Transforming Particle Physics with Machine Learning

Tilman Plehn

Universität Heidelberg

HEPHY, February 2025

Shortest ML-intro ever

Fit-like approximation

- approximate $f_\theta(x) \approx f(x)$
- no function, but very many θ
- data representation θ

Applications

- regression $\qquad x \to f_\theta(x)$
- classification $\qquad x \to f_\theta(x) \in [0, 1]$
- generation $\qquad r \sim \mathcal{N} \to f_\theta(r)$

LHC

- always phase spaces
- symmetries, locality, etc
- accuracy — control — uncertainties
- is LHC data images or language?

$\to$ Benefitting from complexity?

Network training

Remembering fits

- learn scalar field $\quad f_\theta(x) \approx f(x)$
- maximize parameter probability given (f_j, σ_j)

$$\theta = \text{argmax}\; p(\theta|x) = \text{argmax}\; \frac{p(x|\theta)\; p(\theta)}{p(x)}$$

$\to$ Gaussian likelihood loss

$$p(x|\theta) \propto \prod_j \exp\left(- \frac{|f_j - f_\theta(x_j)|^2}{2\sigma_j^2} \right)$$

$$\Rightarrow \qquad \mathcal{L} \equiv - \log p(x|\theta) = \sum_j \frac{|f_j - f_\theta(x_j)|^2}{2\sigma_j^2}$$

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Networks with uncertainty

- uncertainties in NN-training data unknown
- include normalization

$$\mathcal{L} = \frac{|f(x) - f_\theta(x)|^2}{2\sigma_\theta(x)^2} + \log \sigma_\theta(x) + \cdots$$

- if needed replace $\sigma_\theta(x)$ by mixture model

$\to$ Learning function and systematic uncertainty

More network training

Variational inference

- 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

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

More network training

Variational inference

- 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

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

- similarity from minimal KL-divergence

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

- Sampled likelihood + regularization

$$\mathcal{L}_\text{BNN} = - \int d\theta \; q(\theta) \; \log p(A_\text{train}|\theta) + D_\text{KL}[q(\theta), p(\theta)]$$

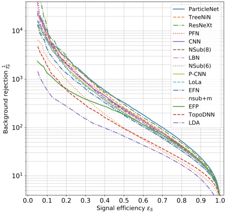
$\rightarrow$ Sampling of statistical uncertainty

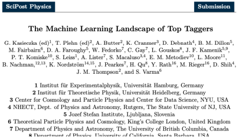
ML in experiment

Top tagging [classification, 2016-today]

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

$\rightarrow$ 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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2 Institut für Theoretische Physik, Universität Heidelberg, Germany
3 Center for Cosmology and Particle Physics and Center for Data Science, NYU, USA
4 NHECT, Dept. of Physics and Astronomy, Rutgers, The State University of NJ, USA
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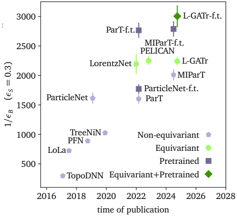
6 Theoretical Particle Physics and Cosmology, King's College London, United Kingdom
7 Department of Physics and Astronomy, The University of British Columbia, Canada



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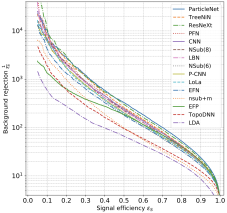

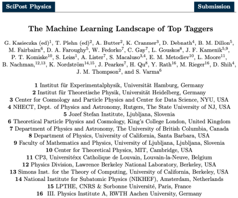
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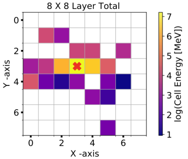
Particle flow [2020-today]

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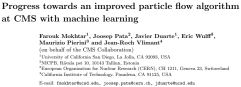
Progress towards an improved particle flow algorithm at CMS with machine learning

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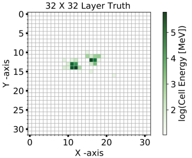
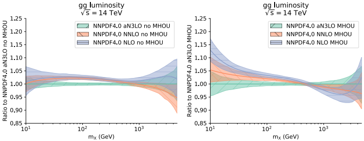


ML in phenomenology

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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[3] *CERN, Theoretical Physics Department, CH-1211 Geneva 23, Switzerland*
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[6] *University of Jyvaskyla, Department of Physics, P.O. Box 35, FI-40014 University of Jyvaskyla, Finland*
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This paper is dedicated to the memory of Stefano Catani, Grand Master of QCD, great scientist and human being

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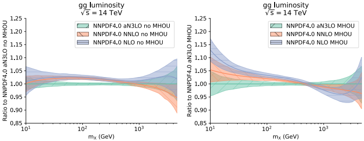

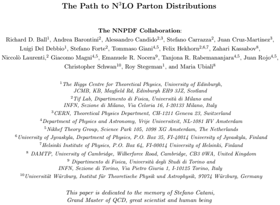

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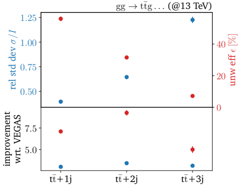
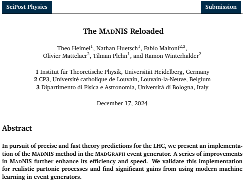
Ultra-fast event generators [Sherpa, MadNIS, MLHad]

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

→ 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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3 Dipartimento di Fisica e Astronomia, Universitá 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.

Transforming Particle Physics

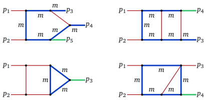
Tilman Plehn

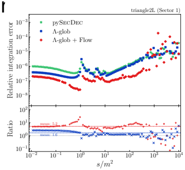
ML in theory

Optimizing integration paths [invertible networks]

- find optimal integration paths
- learn variable transformatior

→ Theory-integrator





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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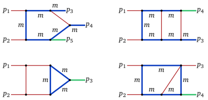

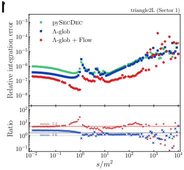

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Navigating string landscape [reinforcement learning]

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

→ Model space sampling

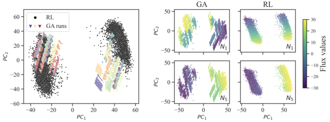

Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_3 and N_5 respectively) in relation to principal components for a PCA fit of the individual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

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

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Abstract

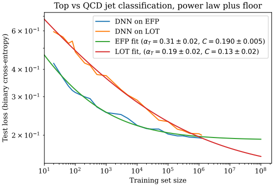
Identifying string theory vacua with desired physical properties at low energies requires searching through high-dimensional solution spaces – collectively referred to as the string landscape. We highlight that this search problem is amenable to reinforcement learning and genetic algorithms. In the context 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

$\rightarrow$ 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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Transforming Particle Physics

Tilman Plehn

ML introduction

Training

Examples

Amplitudes

Generative AI

Transformation

Theory for ML

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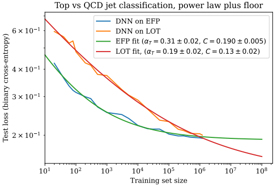

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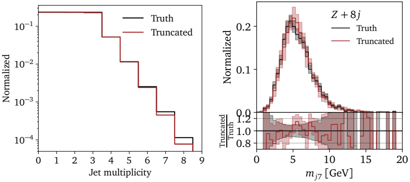
Extrapolating transformers

- 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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December 17, 2024

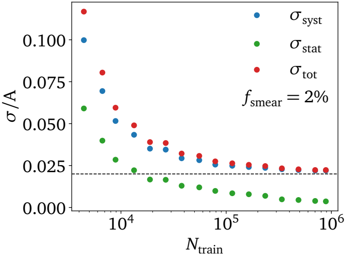
Abstract

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.

Network amplitudes

Loop amplitude $gg \to \gamma\gamma g(g)$

- regression of exact scalar over phase space
- statistics vs systematics
- example systematics: artificial noise



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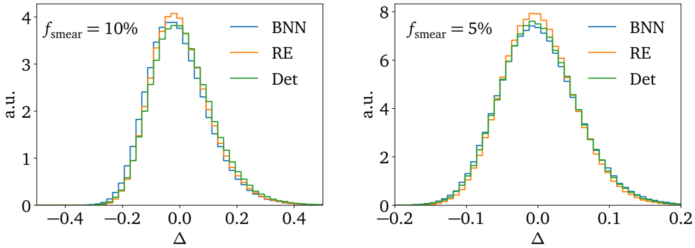

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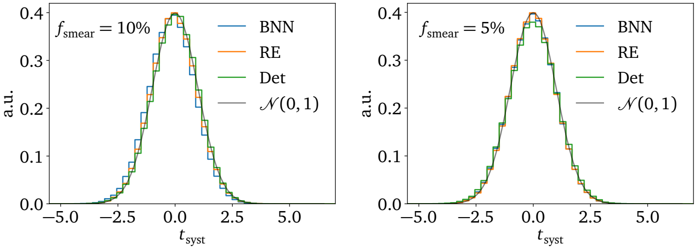
$$t(x) = \frac{A_{\text{NN}}(x) - A_{\text{true}}(x)}{\sigma(x)}$$

$\rightarrow$ calibrated leading systematics



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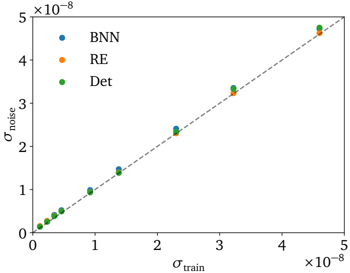
Towards zero noise

- extrapolate to zero noise

$$\sigma^2_\text{noise} = \sigma^2_\text{syst} - \sigma^2_\text{syst,0} \approx \sigma^2_\text{train}$$



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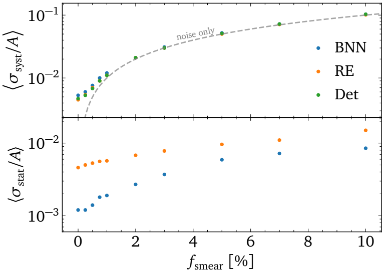
- systematics plateau $\langle \sigma / A \rangle \sim 0.4\%$

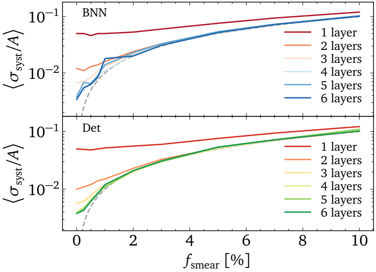
$\to$ Limiting factor??



Improved accuracy

Network expressivity

- large range of amplitude values
- resolution of (collinear) peaks
- network breaks for large amplitudes
- 3 hidden layers needed
- activation function
  machine precision...



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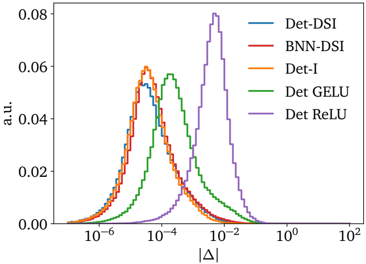
Data pre-processing

- amplitude from invariants
- learn Minkowski metric?
- Deep-sets-invariant network [Heinrich etal]
  L-GATr transformer



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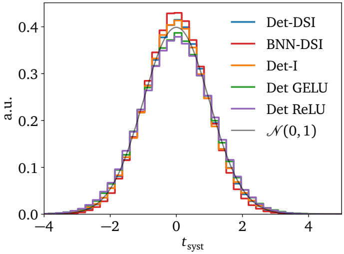
- uncertainty scaling with accuracy
  pull unit Gaussian

$\rightarrow$ Calibrated leading systematics



ATLAS calibration

Energy calibration with uncertainties [ATLAS + Heidelberg]

- 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
  data representation ...

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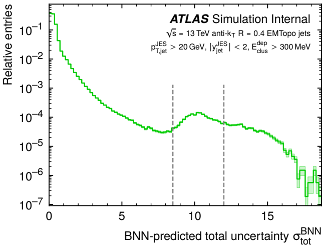
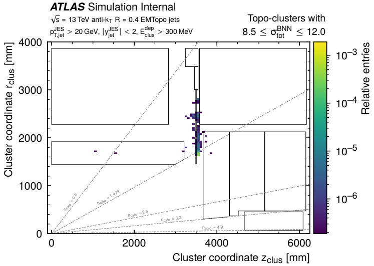
$\rightarrow$ Understand (simulated) detector



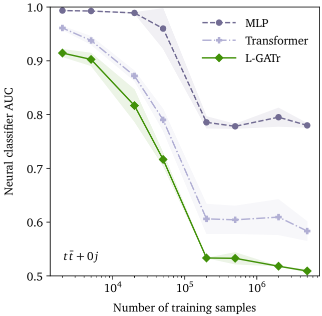


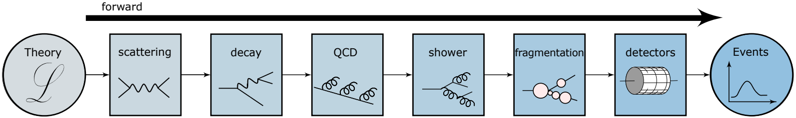
Generative AI

Simulations, MadNIS, calorimeters,... [ask Claudius Krause]

- 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...





Generative AI with uncertainties

Bayesian generative networks

- encoding phase space probabilities
- events with error bars on weights
- learned density & uncertainty
  reflecting network learning

$\rightarrow$ Generative networks like fitted densities

Generative AI with uncertainties

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$\rightarrow$ Generative networks like fitted densities

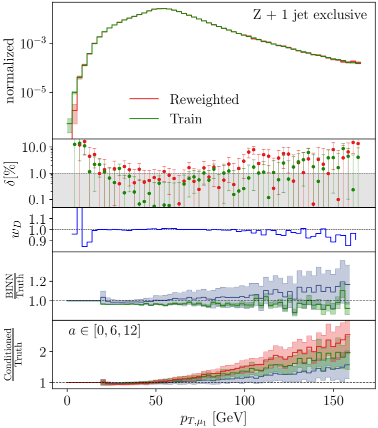
Z+jets events

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

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

- training with condition a sampling including a

$\rightarrow$ Precision and uncertainty control



Controlling generative AI

Compare generated with training data

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

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

$\rightarrow$ Test ratio over phase space

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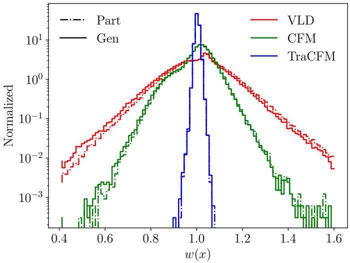
Progress in NN-generators

- 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?

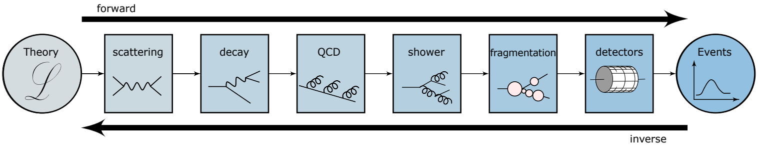
Optimal analyses

- 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

$\rightarrow$ Unfold to suitable level



ML-Unfolding

Basic structure [ask Robert Schöfbeck]

- four phase space distributions

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

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

→ Unbinned and high-dimensional unfolding

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$\to$ Unbinned and high-dimensional unfolding

OmniFold

- learn $p_\text{sim}(x_\text{reco}) \leftrightarrow p_\text{data}(x_\text{reco})$
- 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}) \\
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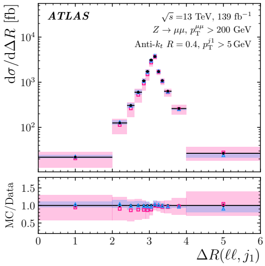

$\to$ Z+jets in 24D [ATLAS]

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

$$
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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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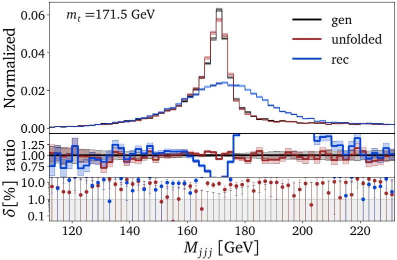
Preliminary unfolding results [TraCFM]

- 4D for calibrated mass measurement



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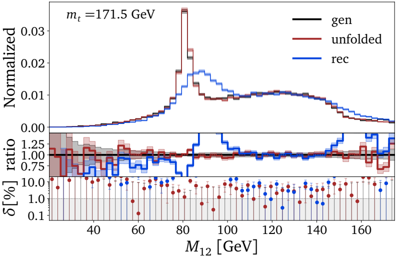
- 4D for calibrated mass measurement
- 12D published data

$\to$ 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

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

→ Complexity a feature, not a problem

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
[c] HEPHY, Austrian Academy of Sciences. Vienna, Austria
[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]