Modern Machine Learning for Jets

Tilman Plehn

Universität Heidelberg

JetMET, Brussels, May 2023

LHC physics vs data scientist

LHC questions

- How to trigger from 3 PB/s to 300 MB/s?
  Data compression [Netflix]
- How to analyze ntuples?
  Graph neural networks [Car cameras]
- How to incorporate symmetries?
  Contrastive learning [Google]
- How to combine tracker and calorimeter?
  Super-resolution [Gaming]
- How to remove pile-up?
  Data denoising [Cars]
- How to look for BSM physics?
  Autoencoders [SAP]
- How to generate jets/events?
  Generative transformer [ChatGPT]
- How to analyse LHC data?
  Simulation-based inference [LHC leading?]
- But how about uncertatinties?

Shortest ML-intro ever

Fit-like approximation [ask NNPDF]

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

Construction and contol

- minimize loss to find best θ
- typically, likelihood generalizing fit χ^2
- compare $x \to f_\theta(x)$ for training/test data

LHC applications

- 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 $r \sim \mathcal{N} \to f_\theta(r|x)$
- ...

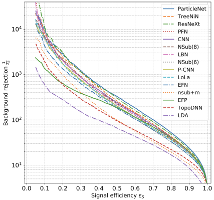
$\to$ Transforming numerical science

Analysis

Jet tagging [supervised classification]

- ‘hello world’ of LHC-ML
- end of QCD-taggers
- powerful NN-architectures

→ ParticleNet & Co established



SciPost Physics — Submission

The Machine Learning Landscape of Top Taggers

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Particle flow [classification, super-resolution]

- mother of jet tools
- combined detector channels
- similar studies in CMS

→ Seriously impressive

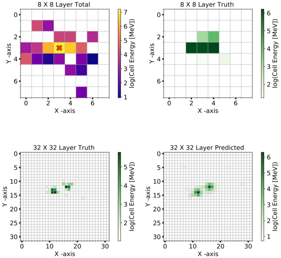

Fig. 7: An event display of total energy shower (within topocluster), as captured by a calorimeter layer of 8×8 granularity, along with the location of the track, denoted by a red cross (left) and the same shower is captured by a calorimeter layer of 32×32 granularity (middle). The bottom right panel shows the corresponding event predicted by the NN. The figure shows that the shower originating from a $\pi^0 \to \gamma\gamma$ is resolved by a 32×32 granularity layer.

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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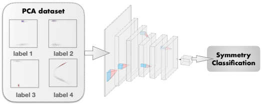
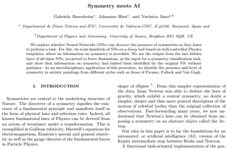
Symmetries

Learning symmetries [representation, visualization]

- (particle) physics is all symmetries
- identify symmetries in 2D systems [paintings]

→ NN-identified symmetries





Symmetry meets AI

Gabriela Barenboim[a], Johannes Hirn[a], and Verónica Sanz[a,b]

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We explore whether Neural Networks (NNs) can *discover* the presence of symmetries as they learn to perform a task. For this, we train hundreds of NNs on a *decoy task* based on well-controlled Physics templates, where no information on symmetry is provided. We use the output from the last hidden layer of all these NNs, projected to fewer dimensions, as the input for a symmetry classification task, and show that information on symmetry had indeed been identified by the original NN without guidance. As an interdisciplinary application of this procedure, we identify the presence and level of symmetry in artistic paintings from different styles such as those of Picasso, Pollock and Van Gogh.

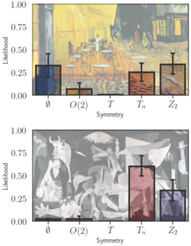
I. INTRODUCTION

Symmetries are central to the underlying structure of Nature. The discovery of a symmetry signifies the existence of a fundamental principle and manifests itself in the form of physical laws and selection rules. Indeed, all known fundamental laws of Physics can be derived from an axiom of invariance under a transformation. This is exemplified in Galilean relativity, Maxwell's equations for electromagnetism, Einstein's special and general relativity as well as the gauge theories of the fundamental forces in Particle Physics.

shape of ellipses [1]. From this simpler representation of the data, Isaac Newton was able to deduce the laws of gravity, which exhibit a central symmetry, no doubt a simpler, deeper and thus more general description of the motion of celestial bodies than the original collection of observations. Fast-forwarding many years, we now understand that Newton's laws can be obtained from imposing a symmetry on an abstract object called the Action.

Our idea in this paper is to lay the foundations for an automated, or artificial intelligence (AI), version of the Kepler intermediate step between Brahe and Newton.

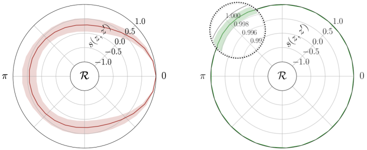
A functional task-oriented implementation of the gen-

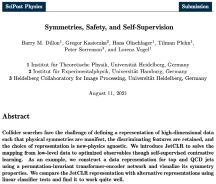


Symmetric networks [contrastive learning, transformer network]

- rotations, translations, permutations, soft splittings, collinear splittings
- learn symmetries/augmentations

→ Symmetric latent representation





SciPost Physics | Submission

Symmetries, Safety, and Self-Supervision

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August 11, 2021

Abstract

Collider searches face the challenge of defining a representation of high-dimensional data such that physical symmetries are manifest, the discriminating features are retained, and the choice of representation is new-physics agnostic. We introduce JetCLR to solve the mapping from low-level data to optimized observables though self-supervised contrastive learning. As an example, we construct a data representation for top and QCD jets using a permutation-invariant transformer-encoder network and visualize its symmetry properties. We compare the JetCLR representation with alternative representations using linear classifier tests and find it to work quite well.

Anomalous jets and parton densities

Anomaly searches [unsupervised training]

- train on QCD-jets, SM-events
- look for non-QCD jets, non-SM events

→ LHC spirit, more later

SciPost Physics Submission

Better Latent Spaces for Better Autoencoders

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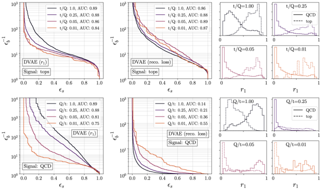
April 20, 2021

Abstract

Autoencoders as tools behind anomaly searches at the LHC have the structural problem that they only work in one direction, extracting jets with higher complexity but not the other way around. To address this, we derive classifiers from the latent space of (variational) autoencoders, specifically in Gaussian mixture and Dirichlet latent spaces. In particular, the Dirichlet setup solves the problem and improves both the performance and the interpretability of the networks.



NNPDF/N3PDF parton densities [full blast]

- starting point: pdfs without functional ansatz
- moving on: cutting-edge ML everywhere

→ Leaders in ML-theory

A data-based parametrization of parton distribution functions

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Received: date / Revised version: date

Abstract. Since the first determination of a structure function many decades ago, all methodologies used to determine structure functions or parton distribution functions (PDFs) have employed a common prefactor as part of the parametrization. The NNPDF collaboration pioneered the use of neural networks to overcome the inherent bias of constraining the space of solution with a fixed functional form while still keeping the same common prefactor as a preprocessing. Over the years various, increasingly sophisticated, techniques have been introduced to counter the effect of the prefactor on the PDF determination. In this paper we present a methodology to remove the prefactor entirely, thereby significantly simplifying the methodology, without a loss of efficiency and finding good agreement with previous results.

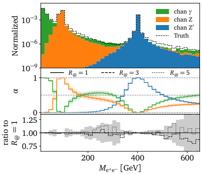
PACS. 12.38.-t Quantum chromodynamics – 12.39.-x Phenomenological quark models – 84.35.+i Neural Networks

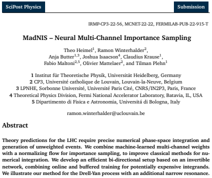
Faster event generators

Speeding up Sherpa and MadNIS [phase space sampling]

- precision simulations limiting factor for Runs 3&4
- fast and efficient sampling key

→ ML-Multichannel-Vegas




SciPost Physics Submission

IRMP-CP3-22-56, MCNET-22-22, FERMILAB-PUB-22-915-T

MadNIS – Neural Multi-Channel Importance Sampling

Theo Heimel[1], Ramon Winterhalder[2], Anja Butter[1,3], Joshua Isaacson[4], Claudius Krause[1], Fabio Maltoni[2,5], Olivier Mattelaer[2], and Tilman Plehn[1]

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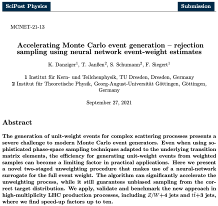
Abstract

Theory predictions for the LHC require precise numerical phase-space integration and generation of unweighted events. We combine machine-learned multi-channel weights with a normalizing flow for importance sampling, to improve classical methods for numerical integration. We develop an efficient bi-directional setup based on an invertible network, combining online and buffered training for potentially expensive integrands. We illustrate our method for the Drell-Yan process with an additional narrow resonance.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MCNET-21-13

Accelerating Monte Carlo event generation – rejection sampling using neural network event-weight estimates

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September 27, 2021

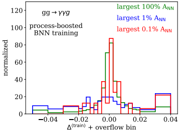
Abstract

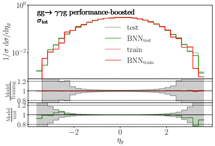
The generation of unit-weight events for complex scattering processes presents a severe challenge to modern Monte Carlo event generators. Even when using sophisticated phase-space sampling techniques adapted to the underlying transition matrix elements, the efficiency for generating unit-weight events from weighted samples can become a limiting factor in practical applications. Here we present a novel two-staged unweighting procedure that makes use of a neural-network surrogate for the full event weight. The algorithm can significantly accelerate the unweighting process, while it still guarantees unbiased sampling from the correct target distribution. We apply, validate and benchmark the new approach in high-multiplicity LHC production processes, including Z/W+4 jets and $t\bar{t}$+3 jets, where we find speed-up factors up to ten.

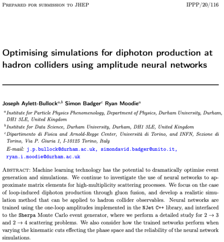
Speeding up amplitudes [phase space regression]

- loop-amplitudes expensive
- interpolation standard

→ Precision NN-regression, more later






PREPARED FOR SUBMISSION TO JHEP IPPP/20/116

Optimising simulations for diphoton production at hadron colliders using amplitude neural networks

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ABSTRACT: Machine learning technology has the potential to dramatically optimise event generation and simulations. We continue to investigate the use of neural networks to approximate matrix elements for high-multiplicity scattering processes. We focus on the case of loop-induced diphoton production through gluon fusion, and develop a realistic simulation method that can be applied to hadron collider observables. Neural networks are trained using the one-loop amplitudes implemented in the NJet C++ library, and interfaced to the Sherpa Monte Carlo event generator, where we perform a detailed study for $2 \to 3$ and $2 \to 4$ scattering problems. We also consider how the trained networks perform when varying the kinematic cuts effecting the phase space and the reliability of the neural network simulations.

Modern ML

Tilman Plehn

ML motivation

ML examples

Regression

Classification

Inference

Resilience

Forward and inverse simulation

Precision NN-generators [INN + Bayesian discriminator]

- control through discriminator [GAN-like]
- uncertainties through Bayesian networks
- phase space prototypical

→ Precision & control

SciPost Physics — Submission

Generative Networks for Precision Enthusiasts

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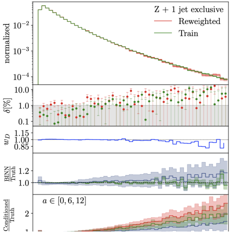
November 16, 2021

Abstract

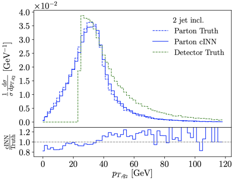
Generative networks are opening new avenues in fast event generation for the LHC. We show how generative flow networks can reach percent-level precision for kinematic distributions, how they can be trained jointly with a discriminator, and how this discriminator improves the generation. Our joint training relies on a novel coupling of the two networks which does not require a Nash equilibrium. We then estimate the generation uncertainties through a Bayesian network setup and through conditional data augmentation, while the discriminator ensures that there are no systematic inconsistencies compared to the training data.



Unfolding and inversion [conditional normalizing flows]

- shower/hadronization unfolded by jet algorithm
- detector/decays unfolded e.g. in tops
- calibrated inverse sampling

→ Inverse generation



SciPost Physics — Submission

Invertible Networks or Partons to Detector and Back Again

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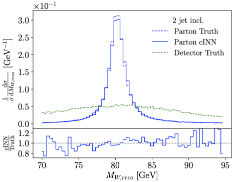
October 2, 2020

Abstract

For simulations where the forward and the inverse directions have a physics meaning, invertible neural networks are especially useful. A conditional INN can invert a detector simulation in terms of high-level observables, specifically for ZW production at the LHC. It allows for a per-event statistical interpretation. Next, we allow for a variable number of QCD jets. We unfold detector effects and QCD radiation to a pre-defined hard process, again with a per-event probabilistic interpretation over parton-level phase space.



Targeting theory

Navigating string landscape [reinforcement learning]

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

→ Model space sampling

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.

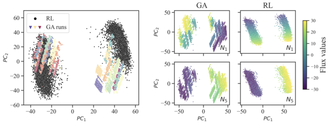

Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_3 and N_5 respectively) in relation to principal components for a PCA fit of the individual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

Learning formulas [genetic algorithm, symbolic regression]

- approximate numerical function through formula
- example: score/optimal observables

→ Useful approximate formulas

compl	dof	function	MSE
3	1	$a\,\Delta\phi$	$1.30 \cdot 10^{-1}$
4	1	$\sin(a\Delta\phi)$	$2.75 \cdot 10^{-1}$
5	1	$a\Delta\phi x_{p,1}$	$9.93 \cdot 10^{-2}$
6	1	$-x_{p,1}\sin(\Delta\phi + a)$	$1.90 \cdot 10^{-1}$
7	1	$(-x_{p,1} - a)\sin(\sin(\Delta\phi))$	$5.63 \cdot 10^{-2}$
8	1	$(a - x_{p,1})x_{p,2}\sin(\Delta\phi)$	$1.61 \cdot 10^{-2}$
14	2	$x_{p,1}(a\Delta\phi - \sin(\sin(\Delta\phi)))(x_{p,2} + b)$	$1.44 \cdot 10^{-2}$
15	3	$-(x_{p,2}(a\Delta\eta^2 + x_{p,1}) + b)\sin(\Delta\phi + c)$	$1.30 \cdot 10^{-2}$
16	4	$-x_{p,1}(a - b\Delta\eta)(x_{p,2} + c)\sin(\Delta\phi + d)$	$8.50 \cdot 10^{-3}$
28	7	$(x_{p,2} + a)(bx_{p,1}(c - \Delta\phi) - x_{p,1}(d\Delta\eta + ex_{p,2} + f)\sin(\Delta\phi + g))$	$8.18 \cdot 10^{-3}$

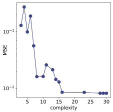

Table 8: Score hall of fame for simplified WBF Higgs production with $f_{W\widetilde{W}} = 0$, including a optimization fit.

SciPost Physics Submission

Back to the Formula — LHC Edition

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2 Center for Data Science, New York University, New York, United States
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November 16, 2021

Abstract

While neural networks offer an attractive way to numerically encode functions, actual formulas remain the language of theoretical particle physics. We use symbolic regression trained on matrix-element information to extract, for instance, optimal LHC observables. This way we invert the usual simulation paradigm and extract easily interpretable formulas from complex simulated data. We introduce the method using the effect of a dimension-6 coefficient on associated ZH production. We then validate it for the known case of CP-violation in weak-boson-fusion Higgs production, including detector effects.

Precision regression

Regression as in jet calibration?

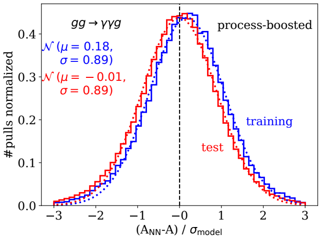
- example: loop amplitudes $gg \to \gamma\gamma g(g)$
- training data $A_j(x)$ exact
- boostable likelihood loss

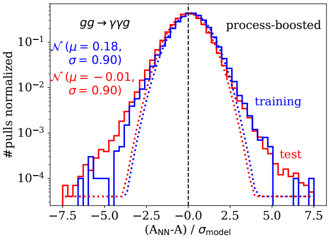
$$L \sim \sum_{\text{points } j} n_j \times \left[\frac{\left| A_j(\omega) - A_j^{\text{truth}} \right|^2}{2\sigma_j(\omega)^2} + \log \sigma_j(\omega) \right] \cdots$$

- pull Gaussian?

$$\frac{A_j(\omega) - A_j^{\text{truth}}}{\sigma_j(\omega)}$$

- NN-fit $\longrightarrow$ NN-interpolation [n_j as function of pull, σ, A,...]





Precision regression

Regression as in jet calibration?

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- pull Gaussian?

$$\frac{A_j(\omega) - A_j^{\text{truth}}}{\sigma_j(\omega)}$$

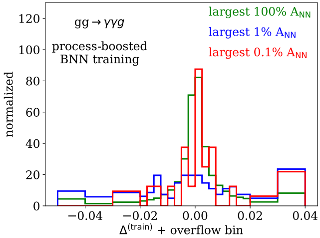
- NN-fit $\longrightarrow$ NN-interpolation [n_j as function of pull, σ, A,...]

Precision

- quality of NN-amplitudes

$$\Delta_j = \frac{\langle A \rangle_j - A_j^{\text{truth}}}{A_j^{\text{truth}}}$$

$\to$ Beyond fit-like regression



Precision regression

Regression as in jet calibration?

- example: loop amplitudes $gg \to \gamma\gamma g(g)$
- training data $A_j(x)$ exact
- boostable likelihood loss

$$L \sim \sum_{\text{points } j} n_j \times \left[\frac{\left| A_j(\omega) - A_j^{\text{truth}} \right|^2}{2\sigma_j(\omega)^2} + \log \sigma_j(\omega) \right] \cdots$$

- pull Gaussian?

$$\frac{A_j(\omega) - A_j^{\text{truth}}}{\sigma_j(\omega)}$$

- NN-fit $\longrightarrow$ NN-interpolation [n_j as function of pull, σ, A,...]

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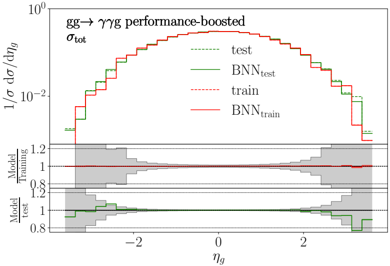
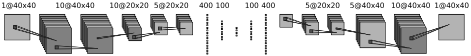


Training on QCD only



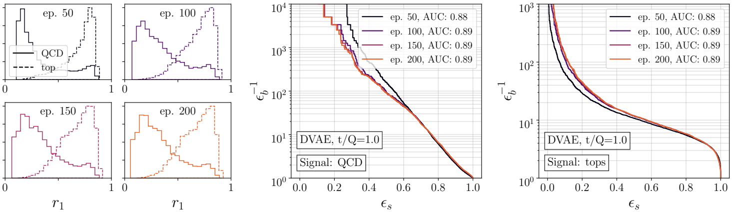
Unsupervised classification

- train on background only
  extract unknown signal from reconstruction error
- reconstruct QCD jets $\to$ top jets hard to describe
  reconstruct top jets $\to$ QCD jets just simple top-like jet
- dark-jets complexity: mass drop vs semivisible constituents

$\to$ Symmetric performance $S \leftrightarrow B$?

Anomaly score from latent space

- VAE $\to$ does not work
  GMVAE $\to$ does not work
  density estimation $\to$ does not work
  Dirichlet VAE $\to$ works okay



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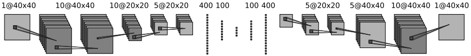

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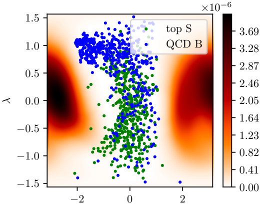


Normalized autoencoder [penalize missing features]

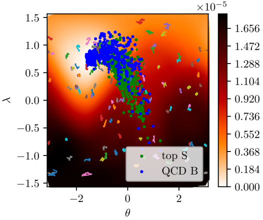
- normalized probability loss
- Boltzmann mapping [E_θ =MSE]

$$p_\theta(x) = \frac{e^{-E_\theta(x)}}{Z_\theta}$$

$$L = -\big\langle \log p_\theta(x) \big\rangle = \big\langle E_\theta(x) + \log Z_\theta \big\rangle$$

- inducing background metric
- small MSE for data, large MSE for model
- Z_θ from (Langevin) Markov Chain

$\rightarrow$ Proper autoencoder, at last...



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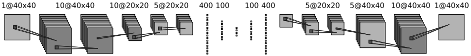

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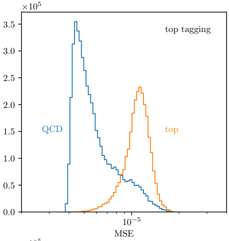
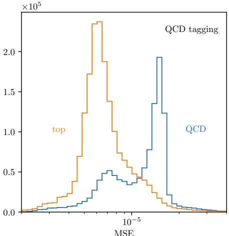




Measuring QCD splitting

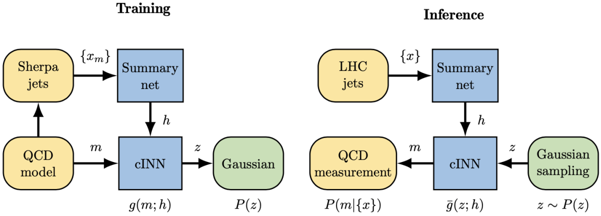
Conditional INN for inference

- condition jets with QCD parameters
  train model parameters $\to$ Gaussian latent space
  test Gaussian sampling $\to$ parameter measurement
- beyond C_A vs C_F [Kluth etal]

$$P_{qq} = C_F \left[D_{qq} \frac{2z(1-y)}{1-z(1-y)} + F_{qq}(1-z) + C_{qq} yz(1-z) \right]$$

$$P_{gg} = 2C_A \left[D_{gg} \left(\frac{z(1-y)}{1-z(1-y)} + \frac{(1-z)(1-y)}{1-(1-z)(1-y)} \right) + F_{gg} z(1-z) + C_{gg} yz(1-z) \right]$$

$$P_{gq} = T_R \left[F_{qq} \left(z^2 + (1-z)^2 \right) + C_{gq} yz(1-z) \right]$$



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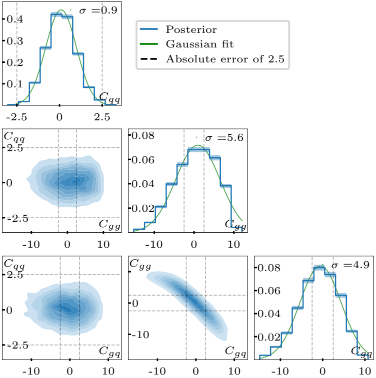
- idealized shower [Sherpa]
- ML-opportunities...



ML for the LHC

ML-applications

- just another numerical tool for a numerical field
- driven by money from data science and medical research
- goals are...

  ...improve established tasks
  ...develop new tools for established tasks
  ...transform through new ideas
- xAI through...

  ...precision control
  ...uncertainties
  ...symmetries
  ...formulas

$\to$ Fun with good old QCD problems

Modern Machine Learning for LHC Physicists

Tilman Plehn[a,*], Anja Butter[a,b], Barry Dillon[a], and Claudius Krause[a,c]

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November 2, 2022

Abstract

Modern machine learning is transforming particle physics, faster than we can follow, and 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 are meant to lead students with basic knowledge of particle physics and significant enthusiasm for machine learning to relevant applications as fast as possible. 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 reflecting the problem at hand 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. Given that these notes will be outdated already at the time of submission, the week of ML4Jets 2022, they will be updated frequently.

Resilient training

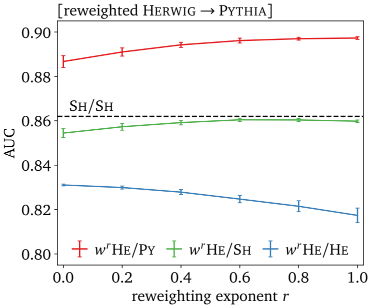
Training on simulation, testing on data

- assume a simulation vs data difference [generalization gap]
  plus, different simulation datasets
- simple question: how train on several datasets?
- adversarial training?
  nuisance parameter?

$\rightarrow$ Uncertain feature same as main discriminator??

Constructing an interpolation parameter

- re-weighted samples: Herwig $\xleftrightarrow{0 \le r \le 1}$ Pythia
- test data, call it Sherpa
- classify conditionally on r
- 1 use r to define working point
  2. vary r to estimate uncertainty
- best AUC for Pythia training



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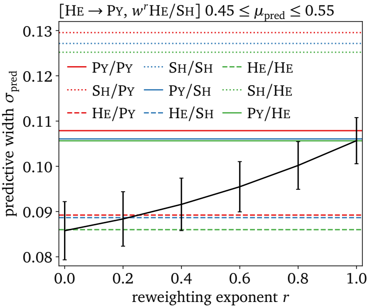
- lowest uncertainty for Herwig training



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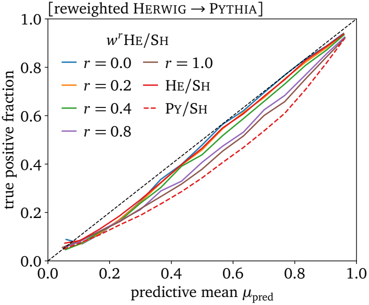
- lowest uncertainty for Herwig training
- best calibration for Herwig



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- continuous approach to calibration?

→ A hammer looking for nails...