LHC Theory as Fun Data Science

Tilman Plehn

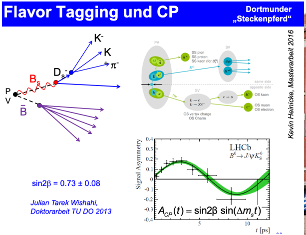
Universität Heidelberg

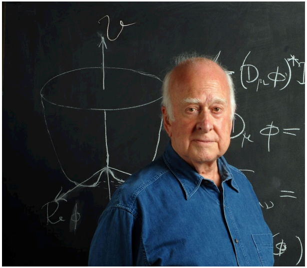
Benasque, September 2022

Modern LHC physics

Classic motivation

- dark matter
- baryogenesis
- Higgs VEV





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LHC physics

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

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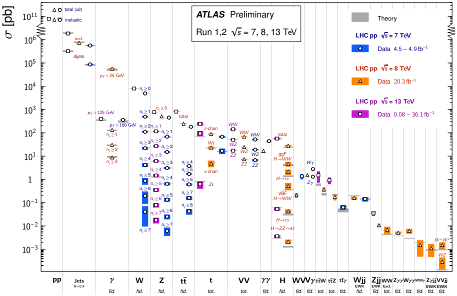
Traditional methods

- discover in rates
- unveil little black holes
- find supersymmetry
- travel extra dimensions
- measure couplings



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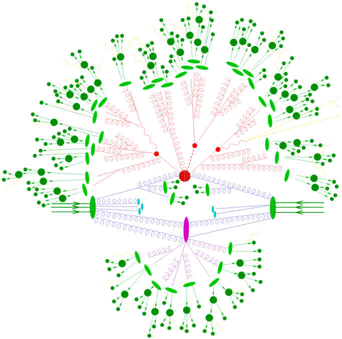
First-principle simulations

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

$\rightarrow$ LHC events in virtual worlds



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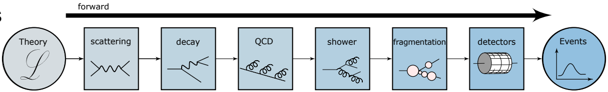
BSM searches

- compare simulations and data
- analyze data systematically [SMEFT]
- understand LHC dataset [SM or BSM]
- publish useable results

$\rightarrow$ With a little help from data science...



Ask a data scientist

LHC questions

- How to get from 3 PB/s to 300 MB/s?

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  Data compression [Netflix]

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...

→ How can we contribute to data science?

Shortest ML-intro ever

Fit-like approximation

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

Construction and contol

- define (well-defined) loss function
- minimize loss to find best θ
- compare $x \to f_\theta(x)$ for training/test data

LHC applications

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

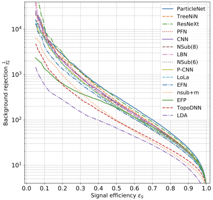
$\to$ Transforming numerical science

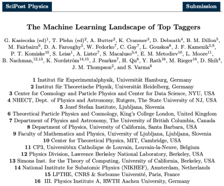
ML-applications for analysis

Top tagging [supervised classification]

- ‘hello world’ of LHC-ML
- the end of QCD
- different NN-architectures

→ Non-NN left in the dust...




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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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
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
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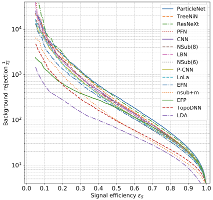

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Particle flow [classification, super-resolution]

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

$\rightarrow$ Seriously impressive

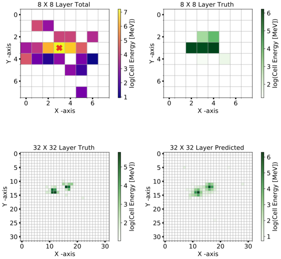


Fig. 7: An event display of total energy shower (within topocluster), as captured by a calorimeter layer of 8×8 granularity, along with the location of the track, denoted by a red cross (left) and the same shower is captured by a calorimeter layer of 32×32 granularity (middle). The bottom right panel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

[1]Weizmann Institute of Science, Rehovot 76100, Israel
[2]CERN, CH 1211, Geneva 23, Switzerland
[3]Università di Roma Sapienza, Piazza Aldo Moro, 2, 00185 Roma, Italy e INFN, Italy
[4]Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405, Orsay, France

LHC Data Science

Tilman Plehn

LHC physics

ML examples

Uncertainties

Inversion

Anomalies

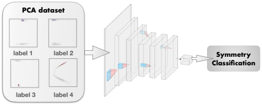
Symbolic reg

Symmetries

Learning symmetries [representation, visualization]

- (particle) physics is all symmetries
- identify symmetries in 2D systems [paintings]
- CNN on PCAs of penultimate network layers

$\to$ Networks represent data patterns



Symmetry meets AI

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

[a] Departament de Física Teòrica and IFIC, Universitat de València-CSIC, E-46100, Burjassot, Spain and

[b] Department of Physics and Astronomy, University of Sussex, Brighton BN1 9QH, UK

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.

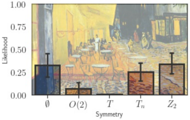
I. INTRODUCTION

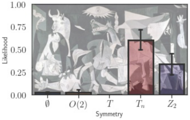
Symmetries are central to the underlying structure of Nature. The discovery of a symmetry signifies the existence of a fundamental principle and manifests itself in the form of physical laws and selection rules. Indeed, all known fundamental laws of Physics can be derived from an axiom of invariance 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-





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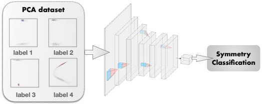

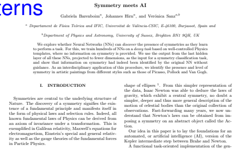

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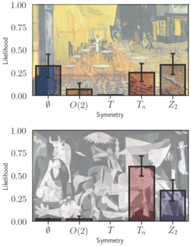
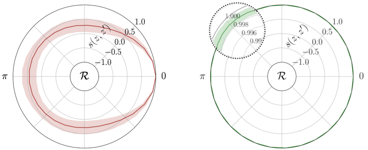
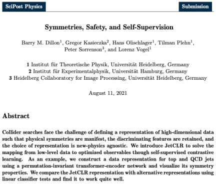


Symmetric networks [contrastive learning, transformer network]

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

→ Symmetry-aware latent space





SciPost Physics Submission

Symmetries, Safety, and Self-Supervision

Barry M. Dillon[1], Gregor Kasieczka[2], Hans Olischlager[1], Tilman Plehn[1], Peter Sorrenson[3], and Lorenz Vogel[1]

1 Institut für Theoretische Physik, Universität Heidelberg, Germany
2 Institut für Experimentalphysik, Universität Hamburg, Germany
3 Heidelberg Collaboratory for Image Processing, Universität Heidelberg, Germany

August 11, 2021

Abstract

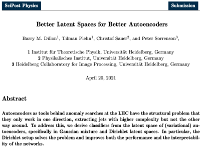
Collider searches face the challenge of defining a representation of high-dimensional data such that physical symmetries are manifest, the discriminating features are retained, and the choice of representation is new-physics agnostic. We introduce JetCLR to solve the mapping from low-level data to optimized 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.

Non-QCD and parton densities

Anomaly searches [unsupervised training, see later]

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

$\to$ Spirit of LHC


SciPost Physics   Submission

Better Latent Spaces for Better Autoencoders

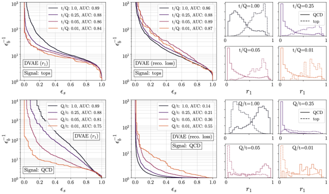
Barry M. Dillon[1], Tilman Plehn[1], Christof Sauer[2], and Peter Sorrenson[3],

1 Institut für Theoretische Physik, Universität Heidelberg, Germany
2 Physikalisches Institut, Universität Heidelberg, Germany
3 Heidelberg Collaboratory for Image Processing, Universität Heidelberg, Germany

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.



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SciPost Physics — Submission

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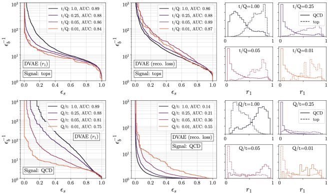


NNPDF/N3PDF parton densities [full blast]

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

→ Leaders in ML-theory

A data-based parametrization of parton distribution functions

Stefano Carrazza[1,2,3], Juan Cruz-Martinez[1], and Roy Stegeman[1]

[1] TIF Lab, Dipartimento di Fisica, Università degli Studi di Milano and INFN Sezione di Milano.
[2] CERN, Theoretical Physics Department, CH-1211 Geneva 23, Switzerland.
[3] Quantum Research Centre, Technology Innovation Institute, Abu Dhabi, UAE.

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

Events and amplitudes

Speeding up Sherpa [sampling]

- precision simulations limiting factor for Runs 3&4
- unweighting critical

→ Phase space sampling

	$gg \to t\bar{t}ggg$	$ug \to t\bar{t}ggu$	$uu \to t\bar{t}guu$	$u\bar{u} \to t\bar{t}gd\bar{d}$
ϵ_{full}	1.1e−2	7.3e−3	6.8e−3	6.6e−4
$\epsilon_{\text{1st,surr}}$	8.7e−3	5.8e−3	4.7e−3	3.6e−4
$\langle t_{\text{full}}\rangle / \langle t_{\text{surr}}\rangle$	39312	2417	199	64
$x_{\max}^{\text{p.m.}}$	52.03	32.52	69.76	326.19
$\epsilon_{\text{2nd,surr}}^{\text{p.m.}}$	2.4e−2	3.8e−2	2.1e−2	5.6e−3
$\alpha^{\text{p.m.}}$	0.9989	0.9984	0.9994	0.9981
$f_{\text{eff}}^{\text{p.m.}}$	2.21	4.89	1.47	0.19
$x_{\max}^{\text{med}}$	30.40	19.14	27.78	25.34
$\epsilon_{\text{2nd,surr}}^{\text{med}}$	4.3e−2	6.4e−2	5.1e−2	7.1e−2
α^{med}	0.9983	0.9966	0.9943	0.9321
$f_{\text{eff}}^{\text{med}}$	3.90	8.26	3.91	2.22

Table 6: Performance measures for partonic channels contributing to $t\bar{t}$+3 jets production at the LHC.

SciPost Physics Submission

MCNET-21-13

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

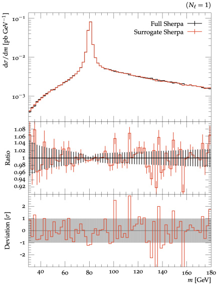
K. Danziger[1], T. Janßen[2], S. Schumann[2], F. Siegert[1]

1 Institut für Kern- und Teilchenphysik, TU Dresden, Dresden, Germany
2 Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

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.



Events and amplitudes

Speeding up Sherpa [sampling]

- precision simulations limiting factor for Runs 3&4
- unweighting critical

→ Phase space sampling

	$gg \to t\bar{t}ggg$	$ug \to t\bar{t}ggu$	$uu \to t\bar{t}guu$	$u\bar{u} \to t\bar{t}gd\bar{d}$
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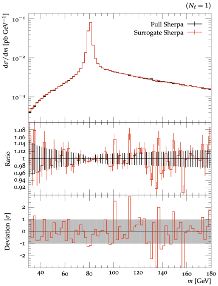
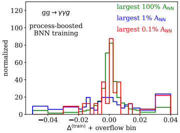
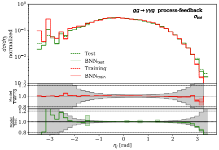


Speeding up amplitudes [precision regression]

- loop-amplitudes expensive
- interpolation standard

→ Network amplitudes





Prepared for submission to JHEP IPPP/20/116

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

Joseph Aylett-Bullock[a,b] Simon Badger[c] Ryan Moodie[a]

[a] Institute for Particle Physics Phenomenology, Department of Physics, Durham University, Durham, DH1 3LE, United Kingdom
[b] Institute for Data Science, Durham University, Durham, DH1 3LE, United Kingdom
[c] Dipartimento di Fisica and Arnold-Regge Center, Università di Torino, and INFN, Sezione di Torino, Via P. Giuria 1, I-10125 Torino, Italy

E-mail: j.p.bullock@durham.ac.uk, simondavid.badger@unito.it, ryan.i.moodie@durham.ac.uk

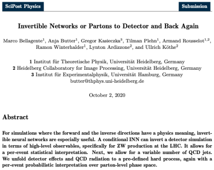
Abstract: Machine learning technology has the potential to dramatically optimise event generation and simulations. We continue to investigate the use of neural networks to approximate matrix elements for high-multiplicity scattering processes. We focus on the case of loop-induced diphoton production 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.

Invertible event generation and errors

Unfolding and inversion [conditional normalizing flows, see later]

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

$\rightarrow$ Backwards generation


SciPost Physics | Submission

Invertible Networks or Partons to Detector and Back Again

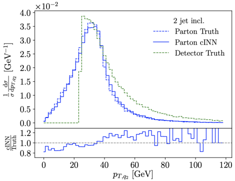
Marco Bellagente[1], Anja Butter[1], Gregor Kasieczka[3], Tilman Plehn[1], Armand Rousselot[1,2], Ramon Winterhalder[1], Lynton Ardizzone[2], and Ullrich Köthe[2]

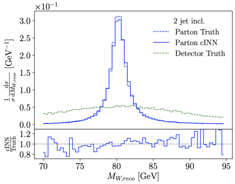
1 Institut für Theoretische Physik, Universität Heidelberg, Germany
2 Heidelberg Collaboratory for Image Processing, Universität Heidelberg, Germany
3 Institut für Experimentalphysik, Universität Hamburg, Germany
butter@thphys.uni-heidelberg.de

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.





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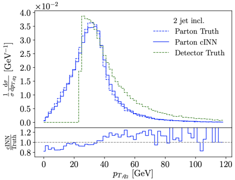
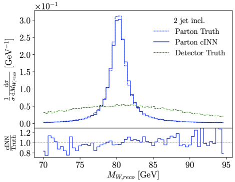




Generative networks with uncertainties [Bayesian discriminator-flows]

- control through discriminator [GAN-like]
- uncertainties through Bayesian networks

→ Precision & control

SciPost Physics Submission

Generative Networks for Precision Enthusiasts

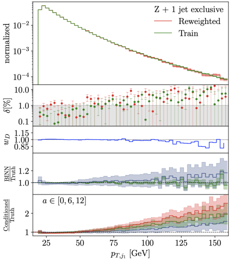
Anja Butter[1], Theo Heimel[1], Sander Hummerich[1], Tobias Krebs[1], Tilman Plehn[1], Armand Rousselot[2], and Sophia Vent[1]

1 Institut für Theoretische Physik, Universität Heidelberg, Germany
2 Heidelberg Collaboratory for Image Processing, Universität Heidelberg, Germany

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.



String landscape and learned formulas

Navigating string landscape [reinforcement learning]

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

$\rightarrow$ Model space sampling

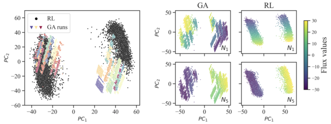


Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_3 and N_5 respectively) in relation to principal components for a PCA fit of the individual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

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

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Gary Shiu
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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.

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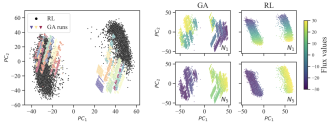

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Learning formulas [genetic algorithm, symbolic regression, see later]

- 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	$(x_{p,2} + a)(bx_{p,1}(c - \Delta\phi) - x_{p,1}(d\Delta\eta + ex_{p,2} + f)\sin(\Delta\phi + g))$	$8.18 \cdot 10^{-3}$

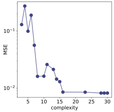

Table 8: Score hall of fame for simplified WBF Higgs production with $f_{W\widetilde{W}} = 0$, including a optimization fit.

SciPost Physics Submission

Back to the Formula — LHC Edition

Anja Butter[1], Tilman Plehn[1], Nathalie Soybelman[1], and Johann Brehmer[2]

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

Abstract

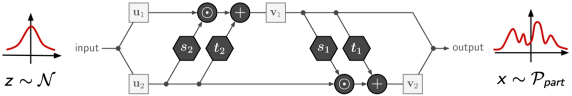
While neural networks offer an attractive way to numerically encode functions, actual formulas remain the language of theoretical particle physics. We use symbolic regression trained on matrix-element information to extract, for instance, optimal LHC observables. This way we invert the usual simulation 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.

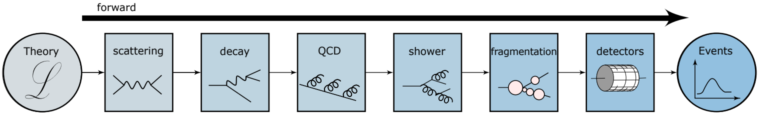
Modern generative networks

Normalizing flows — INN

- phase space density estimation
- trained on event samples
- Gaussian latent space
- bijective mapping
- known Jacobian
- log-likelihood loss

$\to$ Better for physics than VAEs and GANs





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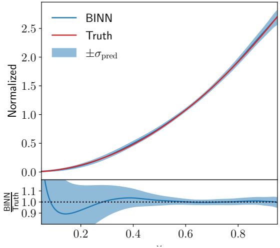
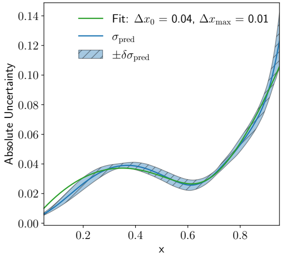


Bayesian networks with uncertainties

- network weight distributions [Gal (2016)]
- sample for output [efficient ensembling]
- working for regression, classification
- events with error bars [density & uncertainty maps]
- 2D: wedge ramp, kicker ramp,...

$\rightarrow$ Bayesian INNs just fits with error bars



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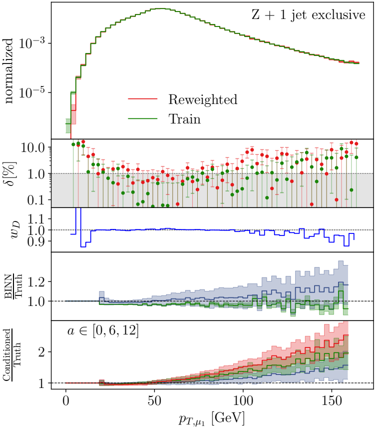

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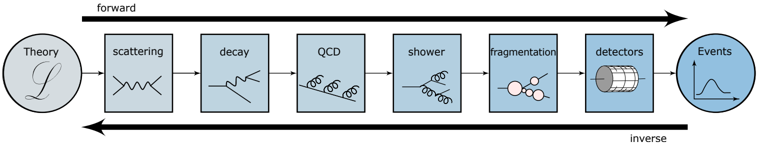
Inverse simulation

Invertible ML-simulation

- forward: $r \rightarrow$ events trained on model
- inverse: $r \rightarrow$ anything trained on model, conditioned on event



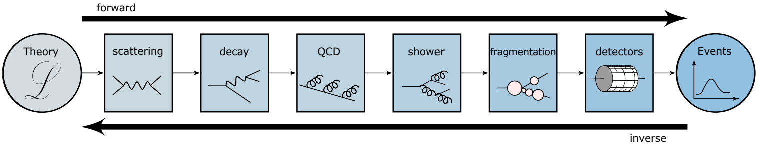
Inverse simulation

Invertible ML-simulation

- forward: $r \to$ events trained on model
- inverse: $r \to$ anything trained on model, conditioned on event
- individual steps known problems

  detector unfolding
  unfolding to QCD parton means jet algorithm
  unfolding jet radiation known combinatorics problem
  unfolding to hard process standard in top groups [needed for global analyses]
  matrix element method an old dream
- improved through coherent ML-method

$\to$ Free choice of data-theory inference point



Inverting to hard process

Conditional INN

- partonic events from $\{r\}$, given detector event
- loss based on likelihood, Bayes' theorem, Jacobian

$$L = -\left\langle \log p(\theta|x_p, x_d) \right\rangle_{x_p, x_d}$$

$$= -\left\langle \log p(g(x_p, x_d)) + \log \left| \frac{\partial g(x_p, x_d)}{\partial x_p} \right| \right\rangle_{x_p, x_d} - \log p(\theta) + \text{const.}$$

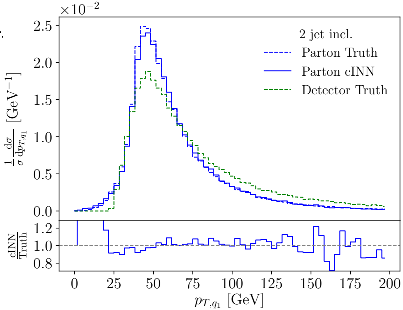
- eventually to be combined with reweighting

→ Stable and statistically calibrated

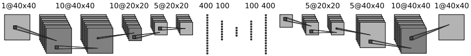
Undo QCD jet radiation in $pp \to ZW$+jets

- nasty jet combinatorics, missing higher-
- hard process given and relevant
- jet radiation universal QCD
- ME vs PS jets from network

→ Report measurement where it matters



Learning background only

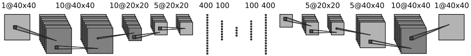


Unsupervised classification

- 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

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

Learning background only



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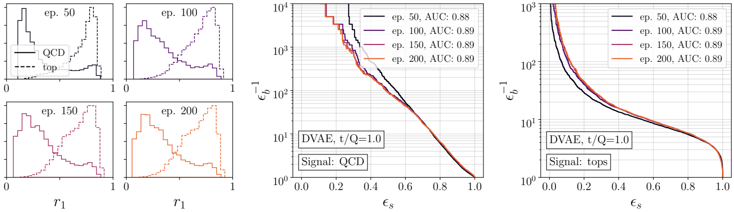
Moving to latent space

- anomaly score from latent space?
- VAE $\to$ does not work
  GMVAE $\to$ does not work
  Dirichlet VAE $\to$ works okay
  density estimation $\to$ does not work



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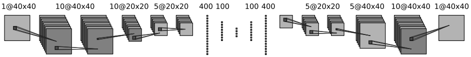

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Normalized autoencoder [penalize missing features]

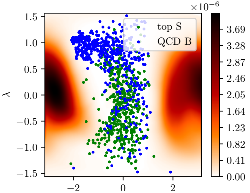
- normalized probability loss
- Boltzmann mapping [E_θ =MSE]

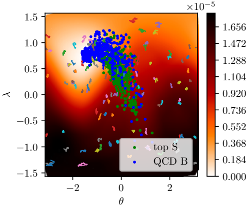
$$p_\theta(x) = \frac{e^{-E_\theta(x)}}{Z_\theta}$$

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

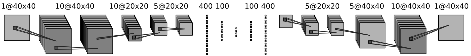
- inducing background metric
- small MSE for data, large MSE for model
- Z_θ from (Langevin) Markov Chain

$\rightarrow$ Symmetric autoencoder, at last





Learning background only



Unsupervised classification

- train on background only
  extract unknown signal from reconstruction error
- reconstruct QCD jets $\rightarrow$ top jets hard to describe
- reconstruct top jets $\rightarrow$ QCD jets just simple top-like jet

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

Normalized autoencoder [penalize missing features]

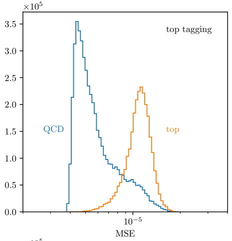
- normalized probability loss
- Boltzmann mapping [E_θ =MSE]

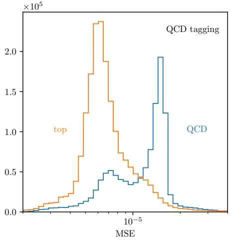
$$p_\theta(x) = \frac{e^{-E_\theta(x)}}{Z_\theta}$$

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

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

$\rightarrow$ Symmetric autoencoder, at last





Optimal observables

Measure model parameter θ optimally

- single-event likelihood

$$p(x|\theta) = \frac{1}{\sigma_{\text{tot}}(\theta)} \frac{d^m\sigma(x|\theta)}{dx^m}$$

- expanded in θ around θ_0, define score

$$\log \frac{p(x|\theta)}{p(x|\theta_0)} \approx (\theta - \theta_0)\, \nabla_\theta \log p(x|\theta)\Big|_{\theta_0} \equiv (\theta - \theta_0)\, t(x|\theta_0) \equiv (\theta - \theta_0)\, \mathscr{O}^{\text{opt}}(x)$$

- leading order parton level

$$p(x|\theta) \approx |\mathcal{M}|_0^2 + \theta |\mathcal{M}|_{\text{int}}^2 \qquad \Rightarrow \qquad t(x|\theta_0) \sim \frac{|\mathcal{M}|_{\text{int}}^2}{|\mathcal{M}|_0^2}$$

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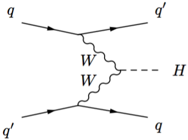
CP-violating Higgs production



- unique CP-observable

$$t \propto \epsilon_{\mu\nu\rho\sigma}\, k_1^\mu\, k_2^\nu\, q_1^\rho\, q_2^\sigma\, \text{sign}\left[(k_1 - k_2)\cdot(q_1 - q_2)\right] \xrightarrow{\text{lab frame}} \sin\Delta\phi_{jj}$$

- CP-effect in $\Delta\phi_{jj}$
  D6-effect in $p_{T,j}$

$\Rightarrow$ Key LHC observable

PySR

Analytic formula for score

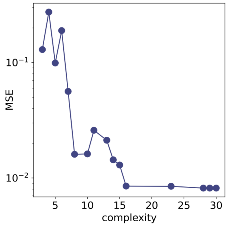
- function to approximate $t(x|\theta)$
- phase space parameters $x_p = p_T/m_H, \Delta\eta, \Delta\phi$ [node]
- operators $\sin x, x^2, x^3, x+y, x-y, x*y, x/y$ [node]
- represent formula as tree [complexity = number of nodes]

⇒ Figures of merit

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\Big[g_i(x) - t(x,z|\theta)\Big]^2 \to \text{MSE} + \text{parsimony}\cdot\text{complexity}$$

Score around Standard Model

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	$(x_{p,2}+a)(bx_{p,1}(c-\Delta\phi)$ $-x_{p,1}(d\Delta\eta + ex_{p,2} + f)\sin(\Delta\phi + g))$	$8.18\cdot 10^{-3}$



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$\Rightarrow$ Figures of merit

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\Big[g_i(x) - t(x,z|\theta)\Big]^2 \to \text{MSE} + \text{parsimony} \cdot \text{complexity}$$

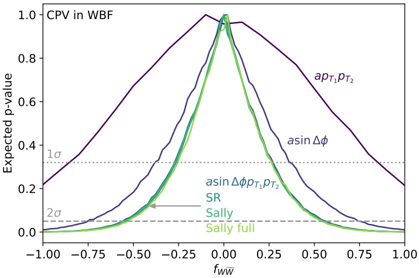
Score around Standard Model

- expected limits:

  very wrong formula
  wrong formula
  right formula
  MadMiner

- same within statistical limitation

$\Rightarrow$ New optimal observables next



ML for LHC Theory

ML-applications in LHC physics

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

  ...improve established tasks
  ...develop new tools for established tasks
  ...transform through new ideas
- link to growing Heidelberg lecture notes

→ Turn HL-LHC into fun!

Machine Learning and LHC Event Generation

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Abstract

First-principle simulations are at the heart of the high-energy physics research program. They link the vast data output of multi-purpose detectors with fundamental theory predictions and interpretation. This review illustrates a wide range of applications of modern machine learning to event generation and simulation-based inference, including conceptional developments driven by the specific requirements of particle physics. New ideas and tools developed at the interface of particle physics and machine learning will improve the speed and precision of forward simulations, handle the complexity of collision data, and enhance inference as an inverse simulation problem.

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