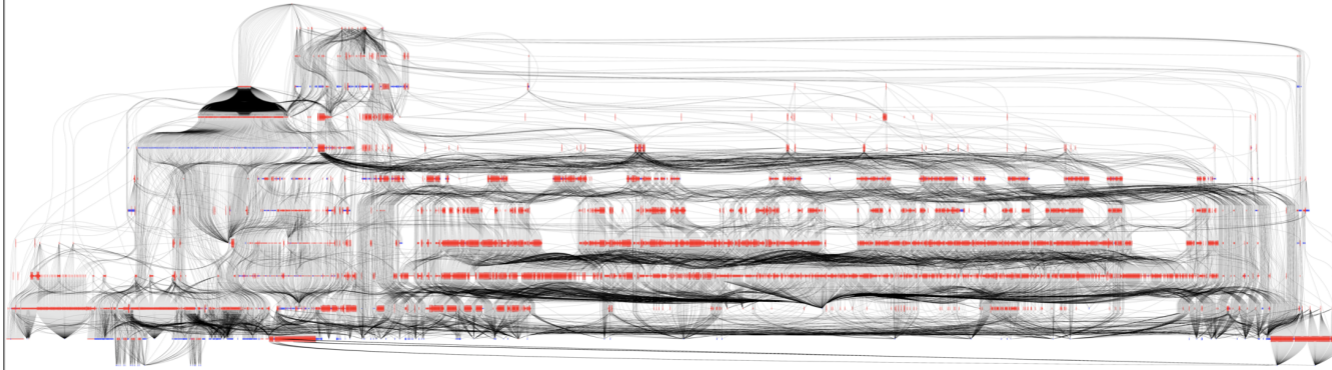
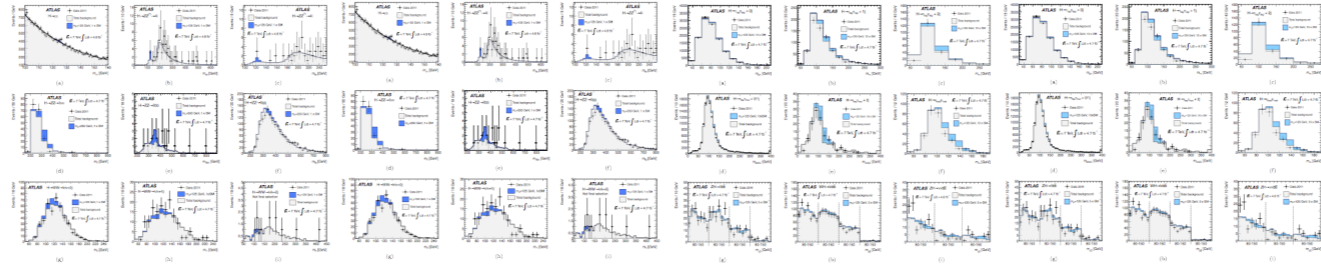
Most measurements and searches for new particles at the LHC are based on the distribution of a single summary statistic

- choosing a good summary statistic (feature engineering) is a task for a skilled physicist and tailored to the goal of measurement or new particle search
- likelihood $p(x|\theta)$ **approximated** using histograms (univariate density estimation)



This doesn't scale if x is high dimensional!

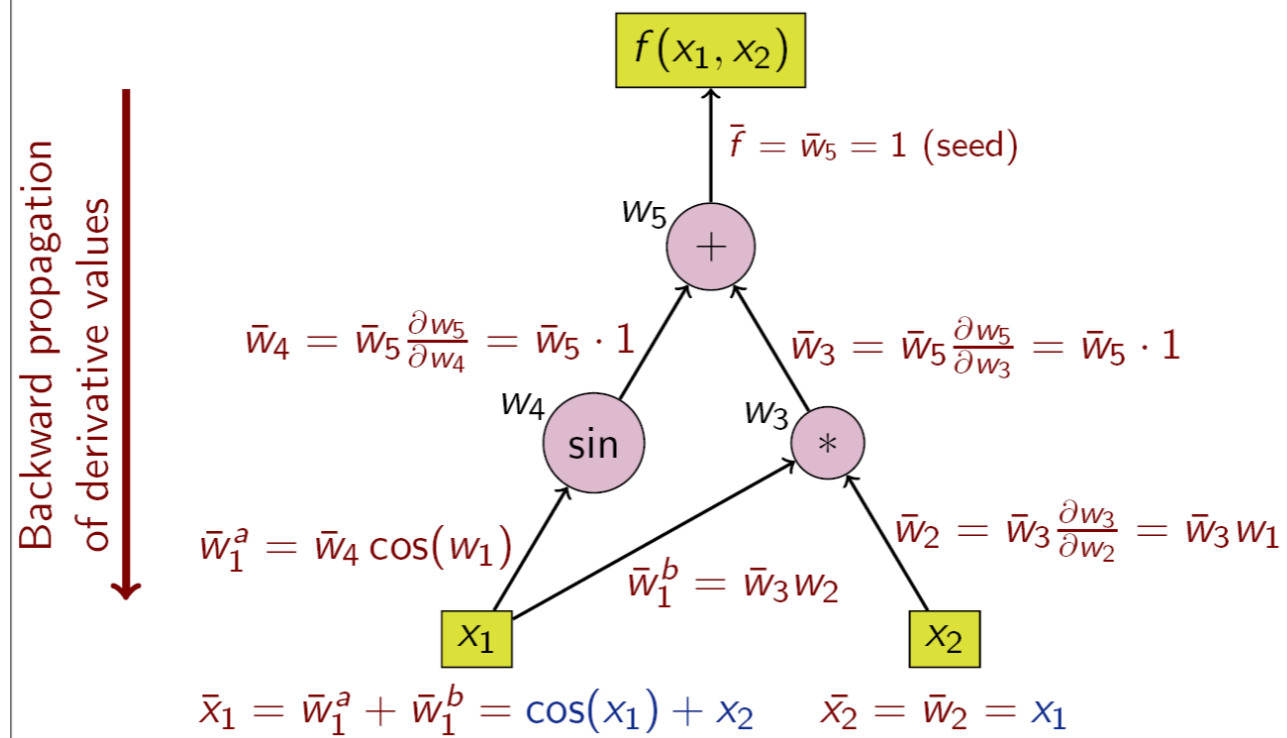
THE DISCOVERY OF THE HIGGS BOSON



$$\mathbf{f}_{\text{tot}}(\mathcal{D}_{\text{sim}}, \mathcal{G} | \boldsymbol{\alpha}) = \prod_{c \in \text{channels}} \left[\text{Pois}(n_c | \nu_c(\boldsymbol{\alpha})) \prod_{e=1}^{n_c} f_c(x_{ce} | \boldsymbol{\alpha}) \right] \cdot \prod_{p \in \mathcal{S}} f_p(a_p | \alpha_p)$$

AUTOMATIC DIFFERENTIATION

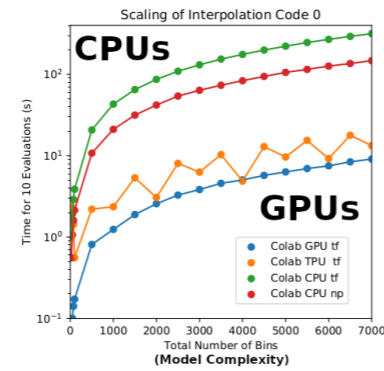
2. **reverse accumulation** computes the recursive relation: $\frac{dy}{dw_i} = \frac{dy}{dw_{i+1}} \frac{dw_{i+1}}{dw_i}$ with $w_0 = x$.



OTHER ADVANTAGES OF USING TENSOR BACKENDS

Slide from Matthew Feickert

- All numerical operations implemented in **tensor backends** through an API of n -dimensional array operations
- Using deep learning frameworks as computational backends allows for **exploitation of auto differentiation (autograd) and GPU acceleration**
- As huge buy in from industry we benefit for free as these frameworks are **continually improved** by professional software engineers



- Preliminary results
- Show hardware acceleration giving **order of magnitude speedup** for some models!
- Hardware acceleration benchmarking planned
- Improvements over traditional
 - 10 hrs to 30 min; 20 min to 10 sec

MAKING IT STANDARD

10 years later: community embraces publishing likelihoods as a standard

- Moved to JSON schema

The screenshot shows the CERN website with a navigation bar at the top containing 'ABOUT', 'NEWS', 'SCIENCE', 'RESOURCES', 'SEARCH', and 'EN'. A news banner at the top right features a photo of the CERN building and the headline 'CERN Council appoints Fabiola Gianotti for second term of office as CERN Director General'. Below this is a 'LATEST NEWS' section with three article thumbnails. The main article on the left is titled 'New open release allows theorists to explore LHC data in a new way' and includes a sub-headline 'The ATLAS collaboration releases full analysis likelihoods, a first for an LHC experiment' and the author 'By Katarina Anthony'. The article features an image of a laptop displaying data on a desk. To the right of the main article is a 'Related Articles' section with three smaller article thumbnails. At the bottom right of the page is the 'pyLHf differentiable Likelihoods' logo, which includes a stylized particle detector diagram and the text 'pyLHf differentiable Likelihoods'. A red diagonal line is drawn across the page from the top left to the bottom right.

New open release allows theorists to explore LHC data in a new way

The ATLAS collaboration releases full analysis likelihoods, a first for an LHC experiment

9 JANUARY, 2020 | By Katarina Anthony



Explore ATLAS open likelihoods on the HEPData platform (Image: CERN)

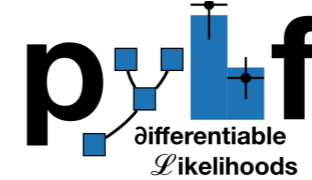
What if you could test a new theory against LHC data? Better yet, what if the expert knowledge needed to do this was captured in a convenient format? This tall order is now on

Display a menu y from the ATLAS collaboration, with the first open release of full analysis likelihoods

Related Articles



[View all news >](#)



FITTING SERVICE

With JSON format, it is much easier to stream necessary data to a fitting service.

- Lukas prototyped this using functions-as-a-service

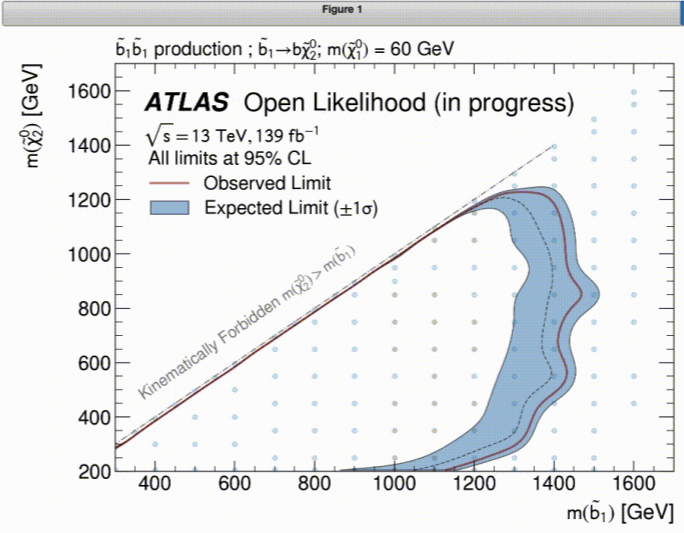
Ideally have a machine with a big GPU or TPU for this

- From 10 min to a few seconds!

Accessing Fitting Service

```
def func(data):
    filename = data['filename']
    region = data['region']
    m = re.compile('bottom_(d+)_(\d+)_(\d+)').search(filename).group(0)
    outname = 'results/region{}.result.{}.json'.format(region,m)
    for i in range(10):
        try:
            d = requests.post(
                '{}/region{}'.format(FITTING_SVC,region),
                data = open(filename), headers = {'Content-Type': 'application/json'})
            .json()
            json.dump(d,open(outname,'w'))
            break
        except:
            pass#retry
```

```
[4]: %matplotlib notebook
fig,ax = plt.subplots(1,1)
fig.set_size_inches(9.33,7)
apply_decorations(ax,label = 'Open Likelihood (in progress)')
```



The figure is a scatter plot with overlaid contours. The x-axis is labeled $m(\tilde{b}_1)$ [GeV] and ranges from 400 to 1600. The y-axis is labeled $m(\tilde{b}_2)$ [GeV] and ranges from 200 to 1600. A diagonal line from the bottom-left to the top-right is labeled 'Kinematically Forbidden $m(\tilde{b}_2) > m(\tilde{b}_1)$ '. The plot contains blue dots representing data points. A red line represents the 'Observed Limit' and a blue shaded region represents the 'Expected Limit ($\pm 1\sigma$)'. Text in the plot includes: 'ATLAS Open Likelihood (in progress)', ' $\sqrt{s} = 13$ TeV, 139 fb^{-1} ', and 'All limits at 95% CL'. The plot title is \tilde{b}_1, \tilde{b}_2 production ; $\tilde{b}_1 \rightarrow b\tilde{\chi}_2^0$; $m(\tilde{\chi}_1^0) = 60$ GeV.

No handles with labels found to put in legend.

```
[*]: for x in glob.glob('results/*.json'):
    os.unlink(x)
cA = [{'region': 'A', 'filename': f} for f in glob.glob('RegionA/patch*_60.json')]
cC = [{'region': 'C', 'filename': f} for f in glob.glob('RegionC/patch*_60.json')]
configs = cA[:] + cC[:]
# np.random.shuffle(configs)

import time
import concurrent.futures
fig.canvas.draw()

with concurrent.futures.ThreadPoolExecutor(max_workers=MAX_WORKERS) as executor:
    for i, _ in enumerate(tqdm(executor.map(func, configs), total = len(configs))):
        if i > 5 and i % 5 == 0:
            make_plot(ax,label = 'Open Likelihood (in progress)', color = 'steelblue', showPoints = True)
            fig.canvas.draw()
            time.sleep(.005)
make_plot(ax, label = 'Open Likelihood', color = 'gold', showPoints = False)
```

35% 91/259 [01:55-01:54, 1.468/s]

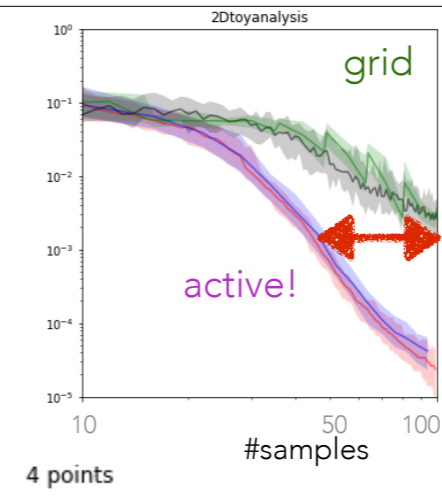
/home/jovyan/interpolate.py:365: UserWarning: No contour levels were found within the data range.
c = ax.contour(xi,yi,zi, [level])

ACTIVE LEARNING

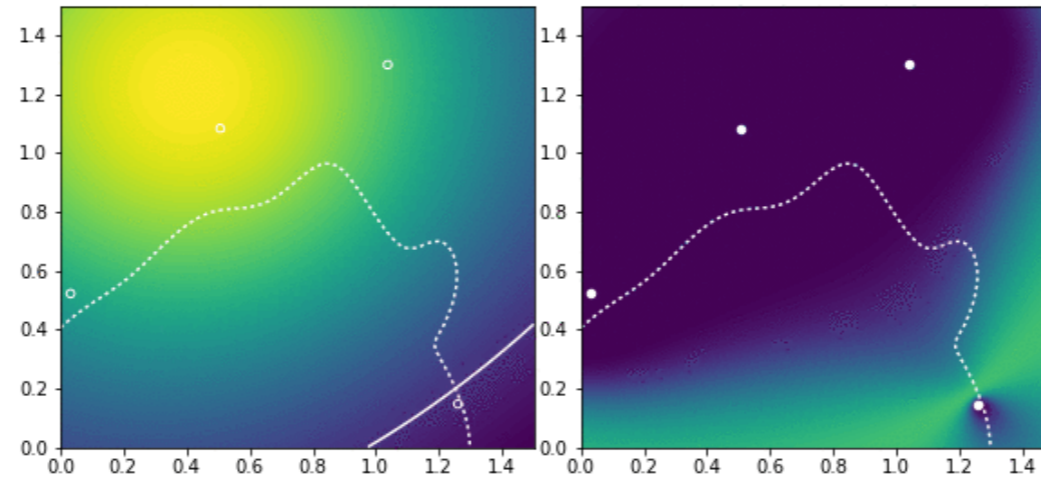
Instead of generating Monte Carlo a priori, generate it on demand where it is relevant!

↓ An algorithm for finding exclusion contours

Drastically more efficient use of computing resources →



K.C., Lukas Heinrich, Gilles Louppe, ACAT2019



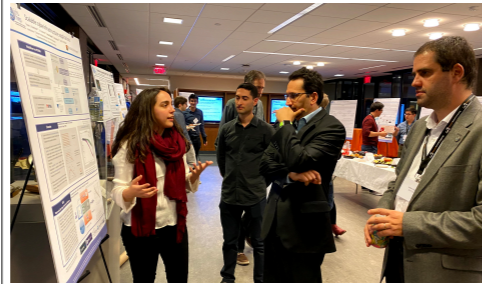
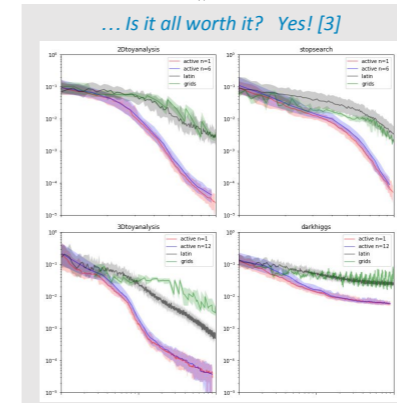


Excursion

in collaboration with G. Louppe² and L. Heinrich³
²University of Liège, ³CERN

diana-hep/excursion
irinaespejo/excursion

- Goal is to find *level sets of black-box functions* that are expensive to evaluate. Examples: test statistics from complex simulations.
- Evaluate the black box function at *interesting points only* instead of evaluating at whole regular grid. We use a *Gaussian process* to: interpolate between samples and model uncertainty in the knowledge of the black box function. The *acquisition function* regulates the exploration vs exploitation tradeoff. Select one that *minimizes global uncertainty* of the location of the excursion set.
- Future: efforts will focus on *scalability* wrt the dimensionality of the function domain space. Example, likelihood ratio as function of mass, charge, spin,...



README.md

<https://indico.cern.ch/event/708041/contributions/3269754/>

excursion — Efficient Excursion Set Estimation

DOI: [10.5281/zenodo.1634427](https://doi.org/10.5281/zenodo.1634427) [launch](#) [binder](#) [build](#) [passing](#)

This package implements a Bayesian Optimization procedure based on Gaussian Processes to efficiently determine excursion sets (or equivalently iso-surfaces) of one or many expensive black-box functions.

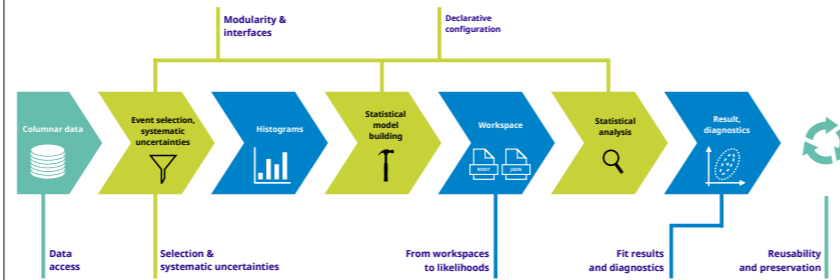
Installation and Example

Install via `pip install excursion==0.0.1a0`.

DIFFERENTIABLE PROGRAMING

Automatic differentiation is not just for Machine Learning!

- Differentiable Programming
- **Attitude:** we can auto-diff through analysis and reconstruction
- End-to-end optimization

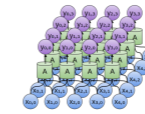


• Convolutional Neural Networks are a close relative of map. A normal map applies a function to every element. Convolutional neural networks also look at neighboring elements, applying a function to a small window around every element.³



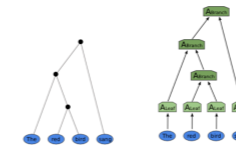
Windowed Map = Convolutional Layer
Haskell: zipWith a xs (tail xs)

Two dimensional convolutional neural networks are particularly notable. They have been behind recent successes in computer vision. (More on conv nets.)



Two Dimensional Convolutional Network

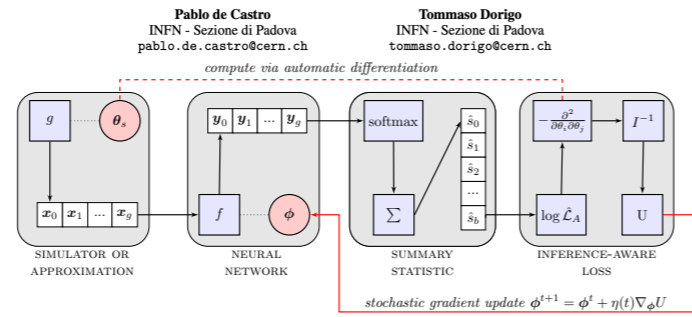
Recursive Neural Networks ("TreeNets") are catamorphisms, a generalization of folds. They consume a data structure from the bottom up. They're mostly used for natural language processing, to allow neural networks to operate on parse trees.



Catamorphism = TreeNet
Haskell: cata a

END-TO-END OPTIMIZATION WITH AUTODIFF

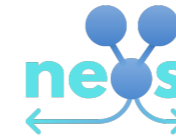
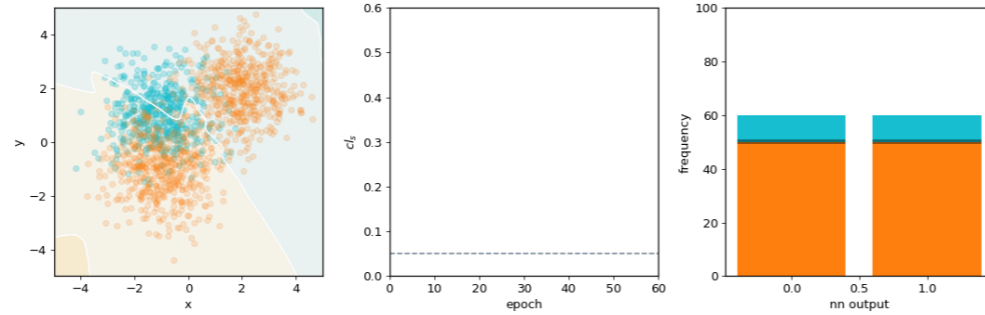
INFERNO: Inference-Aware Neural Optimisation



Kyle Cranmer @KyleCranmer · 19h
 Take note! Here is a nice example of differentiable programming. It shows end-to-end optimization of a NN for event categorization wrt. final statistical analysis (using pyhf). Requires running gradients through results of maximum likelihood with fixed-point differentiation 🍌

Nathan Simpson @ CERN @phi_nate
 I'm *very* excited to share with you what I've been working on recently in collaboration with @lukasheinrich_!
 We've developed a module that performs end-to-end learning with respect to statistical inference in particle physics.
 try it yourself at [github.com/pyhf/neos!](https://github.com/pyhf/neos) :)

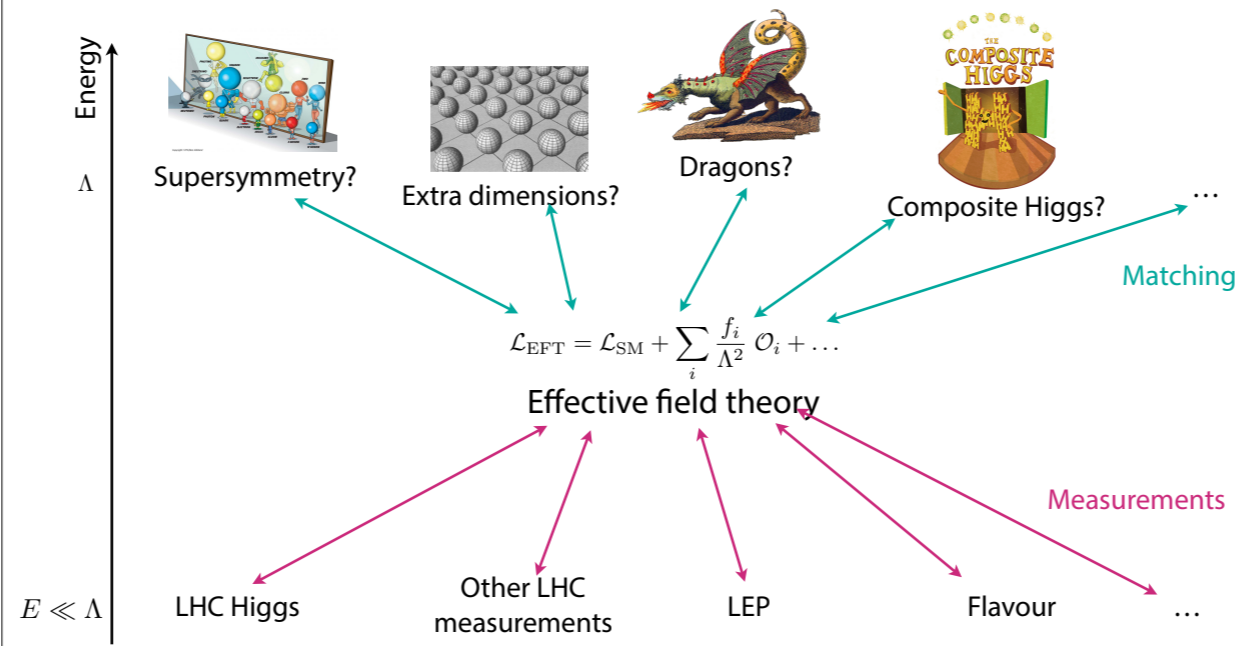
Backpropagate: dLimit / dSelection including full statistical treatment with systematics.



<https://github.com/pyhf/neos>

Effective field theory

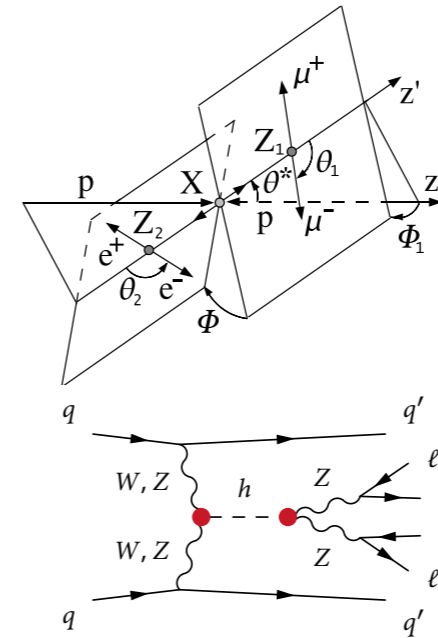
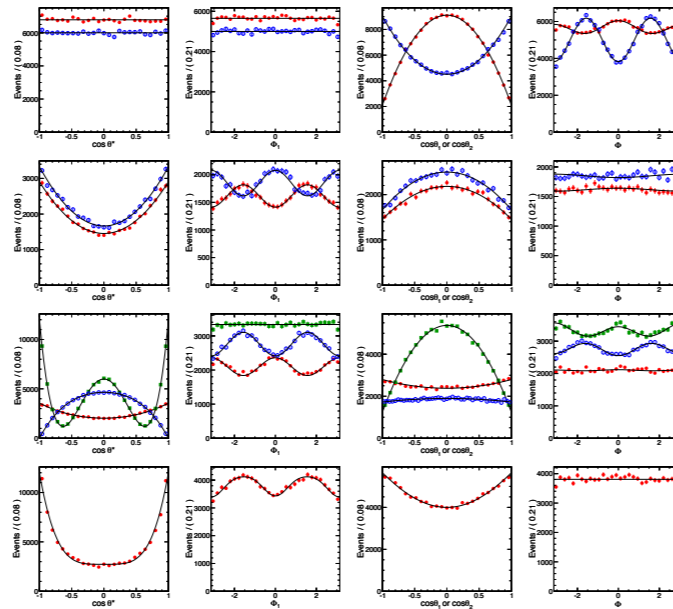
[STFC / Ben Gililand, Sean Carroll, Friedrich Justin Bertuch 1806, symmetry]



HIGH DIMENSIONAL EXAMPLE

When looking for deviations from the standard model Higgs,
we would like to look at all sorts of kinematic correlations

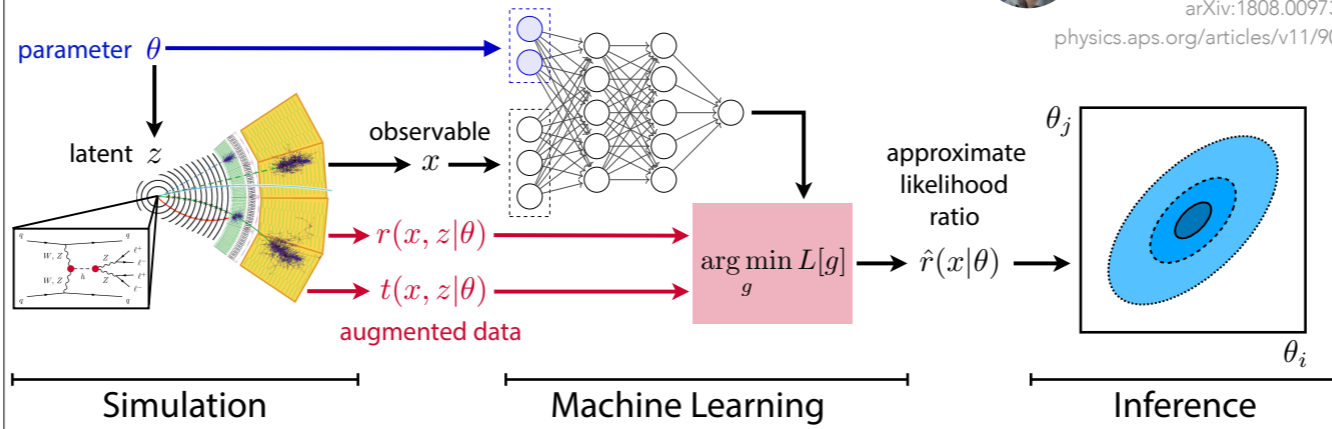
- thus each observation \mathbf{x} is high-dimensional



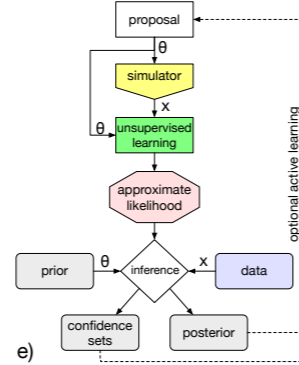
LEARNING THE LIKELIHOOD RATIO



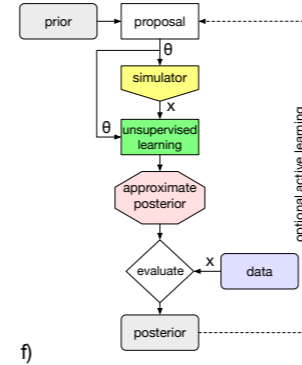
arXiv:1805.12244
 PRL, arXiv:1805.00013
 PRD, arXiv:1805.00020
 arXiv:1808.00973
physics.aps.org/articles/v11/90



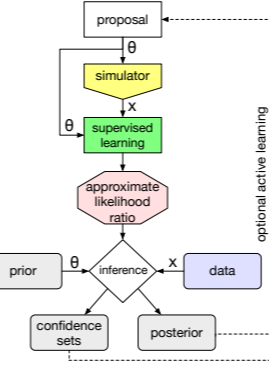
Amortized likelihood



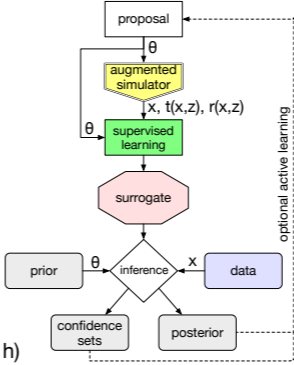
Amortized posterior



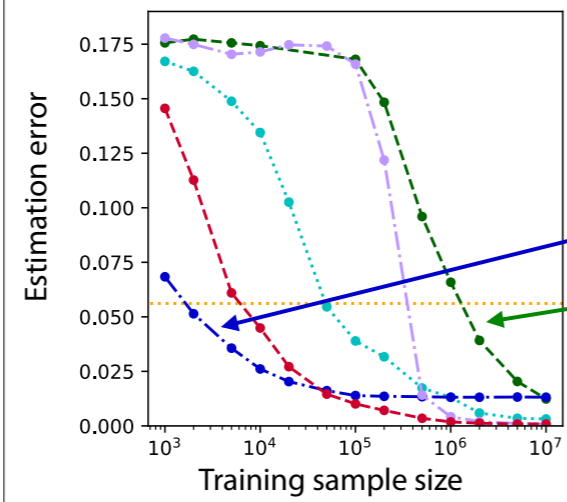
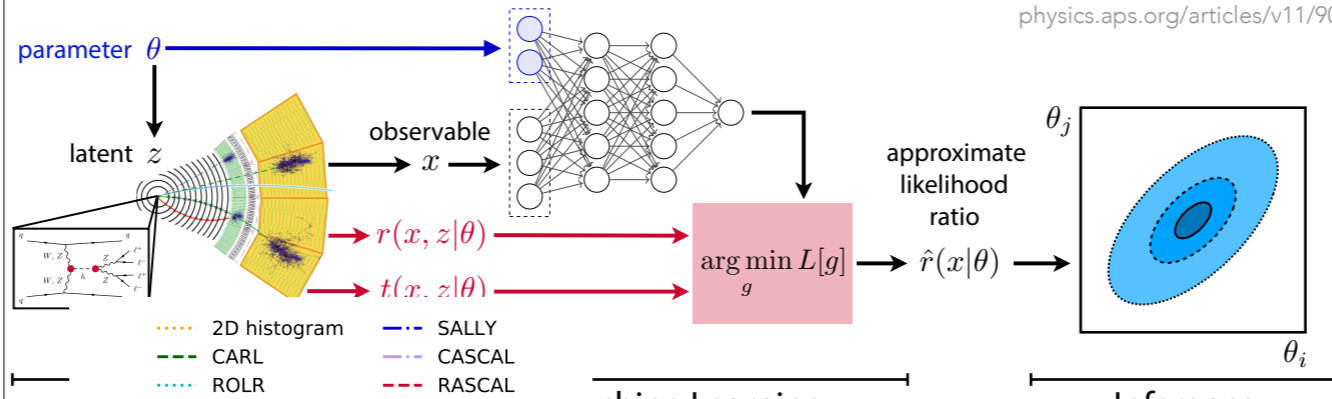
Amortized likelihood ratio



Amortized surrogates trained with augmented data



LIKELIHOOD-FREE INFERENCE



Machine Learning

We can use **augmented data** to dramatically improve training

Inference

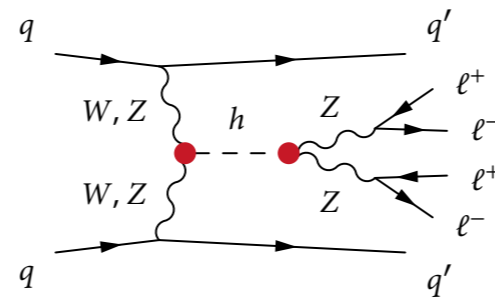
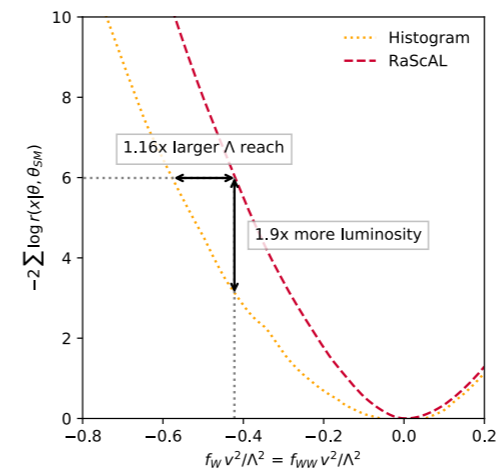
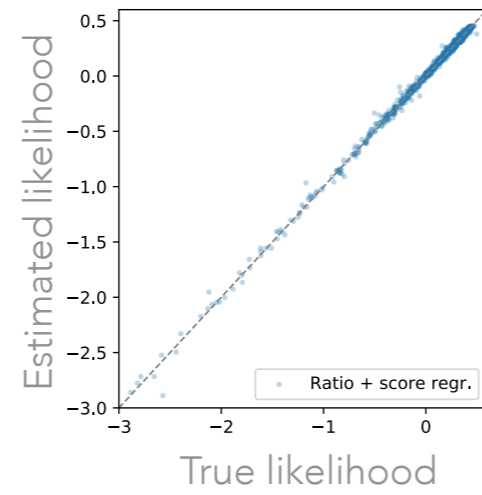
with augmented data

without augmented data

Technically similar to PDF weights

IMPACT ON STUDIES OF THE HIGGS BOSON

(based on a 42-Dim observation x)



J Brehmer, J Pavez, G Louppe, K.C. PRL & PRD 2018 [arXiv:1805.00013 & arXiv:1805.00020]
 "Better Higgs Measurements Through Information Geometry" [arXiv:1612.05261] & CARL [arxiv:1506.02169]

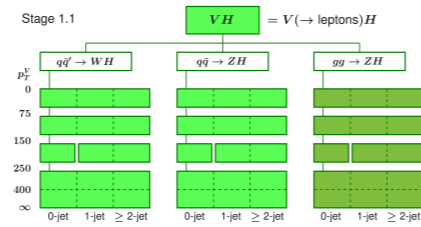


BENCHMARKING STXS IN WH

[JB, S. Dawson, S. Homiller, F. Kling, T. Plehn 1908.06980]

- Simplified Template Cross-Sections (STXS) define observable bins that are supposed to capture as much information on NP as possible

[N. Berger et al. 1906.02754; HXSWG YR4]



- Let's check! How much information on

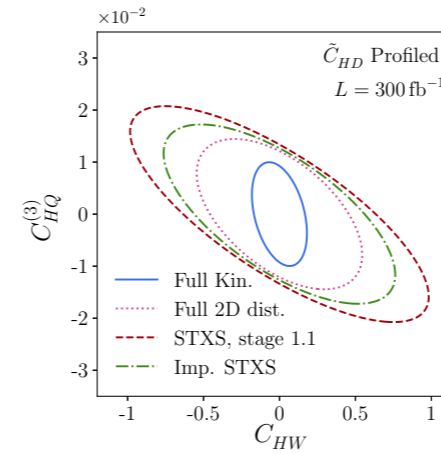
$$\tilde{\mathcal{O}}_{HD} = \mathcal{O}_{H\Box} - \frac{\mathcal{O}_{HD}}{4} = (\phi^\dagger \phi) \Box (\phi^\dagger \phi) - \frac{1}{4} (\phi^\dagger D^\mu \phi)^* (\phi^\dagger D_\mu \phi)$$

$$\mathcal{O}_{HW} = \phi^\dagger \phi W_{\mu\nu}^a W^{\mu\nu a}$$

$$\mathcal{O}_{Hq}^{(3)} = (\phi^\dagger i \overleftrightarrow{D}_\mu \phi) (\bar{Q}_L \sigma^\alpha \gamma^\mu Q_L),$$

can we extract from $pp \rightarrow WH \rightarrow \ell\nu b\bar{b}$?

- Results: **STXS** are indeed sensitive to operators, adding a few more bins improve them, but a **multivariate analysis** is still stronger



HANDS-ON TUTORIAL AT DESY LAST WEEK

We accomplished a lot!

From scratch:

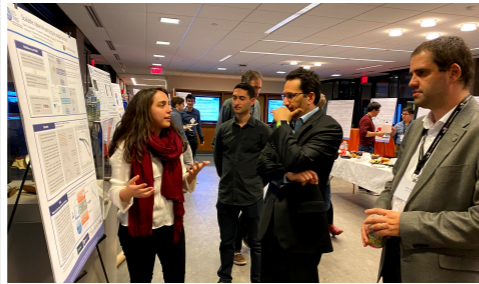
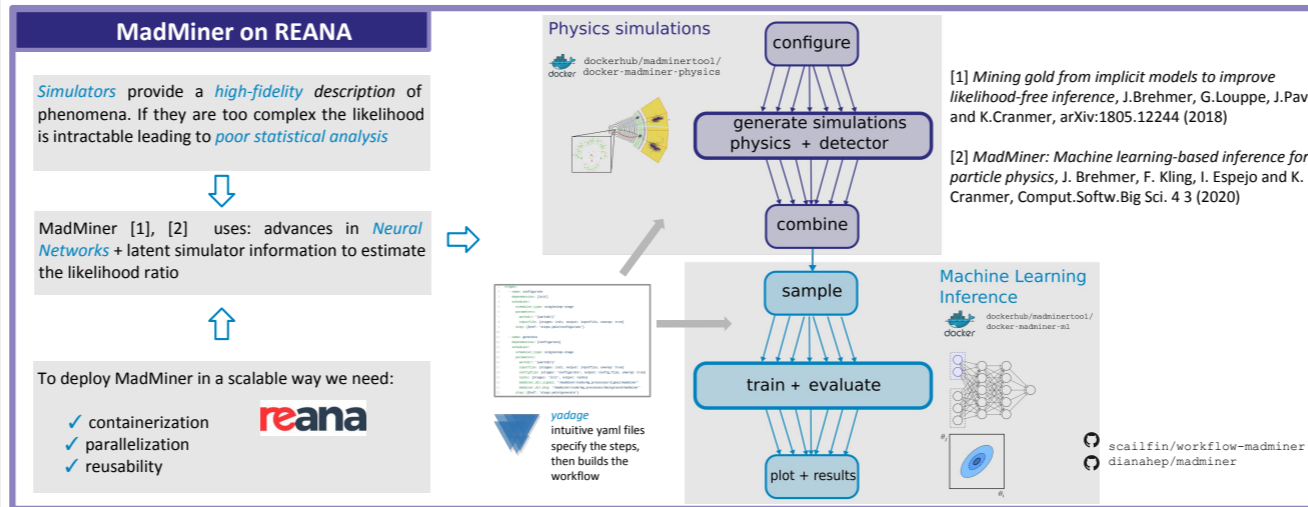
- Generate simulated data for EFT with MadGraph
- Fast detector simulation
- Trained neural network to learn likelihood ratio
- Trained neural network to learn Score (Optimal Observable)
- Calculated expected limit for both approaches and compared to simple 1-d histogram approach
- Calculated Fisher information matrix

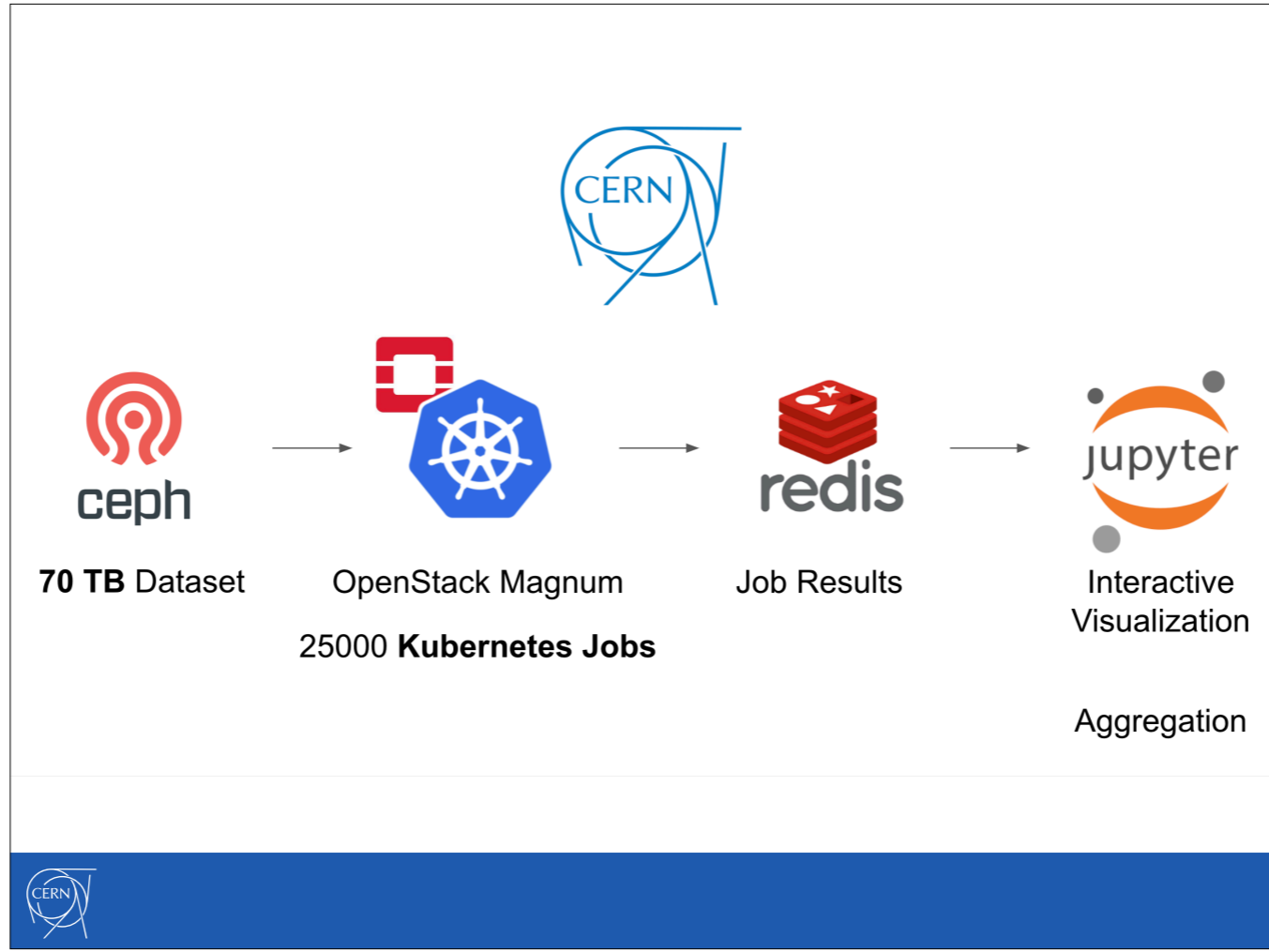
This is workflow for several published papers

- To speed this up, working to streamline MadMiner with REANA

<https://cranmer.github.io/madminer-tutorial/>

The screenshot shows the MadMiner tutorial website. On the left is a navigation menu with the following items: MadMiner Tutorial, Introduction, Preliminaries, Overview, Define process to study * (Morphing, Interactive Morphing Demo), Create training data (Set MadGraph Directory, Parton Level *, With Delphes), Train model (Likelihood Ratio *, Score *, Likelihood), Statistical Analysis (Limits on EFT parameters *, Fisher Information, Information Geometry), and Congratulations. The main content area is titled 'Introduction' and contains the following text: 'MadMiner tutorial. This is a tutorial on MadMiner developed by Johann Brehmer, Felix Kling, Irina Espejo, and Kyle Cranmer. It is built using Jupyter Book.' Below the text is a diagram illustrating the workflow: 'Simulation' (parameters θ and hard process σ leading to observables \mathcal{O} via $f(\mathcal{O}; \theta)$) feeds into 'Machine Learning' (training on \mathcal{O} to learn $L(\theta)$ and $S(\mathcal{O})$), which then leads to 'Inference' (using $L(\theta)$ and $S(\mathcal{O})$ to estimate θ via $f(\theta; \mathcal{O})$ and $S(\mathcal{O})$).







70 TB Dataset



Cluster on GKE
Max **25000 Cores**

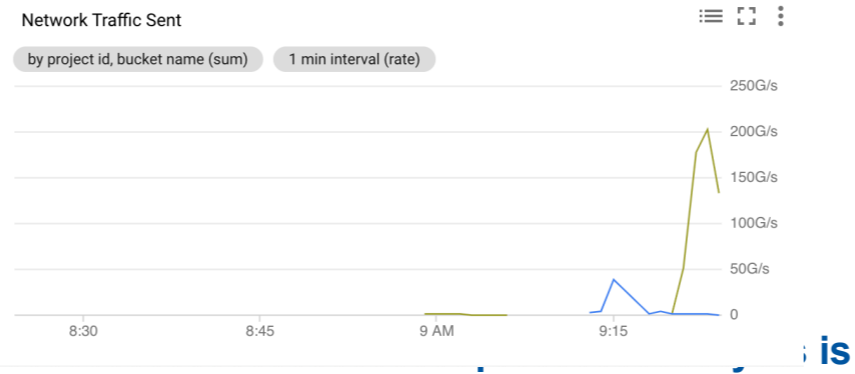


Job Results



Interactive
Visualization
Aggregation

- HEP analysis on Cloud w/ standard ingredients is possible
 - Terabit per second throughput for analysis.



- All using s... is achievable for anyone
 - O(10k)/analysis nodes not an issue on short notice
 - haven't pushed limits yet.



SHIFTING FROM REPRODUCIBILITY TO REUSE





Open is not enough

Xiaoli Chen^{1,2}, Sünje Dallmeier-Tiessen^{1*}, Robin Dasler^{1,3}, Sebastian Feger^{1,3}, Pamfilos Fokianos¹, Jose Benito Gonzalez¹, Harri Hirvonsalo^{1,4,12}, Dinos Kousidis¹, Artemis Lavasa¹, Salvatore Mele¹, Diego Rodriguez Rodriguez¹, Tibor Šimko^{1*}, Tim Smith¹, Ana Trisovic^{1,5*}, Anna Trzcinska¹, Ioannis Tsanaktsidis¹, Markus Zimmermann¹, Kyle Cranmer⁶, Lukas Heinrich⁶, Gordon Watts⁷, Michael Hildreth⁸, Lara Lloret Iglesias⁹, Kati Lassila-Perini⁴ and Sebastian Neubert¹⁰

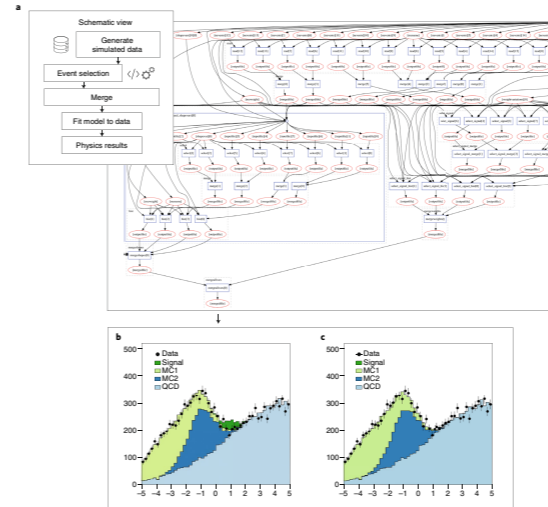
The solutions adopted by the high-energy physics community to foster reproducible research are examples of best practices that could be embraced more widely. This first experience suggests that reproducibility requires going beyond openness.

reana

Reproducible research data analysis platform

<p>Flexible</p> <p>Run many computational workflow engines.</p> 	<p>Scalable</p> <p>Support for remote compute clouds.</p> 	<p>Reusable</p> <p>Containerise once, reuse elsewhere. Cloud-native.</p> 	<p>Free</p> <p>Free Software. MIT licence. Made with ❤️ at CERN.</p> 
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<http://reanahub.io>



1 | Example of a complex computational workflow on REANA mimicking a beyond the standard model (BSM) analysis. This figure shows an example where the experimental data is compared to the predictions of the standard model with an additional hypothesized signal component. The example permits one to study the complex computational workflows used in typical particle physics analyses. **a–c.** The computational workflow (**a**) may consist of several tens of thousands of computational steps that are massively parallelizable and run in a cascading ‘map-reduce’ style of computations distributed across compute clusters. The workflow definition is modelled using the Yastage workflow specification and produces an upper limit on the μ strength of the BSM process. A typical search for BSM physics consists of simulating a hypothetical signal process (**c**), as well as the background estimates predicted by the standard model with properties consistent with the hypothetical signal (marked dark green in **b**). The background often consists of simulated background estimates (dark blue and light green histograms) and data-driven background estimates (light blue histogram). A statistical model involving both signal (dark green histogram) and background components is built and fit to the observed experimental data (black dots). **b.** Results of the model in its pre-fit configuration at nominal signal strength. We can see the excess of the signal over data, meaning that the initial setting does not describe the data well. The post-fit distribution would scale down the signal in order to fit the data. This REANA example is publicly available at ref. 11. For icon credits, see Fig. 1.

<https://doi.org/10.1038/s41567-018-0342-2>

BUILD IT AND THEY WILL COME

In 2010 we identified a use-case with high scientific value for community

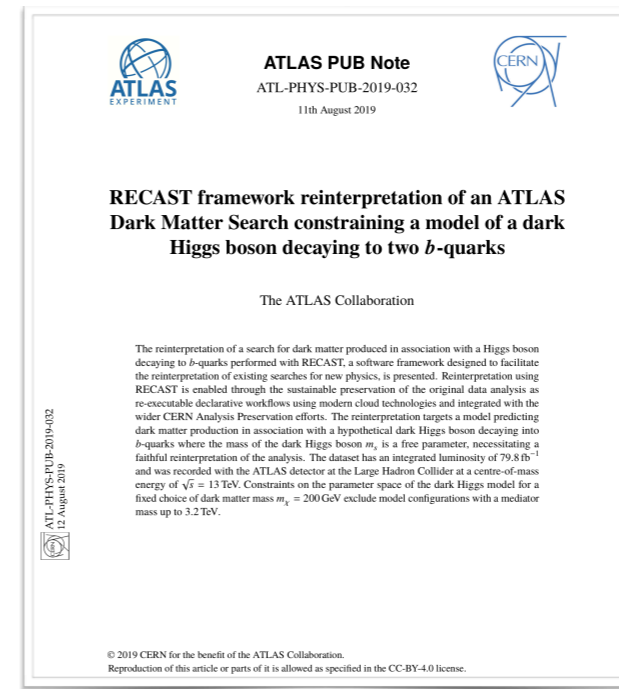
- Conservative narrative compared to “open data”
- Not conservative enough for many. Lots of resistance
- People said it couldn't be done, our workflows are too complicated
- Hard to get effort to work on it.

Got lucky with an amazing student that took a risk and just built it.

- Containers & Cloud technology
- 9 years later ...



Lukas Heinrich



Orig Proposal in 2010: [arXiv.org:1010.2506] 33

TRAINING

Analysis preservation bootcamp



Participants in [Analysis Preservation Bootcamp](#) showing off their ability to reproduce an LHC analysis. Photo Credit: Samuel Meehan

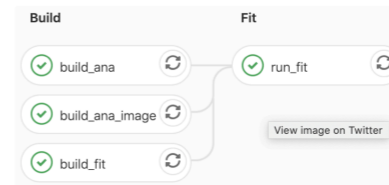
Josh McFayden
@JoshMcFayden

Thoroughly enjoying myself at an [@iris_hep/@diana_hep](#) analysis preservation bootcamp [@CERN](#) today!
[indico.cern.ch/event/854880/o...](#)



Josh McFayden @JoshMcFayden · Feb 18, 2020

Replying to [@JoshMcFayden](#) and 3 others
PROGRESS ✓



Josh McFayden
@JoshMcFayden

Today: REANA ✓
reana

Your workflows

awesome-workflow #7	finished in 4 min 17 sec
Finished a minute ago	step 4/6

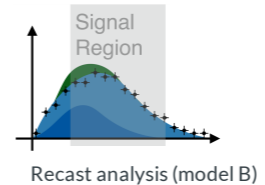
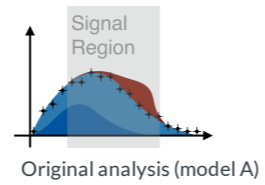


JSON Patch for signal model (reinterpretation)

```
$ pyhf cls example.json | jq .Cls_obs
0.053994246621274014

$ cat new_signal.json
[{"op": "replace",
 "path": "/channels/0/samples/0/data",
 "value": [10.0, 6.0]}]

$ pyhf cls example.json --patch new_signal.json | jq .Cls_obs
0.3536906623262466
```



SYNTHESIS

active learning / sequential design / black box optimization



Active Sciencing



reusable workflows

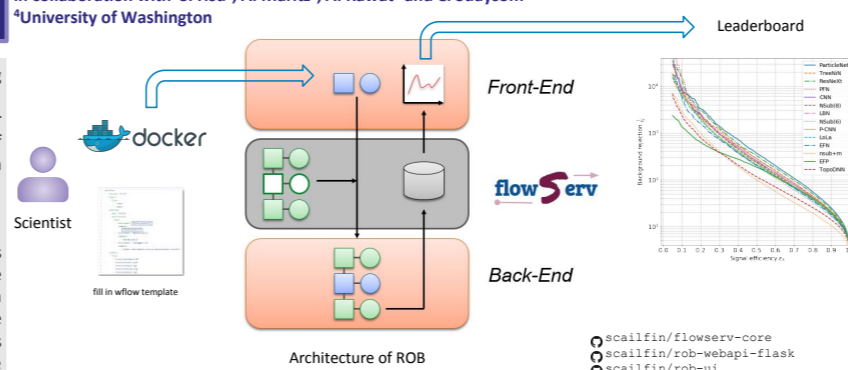


simulation-based /
likelihood-free
inference engines

ROB Reproducible Open Benchmark Platform

- ROB is an experimental prototype for enabling *community benchmarks* of data analysis algorithms. The goal of ROB is to allow user communities to evaluate the performance of their different data analysis algorithms in a *reproducible competition-style* format.
- The *workflow template* and input data are defined by a coordinator. The template contains placeholders for workflow steps that are implemented by the participants (e.g., with Docker containers). The backend processes the submission workflows. The user interface allows participants to *submit new runs* and to view the results.

in collaboration with S. Hsu⁴, A. Maritz⁴, A. Rawat⁴ and C. Suaysom⁴
⁴University of Washington



The diagram illustrates the architecture of the ROB platform. A Scientist interacts with a Docker container to fill in a workflow template. This template is processed by the Front-End, which connects to the Back-End. The Back-End then feeds into a Leaderboard, which displays a graph of background rejection versus signal efficiency for various algorithms. The graph shows several curves representing different methods, with a legend on the right side. Below the graph, there are GitHub repository links for the core components.

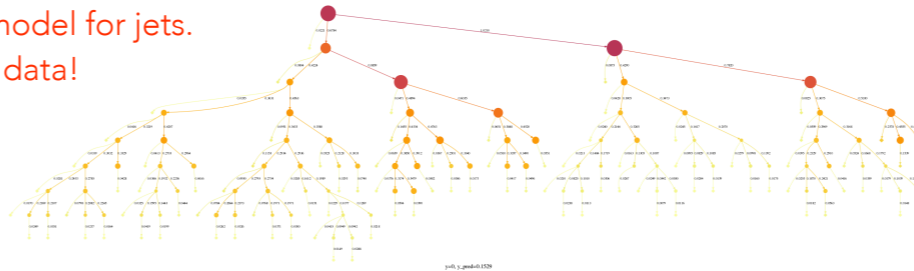
- scailfin/flowserv-core
- scailfin/rob-webapi-flask
- scailfin/rob-ui
- SebastianMacaluso/TopTagComparison

We can use the same technology to streamline comparison of up-stream tools like ML-based jet taggers.

- Building ROB & FlowServe on top of REANA

NN-BASED SIMULATION TRAINED ON DATA

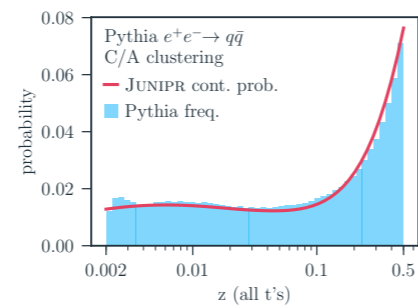
JUNIPR is a generative model for jets.
Can train on real data!



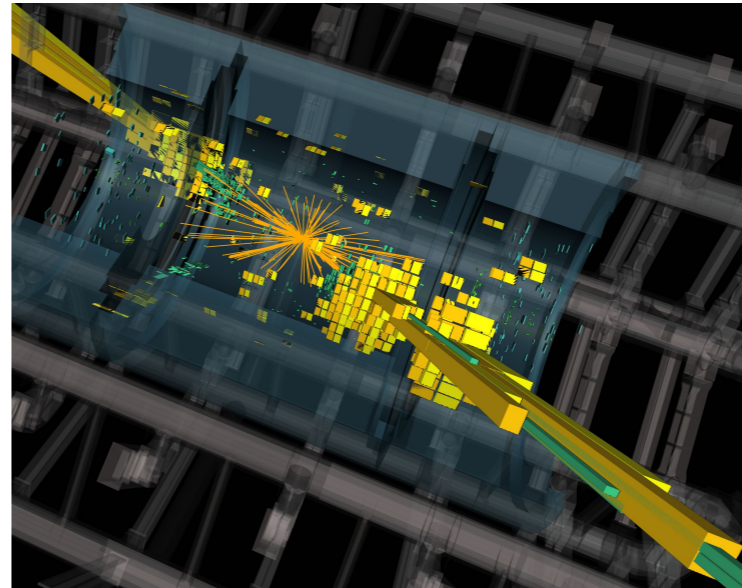
tractable likelihood

$$P_{\text{jet}}(\{p_1, \dots, p_n\}) = \left[\prod_{t=1}^{n-1} P_t(k_1^{(t+1)}, \dots, k_{t+1}^{(t+1)} | k_1^{(t)}, \dots, k_t^{(t)}) \right] \times P_n(\text{end} | k_1^{(n)}, \dots, k_n^{(n)}).$$

... and it is interpretable

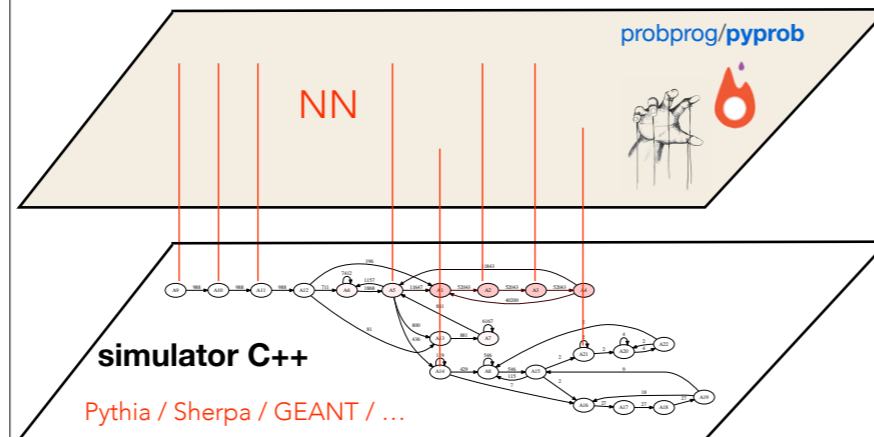


Andreassen, Feige, Frye, Schwartz arXiv:1804.09720

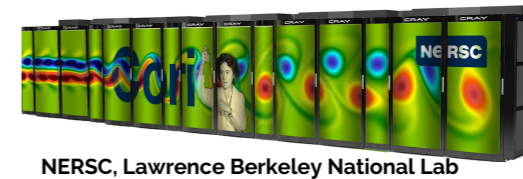
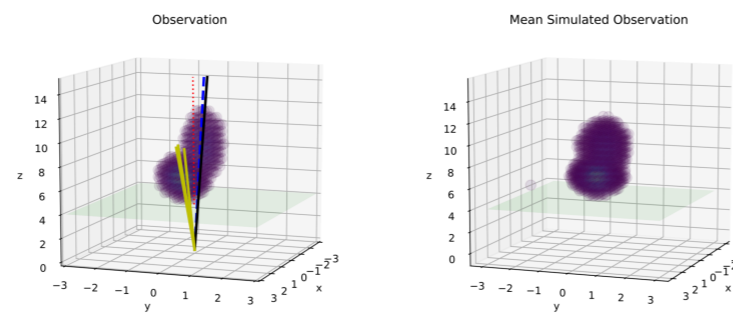


PROBABILISTIC PROGRAMING

Idea: hijack the random number generators and use Neural Network to perform a very fancy type of importance sampling



- Neural Network powered inference engine (python)
- real-world scientific simulator (C++)



NERSC, Lawrence Berkeley National Lab

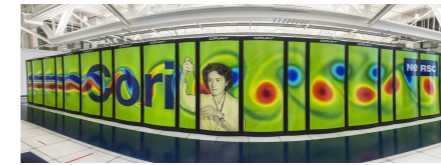
arXiv:1807.07706



Highlight

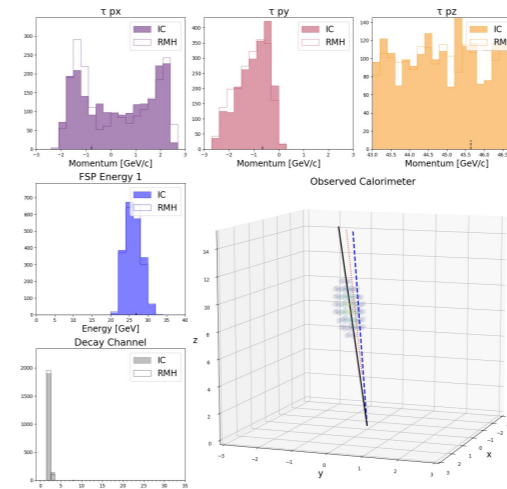


<https://arxiv.org/abs/1907.03382>



Finalist for best paper award at SC19 (Super Computing)

- Largest scale Bayesian inference ever using in a universal probabilistic programming language
 - **Applied to complex LHC Physics use case: Sherpa code base of ~1M lines of code in C++**
- 230x speedup for synchronous data parallel training of a 3DCNN-LSTM neural network
 - **1,024 nodes (32,768 CPU cores)**
 - **128k minibatch size, largest for this NN architecture**
 - **One of the largest-scale use of PyTorch built-in MPI**
- Novel protocol (PPX) to execute & control existing, large-scale, scientific simulator code bases



SUMMARY

Accelerating analysis design

- more powerful observables
- end-to-end optimization
- benchmarking of algorithms

Accelerating fitting

- pyhf and a fitting service

More efficient simulation

- excursion
- Probabilistic programming

Extending impact of results

- RECAST

Core technologies:

- automatic differentiation
- GPUs & TPUs
- Cloud-native : docker, kubernetes
- Workflows & REANA
- Functions as a service Accelerating analysis design

Sorry if this is a little disorganized, COVID has complicated work life

