Ride the ML-Wave or Drown?
(How To Not Become a Physics Museum)

Tilman Plehn

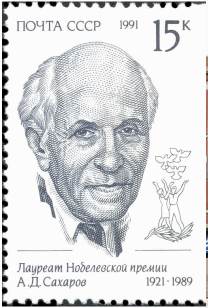
Universität Heidelberg

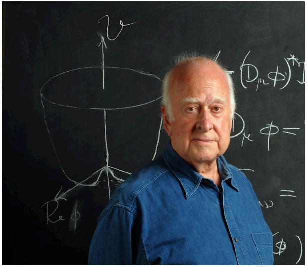
Annual Theory Meeting, IPPP, 2024

All about LHC physics

Classic motivation

- dark matter?
- matter vs antimatter?
- origin of Higgs boson?





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LHC physics

- fundamental questions
- huge data set
- first-principle, precision simulations
- complete uncertainty control

Successful past

- measurements of total rates
- analyses inspired by simulation
- model-driven Higgs discovery

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First-principle, precision simulations

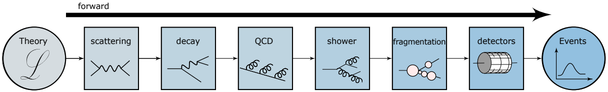
- start with Lagrangian
- calculate scattering using QFT
- simulate collisions
- simulate detectors

→ LHC collisions in virtual worlds

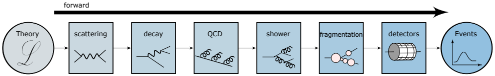
(Instead of) BSM searches

- compare simulations and data
- infer underlying theory [SM or BSM]
- publish results/data meaningfully

→ Understand LHC data systematically



LHC Theory

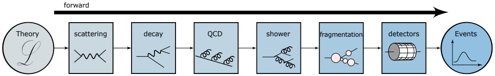


Turning data to knowledge

- Quantum Field Theory
  start with Lagrangian
- compute hard scattering
  compute decays
  compute jet radiation
- parton densities [NNPDF]
  hadron-level QCD

→ First-principle simulations, with help from ML

LHC Theory



Turning data to knowledge

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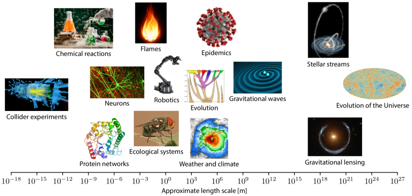
$\rightarrow$ First-principle simulations, with help from ML

HL-LHC: inference with 10$\times$ more data

- SBI starts with Simulation...
- statistical improvement $\sqrt{10} = 3$
- rate over phase space to $< 0.1\%$
- theory to follow
- precision = QFT $\times$ Compute

$\rightarrow$ Everything, faster and better...



Shortest ML-intro ever

Fit-like approximation

- approximate $f_\theta(x) \approx f(x)$
- no parametrization, just very many θ
- new representation/latent space θ

Applications

- applications all over experiment
- regression $x \to f_\theta(x)$
- classification $x \to f_\theta(x) \in [0, 1]$
- generation $r \sim \mathcal{N} \to f_\theta(r)$
- conditional generation $r \sim \mathcal{N} \to f_\theta(r|x)$

Architectures

- physics-aware questions and data representation
- symmetries, locality, etc
- accuracy, control, error bars?
- is LHC data images or language?

$\to$ Complexity a feature, not a problem

Network training

Encoding a transtition amplitude-squared

- expectation value from probability

$$\langle A \rangle (x) = \int dA \; A \; p(A|x)$$

- internal representation θ

$$\langle A \rangle = \int dA \; A \int d\theta \; p(A|\theta) \; p(\theta|A_\text{train})$$

- training a generalization of θ-probability

$$\int d\theta \; p(A|\theta) \; p(\theta|A_\text{train}) \approx \int d\theta \; p(A|\theta) \; q(\theta)$$

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$$\int d\theta \; p(A|\theta) \; p(\theta|A_\text{train}) \approx \int d\theta \; p(A|\theta) \; q(\theta)$$

- similarity from minimal KL-divergence

$$\begin{aligned} D_\text{KL}[q(\theta), p(\theta|A_\text{train})] &\equiv \int d\theta \; q(\theta) \; \log \frac{q(\theta)}{p(\theta|A_\text{train})} \\ &= \int d\theta \; q(\theta) \; \log \frac{q(\theta) p(A_\text{train})}{p(A_\text{train}|\theta) p(\theta)} \\ &= - \int d\theta \; q(\theta) \; \log p(A_\text{train}|\theta) + \int d\theta \; q(\theta) \log \frac{q(\theta)}{p(\theta)} + \cdots \end{aligned}$$

$\to$ Simplification: likelihood + regularization + dropout

$$\begin{aligned} \mathcal{L}_\text{BNN} &= - \int d\theta \; q(\theta) \; \log p(A_\text{train}|\theta) + D_\text{KL}[q(\theta), p(\theta)] \\ &\to (A_\theta - A_\text{train})^2 + c(\theta - \theta_0)^2 \end{aligned}$$

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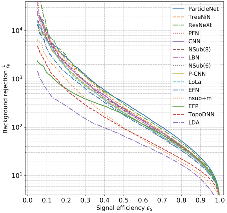
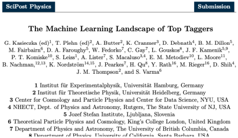
Top tagging [classification, 2016-today]

- ‘hello world’ of LHC-ML
- end of QCD-taggers
- ever-improving [Huilin Qu]

→ Driving NN-architectures





SciPost Physics Submission

The Machine Learning Landscape of Top Taggers

G. Kasieczka (ed)[1], T. Plehn (ed)[2], A. Butter[2], K. Cranmer[3], D. Debnath[4], B. M. Dillon[5], M. Fairbairn[6], D. A. Faroughy[5], W. Fedorko[7], C. Gay[7], L. Gouskos[8], J. F. Kamenik[5,9], P. T. Komiske[10], S. Leiss[1], A. Lister[7], S. Macaluso[3,4], E. M. Metodiev[10], L. Moore[11], B. Nachman,[12,13], K. Nordström[14,15], J. Pearkes[7], H. Qu[8], Y. Rath[16], M. Rieger[16], D. Shih[4], J. M. Thompson[2], and S. Varma[6]

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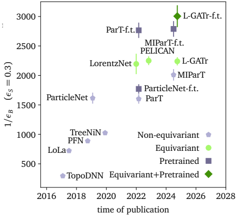
4 NHECT, Dept. of Physics and Astronomy, Rutgers, The State University of NJ, USA
5 Jozef Stefan Institute, Ljubljana, Slovenia
6 Theoretical Particle Physics and Cosmology, King’s College London, United Kingdom
7 Department of Physics and Astronomy, The University of British Columbia, Canada
8 Department of Physics, University of California, Santa Barbara, USA



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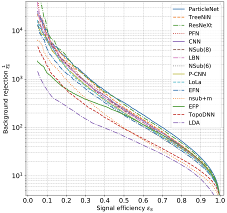

SciPost Physics — Submission

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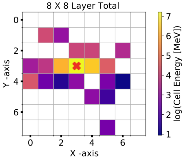
10 Center for Theoretical Physics, MIT, Cambridge, USA
11 CP3, Universitéxx Catholique de Louvain, Louvain-la-Neuve, Belgium
12 Physics Division, Lawrence Berkeley National Laboratory, Berkeley, USA
13 Simons Inst. for the Theory of Computing, University of California, Berkeley, USA
14 National Institute for Subatomic Physics (NIKHEF), Amsterdam, Netherlands
15 LPTHE, CNRS & Sorbonne Université, Paris, France
16 III. Physics Institute A, RWTH Aachen University, Germany

Particle flow [2020-today]

- mother of jet analyses
- combining detectors with different resolution
- optimality the key

→ Modern jet analysis basics



Towards a Computer Vision Particle Flow ⋆

Francesco Armando Di Bello[a,3], Sanmay Ganguly[b,1], Eilam Gross[1], Marumi Kado[3,4], Michael Pitt[2], Lorenzo Santi [3], Jonathan Shlomi[1]

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[4]Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405, Orsay, France

Progress towards an improved particle flow algorithm at CMS with machine learning

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(on behalf of the CMS Collaboration)
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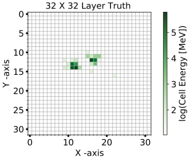

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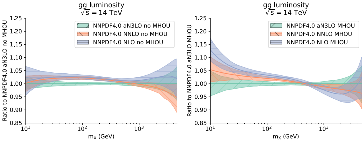
ML in phenomenology

Parton densities [NNPDF, 2002-today]

- pdfs without functional bias and full uncertainties
- precision and calibrated uncertainties

→ Drivers of ML-theory



The Path to N^{3}LO Parton Distributions

The NNPDF Collaboration:
Richard D. Ball[1], Andrea Barontini[2], Alessandro Candido[2,3], Stefano Carrazza[2], Juan Cruz-Martinez[3], Luigi Del Debbio[1], Stefano Forte[2], Tommaso Giani[4,5], Felix Hekhorn[2,6,7], Zahari Kassabov[8], Niccolò Laurenti,[2] Giacomo Magni[4,5], Emanuele R. Nocera[9], Tanjona R. Rabemananjara[4,5], Juan Rojo[4,5], Christopher Schwan[10], Roy Stegeman[1], and Maria Ubiali[8]

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[10] *Universität Würzburg, Institut für Theoretische Physik und Astrophysik, 97074 Würzburg, Germany*

This paper is dedicated to the memory of Stefano Catani, Grand Master of QCD, great scientist and human being

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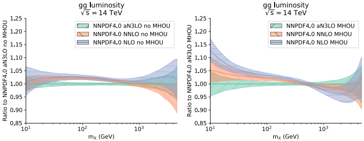

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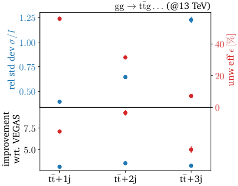
Ultra-fast event generators [Sherpa, MadNIS, MLHad]

- event generation modular
- improve and replace by ML-modules

$\rightarrow$ Beat state of the art

Triple-W	$u\bar{d} \to W^+W^+W^-$		
VBS	$uc \to W^+W^+ ds$		
W+jets	$gg \to W^+d\bar{u}$	$gg \to W^+d\bar{u}g$	$gg \to W^+d\bar{u}gg$
$t\bar{t}$+jets	$gg \to t\bar{t} + g$	$gg \to t\bar{t} + gg$	$gg \to t\bar{t} + ggg$,



SciPost Physics Submission

The MadNIS Reloaded

Theo Heimel[1], Nathan Huetsch[1], Fabio Maltoni[2,3], Olivier Mattelaer[2], Tilman Plehn[1], and Ramon Winterhalder[2]

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2 CP3, Université catholique de Louvain, Louvain-la-Neuve, Belgium
3 Dipartimento di Fisica e Astronomia, Università di Bologna, Italy

December 17, 2024

Abstract

In pursuit of precise and fast theory predictions for the LHC, we present an implementation of the MadNIS method in the MadGraph event generator. A series of improvements in MadNIS further enhance its efficiency and speed. We validate this implementation for realistic partonic processes and find significant gains from using modern machine learning in event generators.

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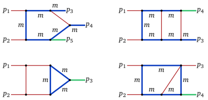
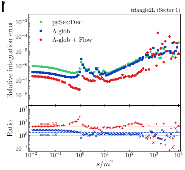
ML in theory

Optimizing integration paths [invertible networks]

- find optimal integration paths
- learn variable transformation

$\rightarrow$ Theory-integrator





SciPost — SciPost Phys. 12, 129 (2022)

Targeting multi-loop integrals with neural networks

Ramon Winterhalder[1,2,3], Vitaly Magerya[4], Emilio Villa[4], Stephen P. Jones[5], Matthias Kerner[4,6], Anja Butter[1,2], Gudrun Heinrich[2,4] and Tilman Plehn[1,2]

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2 HEiKA - Heidelberg Karlsruhe Strategic Partnership, Heidelberg University, Karlsruhe Institute of Technology (KIT), Germany
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6 Institut für Astroteilchenphysik, Karlsruher Institut für Technologie, Germany

Abstract

Numerical evaluations of Feynman integrals often proceed via a deformation of the integration contour into the complex plane. While valid contours are easy to construct, the numerical precision for a multi-loop integral can depend critically on the chosen contour. We present methods to optimize this contour using a combination of optimized, global complex shifts and a normalizing flow. They can lead to a significant gain in precision.

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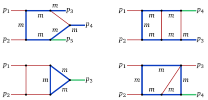

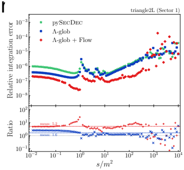

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Navigating string landscape [reinforcement learning]

- searching for viable vacua
- high dimensions, unknown global structure

→ Model space sampling

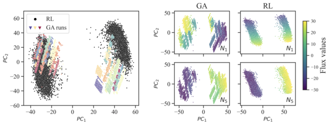

Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_3 and N_5 respectively) in relation to principal components for a PCA fit of the individual output of GA and RL.

Probing the Structure of String Theory Vacua with Genetic Algorithms and Reinforcement Learning

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Abstract

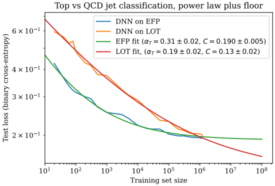
Identifying string theory vacua with desired physical properties at low energies requires searching through high-dimensional solution spaces – collectively referred to as the string landscape. We highlight that this search problem is amenable to reinforcement learning and genetic algorithms. In the context of flux vacua, we are able to reveal novel features (suggesting previously unidentified symmetries) in the string theory solutions required for properties such as the string coupling. In order to identify these features robustly, we combine results from both search methods, which we argue is imperative for reducing sampling bias.

Theory for ML

Scaling laws for classification networks [statistical learning]

- networks are complex systems
- training as statistical process

$\to$ Now solving problems



SCALING LAWS IN JET CLASSIFICATION

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ABSTRACT

We demonstrate the emergence of scaling laws in the benchmark top versus QCD jet classification problem in collider physics. Six distinct physically-motivated classifiers exhibit power-law scaling of the binary cross-entropy test loss as a function of training set size, with distinct power law indices. This result highlights the importance of comparing classifiers as a function of dataset size rather than for a fixed training set, as the optimal classifier may change considerably as the dataset is scaled up. We speculate on the interpretation of our results in terms of previous models of scaling laws observed in natural language and image datasets.

Collective variables of neural networks: empirical time evolution and scaling laws

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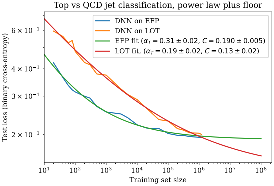
Theory for ML

Scaling laws for classification networks [statistical learning]

- networks are complex systems
- training as statistical process

$\rightarrow$ Now solving problems



SCALING LAWS IN JET CLASSIFICATION

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ABSTRACT

We demonstrate the emergence of scaling laws in the benchmark top versus QCD jet classification problem in collider physics. Six distinct physically-motivated classifiers exhibit power-law scaling of the binary cross-entropy test loss as a function of training set size, with distinct power law indices. This result highlights the importance of comparing classifiers as a function of dataset size rather than for a fixed training set, as the optimal classifier may change considerably as the dataset is scaled up. We speculate on the interpretation of our results in terms of previous models of scaling laws observed in natural language and image datasets.

Collective variables of neural networks: empirical time evolution and scaling laws

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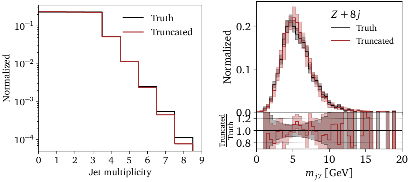
Extrapolating transformers

- train on QCD jet radiation
- learn to generate universal patterns

$\rightarrow$ Extrapolation at work



SciPost Physics Submission

Extrapolating Jet Radiation with Autoregressive Transformers

Anja Butter[1,2], François Charton[3], Javier Mariño Villadamigo[1], Ayodele Ore[1], Tilman Plehn[1,4], and Jonas Spinner[1]

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2 LPNHE, Sorbonne Université, Université Paris Cité, CNRS/IN2P3, Paris, France
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4 Interdisciplinary Center for Scientific Computing (IWR), Universität Heidelberg, Germany

December 17, 2024

Abstract

Generative networks are an exciting tool for fast LHC event generation. Usually, they are used to generate configurations with a fixed number of particles. Autoregressive transformers allow us to generate events with variable numbers of particles, very much in line with the physics of QCD jet radiation. We show how they can learn a factorized likelihood for jet radiation and extrapolate in terms of the number of generated jets. For this extrapolation, bootstrapping training data and training with modifications of the likelihood loss can be used.

Amplitude regression

An IPPP story...

- $gg \to ZZ$ [Bishara & Montull (2019)] $\longrightarrow$ BDTs as a start
- $e^+e^- \to 5$ jets [Badger, Bullock (2020)] $\longrightarrow$ ensembles and K-factors
- $gg \to \gamma\gamma g(g)$ [Aylett-Bullock, Badger, Moodie (2021)] $\longrightarrow$ speed gain 10^4
- $e^+e^- \to 5$ jets [Maitre & Truong (2021)] $\longrightarrow$ Catani-Seymour coefficients
- $e^+e^- \to 5$ [Maitre & Truong (2023)] $\longrightarrow$ antenna functions
- $gg \to \gamma\gamma g(g)$ [Badger+Heidelberg (2024] $\longrightarrow$ boosted training
- $t\bar{t}H$ NNLO tests [Breso, Heinrich, Magerya, Olsson] $\longrightarrow$ race for best performance

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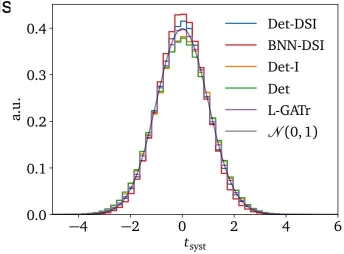
Learned uncertainties [Bahl, Elmer, Favaro, Haussmann, TP, Winterhalder]

- systematic: (added) noise, expressivity, data representation
  learned by heteroscedastic loss and BNNs
- statistical: too little training data
  learned by BNN or repulsive ensembles
- calibration of learned uncertainties?



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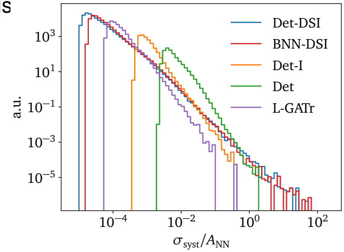
$\to$ Path to 10^{-5} accuracy



ATLAS calibration

Energy calibration with uncertainties [ATLAS + Vogel, 2412.04370]

- interpretable calorimeter phase space x
- learned calibration function

$$\mathcal{R}^{\text{BNN}}(x) \pm \Delta\mathcal{R}^{\text{BNN}}(x) \approx \frac{E^{\text{obs}}(x)}{E^{\text{dep}}(x)}$$

- uncertainties: noise in data
  network expressivity
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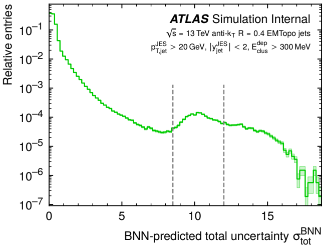
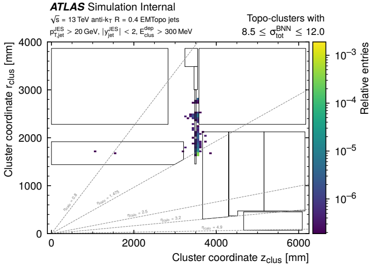
$\to$ Understand (simulated) detector



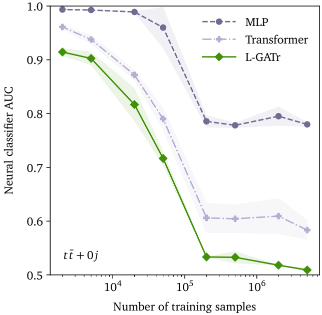


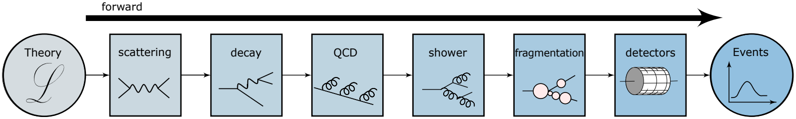
Generative AI

Simulations, MadNIS, calorimeters,...

- learn phase space density
  fast sampling Gaussian $\to$ phase space
- Variational Autoencoder
  $\to$ low-dimensional physics
- Generative Adversarial Network
  $\to$ generator trained by classifier
- Normalizing Flow/Diffusion
  $\to$ (bijective) mapping
- JetGPT, ViT
  $\to$ non-local structures
- Equivariant L-GATr
  $\to$ Lorentz symmetry for efficiency

$\to$ Equivariant transformer CFM... [Maitre, Ngairangbam, Spannowsky,...]





Generative AI with uncertainties

Bayesian generative networks [Bellagente, Haussmann, Luchmann, TP]

- network weight distributions for density
- sampling phase space
  events with error bars on weights
- learned density & uncertainty
  reflecting network learning?

$\rightarrow$ Generative networks like fitted densities

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$\rightarrow$ Generative networks like fitted densities

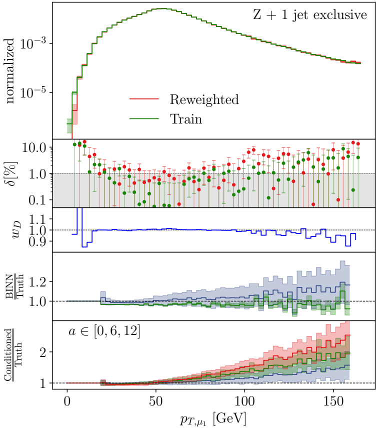
Z+jets events [Heimel, Vent...]

- per-cent accuracy on density
- statistical uncertainty from BNN
- systematics in training data

$$w = 1 + a \left(\frac{p_{T,j_1} - 15 \text{ GeV}}{100 \text{ GeV}} \right)^2$$

sampling a conditionally

$\rightarrow$ Precision and uncertainty control



Controlling generative AI

Compare generated with training data

- regression accuracy $\Delta = (A_\text{data} - A_\theta)/A_\text{data}$
- harder for generation, unsupervised density
  classify training vs generated events $D(x)$
  learned density ratio [Neyman-Pearson]

$$w(x_i) = \frac{D(x_i)}{1 - D(x_i)} = \frac{p_\text{data}(x_i)}{p_\text{model}(x_i)}$$

$\to$ Test ratio over phase space

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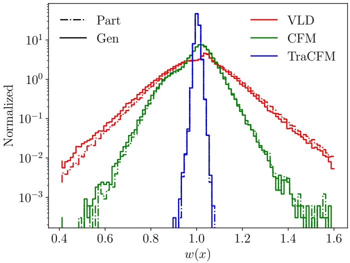
$\rightarrow$ Test ratio over phase space

Progress in NN-generators

- any generative AI task
- compare different architectures
- accuracy from width of weight distribution
- tails indicating failure mode

$\rightarrow$ Systematic performance test



Transforming LHC physics

Number of searches

- optimal inference: signal and background simulations
- CPU-limitation for many signals?

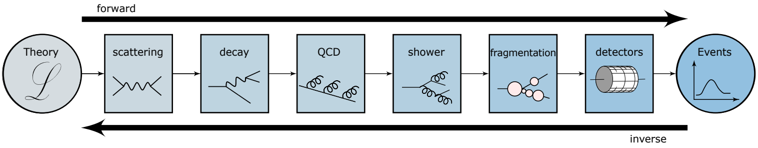
Optimal analyses

- theory limiting many analyses
- include predictions not in event generators

Public LHC data

- common lore:
  LHC data too complicated for amateurs
- in truth:
  hard scattering and decay simulations public
  BSM physics not in hadronization and detector

→ Unfold to suitable level



ML-Unfolding

Basic structure [Butter, Köthe, TP, Winterhalder]

- four phase space distributions

$$\begin{tikzcd}
p_\text{sim}(x_\text{part}) \arrow[r, leftrightarrow, "\text{unfolding inference}"] \arrow[d, "p(x_\text{reco}|x_\text{part})"'] & p_\text{unfold}(x_\text{part}) \\
p_\text{sim}(x_\text{reco}) \arrow[r, leftrightarrow, "\text{forward inference}"] & p_\text{data}(x_\text{reco}) \arrow[u, "p(x_\text{part}|x_\text{reco})"']
\end{tikzcd}$$

- learn conditional probabilities from $(x_\text{part}, x_\text{reco})$ [forward-inverse symmetric]

$\to$ ML for unbinned and high-dimensional unfolding?

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OmniFold [Andreassen, Komiske, Metodiev, Nachman, Thaler + ATLAS]

- learn $p_\text{sim}(x_\text{reco}) \leftrightarrow p_\text{data}(x_\text{reco})$ [Neyman-Pearson]
- reweight $p_\text{sim}(x_\text{part}) \to p_\text{unfold}(x_\text{part})$

$$\begin{tikzcd}
p_\text{sim}(x_\text{part}) \arrow[rr, "\text{classifier weights}"] \arrow[d, leftrightarrow, "\text{pull/push weights}"'] & & p_\text{unfold}(x_\text{part}) \\
p_\text{sim}(x_\text{reco}) \arrow[rr, leftrightarrow, "\text{classifier weights}"] & & p_\text{data}(x_\text{reco})
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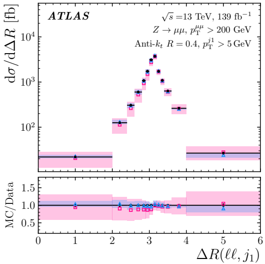

$\to$ Z+jets in 24D [ATLAS]

Unfolding top decays

A challenge [Favaro, Kogler, Paasch, Palacios Schweitzer, TP, Schwarz]

- first measure m_t in unfolded data
  then unfold full kinematics
- model dependence: simulation m_s vs data m_d

$$\begin{tikzcd}
p_\text{sim}(x_\text{part}|m_s) \arrow[d, "p(x_\text{reco}|x_\text{part})"'] & & p_\text{unfold}(x_\text{part}|m_s, m_d) \\
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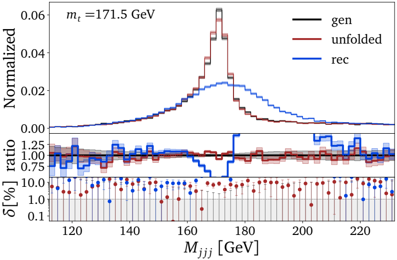
Preliminary unfolding results [TraCFM]

- 4D for calibrated mass measurement



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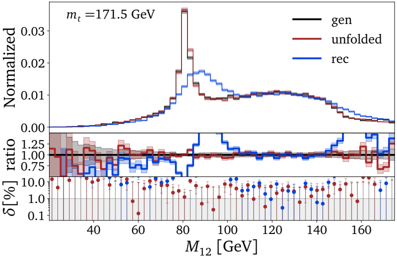
Preliminary unfolding results [TraCFM]

- 4D for calibrated mass measurement
- 12D published data

$\to$ CMS data next



ML for LHC Theory

Developing ML for the best science

1 just another numerical tool for a numerical field

2 completely transformative new language

- driven by money from data science and medical research
- physics should be leading scientific AI
- 1000 Einsteins...

...improving established tools
...developing new tools for established tasks
...transforming through new ideas

→ You can be the golden generation!

Modern Machine Learning for LHC Physicists

Tilman Plehn[a*], Anja Butter[a,b], Barry Dillon[a],
Theo Heimel[a], Claudius Krause[c], and Ramon Winterhalder[d]

[a] Institut für Theoretische Physik, Universität Heidelberg, Germany
[b] LPNHE, Sorbonne Université, Université Paris Cité, CNRS/IN2P3, Paris, France
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[d] CP3, Université catholique de Louvain, Louvain-la-Neuve, Belgium

March 19, 2024

Abstract

Modern machine learning is transforming particle physics fast, bullying its way into our numerical tool box. For young researchers it is crucial to stay on top of this development, which means applying cutting-edge methods and tools to the full range of LHC physics problems. These lecture notes lead students with basic knowledge of particle physics and significant enthusiasm for machine learning to relevant applications. They start with an LHC-specific motivation and a non-standard introduction to neural networks and then cover classification, unsupervised classification, generative networks, and inverse problems. Two themes defining much of the discussion are well-defined loss functions and uncertainty-aware networks. As part of the applications, the notes include some aspects of theoretical LHC physics. All examples are chosen from particle physics publications of the last few years.[1]