

Generative Networks in Particle Physics

Tilman Plehn

Universität Heidelberg

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Particle physics goals

Particle physics defined by

- fundamental questions
- lot of data
- first-principles predictions
- precision analysis

Fundamental questions

- particle nature of dark matter?
- origin of the Higgs mechanism?
- matter-antimatter asymmetry?
- Standard Model all there is?

LHC

Some ML...

GAN

GANplification

Statistical gains

VAE

Calomplification

INN

Uncertainties

Inverting



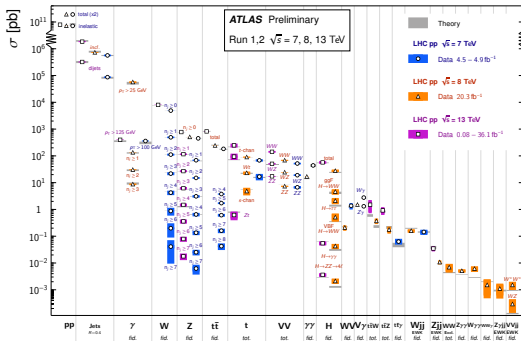
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Rate measurements

- many processes
- vastly different rates
- high precision
- predicted by theory



Particle physics goals

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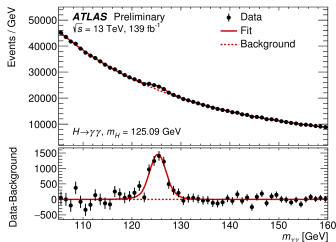
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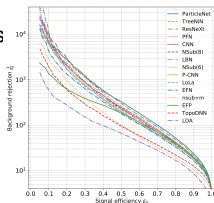
Rates not interesting

- new physics rare and heavy
 - phase space vast
- ⇒ bumps, tails, kinematics instead



Top tagging [supervised classification]

- different NN-architectures
 - tagger comparison
- ⇒ Just do it right...



SciPost Physics

Submissions

The Machine Learning Landscape of Top Taggers

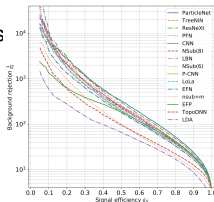
G. Kasieczka (a), T. Plehn (a,b), A. Bhattarai, K. Chatterjee, D. DeLoraine, R. M. Dörmal, M. Hübner, D. A. Paganoni, M. Paganoni, C. Pap, L. Gornow, J. F. Kaniak, P. T. Komiske, S. Linn, A. List, S. Mariani, E. M. Metodiev, L. Moore, B. Nachman, K. Nourbakhsh, J. Papan, H. Qu, V. Rath, M. Reher, D. Shaw, J. M. Thompson, and S. Varma

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- 2 Institut für Theoretische Physik, Universität Bonn/Bonn, Germany
- 3 Center for Cosmology and Particle Physics and Center for Data Science, NYU, USA
- 4 NHEEC, Dept. of Physics and Astronomy, Belgium, The State University of NJ, USA
5 Juelj Station Institute, Ljiljana, Slovenia
- 6 Theoretical Particle Physics and Cosmology, King's College London, United Kingdom
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- 8 Department of Physics, University of California, Santa Barbara, USA
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- 10 Center for Theoretical Physics, MIT, Cambridge, USA
- 11 CPUL, Universit t Catholique de Louvain, Louvain-la-Neuve, Belgium
- 12 Physics Division, Lawrence Berkeley National Laboratory, Berkeley, USA
- 13 Simons Inst. for the Theory of Computing, University of California, Berkeley, USA
- 14 National Institute for Subatomic Physics (NIKHEF), Amsterdam, Netherlands
- 15 LPJHE, CNRS & Sorbonne Universit , Paris, France
- 16 III. Physikalisches A, RWTH Aachen University, Germany



Top tagging [supervised classification]

- different NN-architectures
 - tagger comparison
- ⇒ Just do it right...



SciPost Physics

Submissions

The Machine Learning Landscape of Top Taggers

G. Kaselka^{1(a)}, T. Plehn^{1(a)}, A. Bharath², K. Chatterjee³, D. DeLaney⁴, B. M. Dolan⁵, M. Hartzman⁶, D. A. Pongracz⁷, M. Soderstrom⁸, C. Vogt⁹, L. Gonzalez¹⁰, J. F. Kaniwal¹¹, P. T. Komarath¹², S. Linn¹³, A. Lister¹⁴, S. Mariani¹⁵, E. M. Metodiev¹⁶, L. Moore¹⁷, B. Nossaman^{18(a)}, K. Nourbakhsh^{19(a)}, J. Penning²⁰, H. Qu²¹, Y. Bai²², M. Regier²³, D. Shih²⁴, J. M. Thompson²⁵, and S. Varma²⁶

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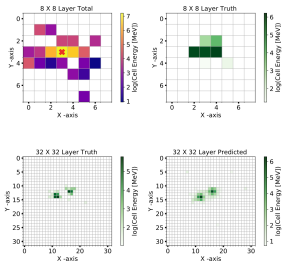
14 National Institute for Subatomic Physics (NIKHEF), Amsterdam, Netherlands

15 LPFIB, CNRS & Sorbonne Université, Paris, France

16 III-Physikalisches Institut, RWTH Aachen University, Germany

Particle flow [classification, super-resolution]

- mother of jet tools
 - combined detector channels
- ⇒ Seriously impressive



Towards a Computer Vision Particle Flow *

Francesco Aramo Di Belle^{1(a)}, Samay Ganguly^{1(a)}, Eliam Gross², Marumi Kado^{3(a)}, Michael Pitt⁴, Lorenzo Santoni⁵, Jonathan Shlomi⁶

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²CBRN, CERN, Geneva 23, Switzerland

³Università di Roma Sapienza, Piazza Aldo Moro, 2, 00185 Roma, Italy & INFN, Italy

⁴Université Paris-Saclay, CNRS/IN2P3, UCLab, 91195, Orsay, France

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 $g \rightarrow \gamma\gamma$ is resolved by a 32×32 granularity layer.



Jets, QCD, symmetries

Lund plane representation [input preprocessing]

- QCD-inspired input with cutting-edge networks
- angular separation vs transverse momentum

⇒ Understanding data helps

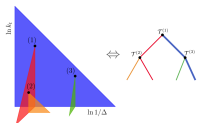
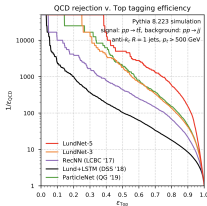


Figure 1. The Lund plane representation of a jet (left) where each cascade is positioned according to its k_T and k_\perp coordinates, and the corresponding mapping in a binary Lund tree of triplets (right). The thick blue line represents the primary sequence of triplets C_{\min} .



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06/17/2017

Jet tagging in the Lund plane with graph networks

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^bCERN, EP Department, CH-1211 Geneva 23, Switzerland

ABSTRACT: The identification of boosted heavy particles such as top quarks or vector bosons is one of the key problems arising in experimental studies at the Large Hadron Collider. In this article, we introduce LundNet, a novel jet tagging method which relies on graph neural networks and an efficient description of the radiation patterns within a jet to optimally disentangle signatures of boosted objects from background events. We apply this framework to a number of different benchmarks, showing significantly improved performance for top tagging compared to existing state-of-the-art algorithms. We study the robustness of the LundNet taggers to non-perturbative and detector effects, and show how kinematic cuts in the Lund plane can mitigate overfitting of the neural network to model-dependent distributions. Finally, we consider the computational complexity of this method and its scaling as a function of kinematic Lund plane cuts, showing an order of magnitude improvement in speed over previous graph-based taggers.



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- QCD-inspired input with cutting-edge networks
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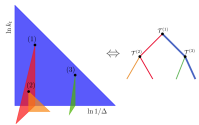
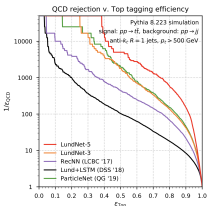


Figure 1. The Lund plane representation of a jet (left) where each vertex is positioned according to its Δ and $1/\Delta$ coordinates, and the corresponding mapping to a binary Lund tree of triplets (right). The thick blue line represents the primary sequence of triplets $\mathcal{L}_{\text{primary}}$.



PREPARED FOR SUBMISSION TO JHEP

03/77-36-1P

Jet tagging in the Lund plane with graph networks

Frédéric A. Dreyer,^a Heiko Qu^b

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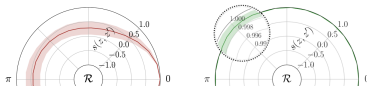
^bCERN, EP Department, CH-1211 Geneva 23, Switzerland

ABSTRACT: The identification of boosted heavy particles such as top quarks or vector bosons is one of the top priorities arising in experimental studies at the Large Hadron Collider. In this article, we introduce LundNet, a novel jet tagging method which relies on graph neural networks and an efficient description of the radiation patterns within a jet to optimally disentangle signatures of boosted objects from background events. We apply this framework to a number of different benchmarks, showing significantly improved performance for top tagging compared to existing state-of-the-art algorithms. We study the robustness of the LundNet taggers to non-perfective and detector effects, and show how kinematic cuts in the Lund plane can mitigate overfitting of the neural network to model-dependent contributions. Finally, we consider the computational complexity of this method and its scaling as a function of kinematic Lund plane cuts, showing an order of magnitude improvement in speed over previous graph-based taggers.

Self-supervised training [contrastive learning, transformer network]

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

⇒ Symmetry-aware latent space



Full Paper Physics

Introduction

Symmetries, Safety, and Self-Supervision

Henry M. Dörmal¹, Gregor Kasieczka², Hans Okawa³, Tilman Plehn¹, Peter Sommerer², and Lorenz Vogl²

¹ Institut für Theoretische Physik, Universität Heidelberg, Germany
² Institut für Experimentelle Physik, Universität Hamburg, Germany
³ Heidelberg Collaborator for Particle Physics, 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 non-polyakov agnostic. We introduce JetCLR to solve the mapping from low-level data to optimized observables through 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.



Anomaly searches [unsupervised training]

- look for non-QCD jets, non-SM events
- idea of BSM searches, trigger

⇒ Latent density?

Better Latent Spaces for Better Anomalous

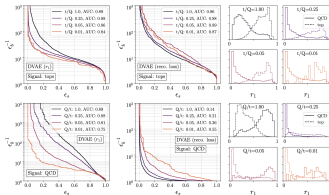
Henry M. Wickham¹, Tilman Plehn¹, Christof Haack², and Peter Schwenn³,

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² Physikalisches Institut, Universität Heidelberg, Germany
³ Heidelberg Collaboratory for Large Accelerator, Universität Heidelberg, Germany

April 26, 2020

Abstract

Anomalous events behind anomaly searches at the LHC face the structural problem that they only work in one direction, returning jets with higher complexity but not the other way around. To address this, we derive classifiers from the latent space of (restricted) 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.



Non-QCD and parton densities

Anomaly searches [unsupervised training]

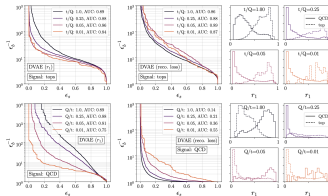
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⇒ Latent density?



Abstract

Autoencoders on tasks behind anomaly searches at the LHC face the structural problem that they only work in one direction, reconstructing 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 mixtures and Dirichlet latent spaces. In particular, the Dirichlet setup solves the problem and improves both the performance and the interpretability of the autoencoders.



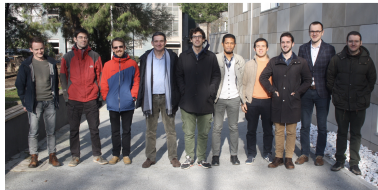
NNPDF/N3PDF parton densities [full blast]

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

⇒ Leaders in ML-theory

N3PDF
Neural Network Parton Distribution Functions

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A data-based parametrization of parton distribution functions

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² DESY, Theoretical Physics Department, DESY 111 (Theorie 2), DESY-Hamburg.
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 describe structure functions or parton distribution functions (PDFs) have employed a common paradigm as part of the parametrization. The NNPDF collaboration pioneered the use of neural networks to overcome the inherent bias of constraining the space of solutions with a fixed functional form while still keeping the same common practice as a preprocessing. Over the years various, increasingly sophisticated, techniques have been introduced to control the effect of the network on the PDF determination. In this paper we present a methodology to remove the particular arbitrariness, identify significantly simplifying the workability, without a loss of efficiency and facing good agreement with previous results.

PACS. 23.20.+g Quantum chromodynamics – 1.23.0+ Phenomenological models – 85.35.+t Neural Networks

- LHC
- Some ML...
- GAN
- GANplification
- Statistical gains
- VAE
- Calomplification
- INN
- Uncertainties
- Inverting



Events and amplitudes

Speeding up event generation [sampling]

- precision simulations limiting factor for Runs 3&4
 - unweighting critical
- ⇒ Phase space sampling

	gg → tt̄gg	gg → tt̄ggg	gg → tt̄gggg	gg → tt̄ggggg
σ_{tot}	$1.1e-2$	$7.3e-3$	$6.8e-3$	$6.6e-4$
$\sigma_{\text{tot,MC}}$	$8.7e-3$	$5.8e-3$	$4.7e-3$	$3.5e-4$
$(\sigma_{\text{tot}})/(\sigma_{\text{tot,MC}})$	20312	2417	199	64
$\sigma_{\text{tot}}^{\text{MC}}$	52.03	32.52	49.78	306.19
$\sigma_{\text{tot}}^{\text{MC,unw}}$	$5.4e-2$	$3.5e-2$	$2.1e-2$	$5.6e-2$
$\sigma_{\text{tot}}^{\text{MC,unw}}$	0.5669	0.9994	0.9994	0.9991
$\sigma_{\text{tot}}^{\text{MC,unw}}$	2.21	4.89	1.47	0.19
$\sigma_{\text{tot}}^{\text{MC,unw}}$	30.40	19.14	27.78	35.24
$\sigma_{\text{tot}}^{\text{MC,unw}}$	$4.3e-2$	$6.4e-2$	$3.1e-2$	$7.1e-2$
$\sigma_{\text{tot}}^{\text{MC,unw}}$	0.5663	0.9960	0.9950	0.9921
$\sigma_{\text{tot}}^{\text{MC,unw}}$	3.50	8.26	3.31	2.22

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

SciPost, Plehn

Subramanian

MCNET-21-11

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

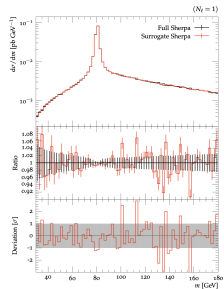
K. Danziger¹, T. Jochim², S. Kuhnke², F. Sjöberg¹

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 unweighted 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 unweighted events from weighted samples can become a limiting factor in practical applications. Here we present a novel two-stage 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 $2\text{W}+4$ jets and $0+3$ jets, where we find speed-up factors up to ten.



Events and amplitudes

Speeding up event generation [sampling]

- precision simulations limiting factor for Runs 3&4
- unweighting critical
- ⇒ Phase space sampling

	gg → Higgs	gg → ZHiggs	gg → ZHiggs	gg → HiggsZ
ϵ_{cut}	1.1e-2	7.3e-3	6.8e-3	6.6e-4
$\epsilon_{\text{stat,stat}}$	8.7e-3	5.8e-3	4.7e-3	3.9e-4
$\langle \text{ratio} \rangle / \langle \text{ratio} \rangle$	20012	2017	199	60
$\epsilon_{\text{stat}}^{\text{full}}$	52.03	32.32	69.76	226.19
$\epsilon_{\text{stat}}^{\text{surrogate}}$	2.4e-2	3.8e-2	2.1e-2	5.6e-3
$\epsilon_{\text{stat}}^{\text{full}} / \epsilon_{\text{stat}}^{\text{surrogate}}$	0.9889	0.9984	0.9994	0.9981
$\epsilon_{\text{stat}}^{\text{full}} / \epsilon_{\text{stat}}^{\text{surrogate}}$	2.21	4.89	1.47	0.19
$\epsilon_{\text{stat}}^{\text{full}} / \epsilon_{\text{stat}}^{\text{surrogate}}$	30.40	19.11	37.78	25.24
$\epsilon_{\text{stat}}^{\text{full}} / \epsilon_{\text{stat}}^{\text{surrogate}}$	4.3e-2	6.4e-2	3.1e-2	2.1e-2
$\epsilon_{\text{stat}}^{\text{full}} / \epsilon_{\text{stat}}^{\text{surrogate}}$	0.9983	0.9986	0.9983	0.9921
$\epsilon_{\text{stat}}^{\text{full}} / \epsilon_{\text{stat}}^{\text{surrogate}}$	3.50	8.26	3.91	2.22

Table 4: Performance measures for partonic channels contributing to tt - 3 jets production at the LHC.

SciPost Physics

MCNET-21-33

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

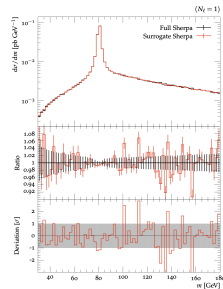
K. Danziger¹, T. Jaden¹, S. Schumann², F. Singer¹

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

September 27, 2021

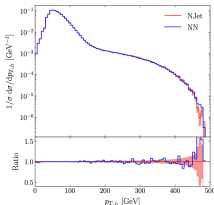
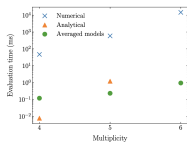
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The generation of multi-weight events for complex scattering processes presents a severe challenge to modern Monte Carlo event generators. Even when using sophisticated phase-space sampling techniques adapted to the underlying transition matrix elements, the efficiency for generating multi-weight events from weighted samples can become a limiting factor in practical applications. Here we present a novel two-stage 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 $2^m W + 4$ jets and $n+3$ jets, where we find speed-up factors up to ten.



Speeding up amplitudes [regression]

- loop-amplitudes expensive
- interpolation standard
- ⇒ Network amplitudes



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07PP/20/110

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 multi-resolution method that can be applied to hadron collider observables. Neural networks are trained using the one-loop amplitudes implemented in the Rivet \mathcal{O} -library, and interfaced to the Sherpa Monte Carlo event generator, where we perform a detailed study for $2+3$ and $2+4$ scattering processes. We also consider how the trained networks perform when varying the kinematic cuts affecting the phase space and the reliability of the neural network simulations.



String landscape and learned formulas

Navigating string landscape [reinforcement learning]

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

⇒ Model space sampling

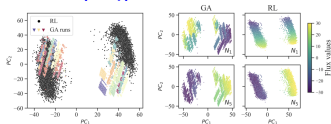


Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_1 and N_2 respectively) in relation to principal components for a PCA fit of the individual 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 unacknowledged 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.



String landscape and learned formulas

Navigating string landscape [reinforcement learning]

- searching for viable vacua
 - high dimensions, unknown global structure
- ⇒ **Model space sampling**

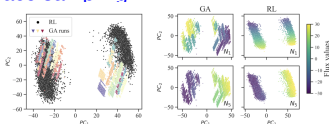


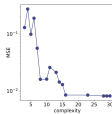
Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_3 and N_5 respectively) in relation to principal components for a PCA fit of the individual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

Learning formulas [genetic algorithm, symbolic regression]

- approximate numerical function through formula
 - example: score/optimal observables
- ⇒ **Useful approximate formulas**

compil	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	$a \Delta \phi \exp_1$	$9.50 \cdot 10^{-2}$
6	1	$-x_{p,1} \sin(\Delta \phi + a)$	$1.90 \cdot 10^{-1}$
7	1	$(-x_{p,1} - a) \sin(\sin(\Delta \phi))$	$5.63 \cdot 10^{-3}$
8	1	$(a - 2x_{p,1}) \exp_2 \sin(\Delta \phi)$	$1.61 \cdot 10^{-3}$
14	2	$x_{p,1}(a \Delta \phi - \sin(\sin(\Delta \phi)))(x_{p,2} + b)$	$1.44 \cdot 10^{-2}$
15	3	$(-f_{p,2}(a \Delta \phi^2 + x_{p,1} + b) \sin(\Delta \phi + c))$	$1.30 \cdot 10^{-2}$
16	4	$(x_{p,2} + a)(\exp_1(x_{p,2} + c) \sin(\Delta \phi + d) - x_{p,2} + b)$	$8.50 \cdot 10^{-3}$
28	7	$(x_{p,2} + a)(\exp_1(x_{p,2} + c) \sin(\Delta \phi + d) - x_{p,2} + b)(\exp_2 + f) \sin(\Delta \phi + g)$	$8.18 \cdot 10^{-3}$

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



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

Alex Cole
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Seon Krippendorfer
Arnold Sommerfeld Center for Theoretical Physics
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Center for Mathematical Sciences
University of Cambridge
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University of Wisconsin-Madison
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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 unacknowledged 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.

ECPHUS Physics

Schedulin

Back to the Formulas — LHC Edition

Anja Butter¹, Tilman Plehn¹, Nathalie Seydoux¹, and Johann Boehmer²

¹ Institut für Theoretische Physik, Universität Heidelberg, Germany
² Center for Data Science, New York University, New York, United States
nathalie@hep.wisc.edu

November 16, 2021

Abstract

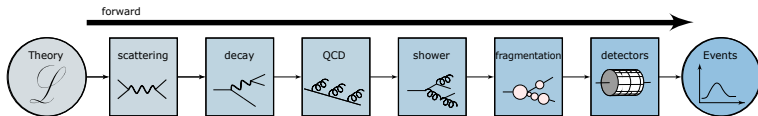
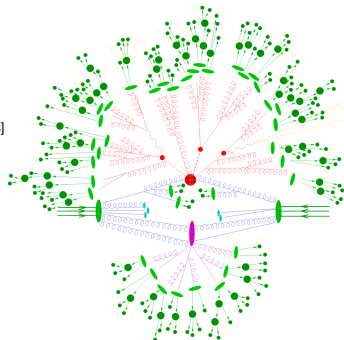
While neural networks offer an attractive way to numerically encode functions, actual formulas remain the language of theoretical particle physics. We use symbolic regression trained on matrix-element information to extract, for instance, optimal LHC observables. This way we invert the usual simulation paradigm and extract easily interpretable formulas from complex simulated data. We introduce the method using the effect of a dimension-4 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.



LHC simulations

Simulation-based inference

- start with Lagrangian
 - calculate scattering in perturbative QFT
 - simulate events [theory: Sherpa, Madgraph, Pythia]
 - simulate detectors [experiment: ATLAS, CMS, Delphes]
- ⇒ LHC events in virtual worlds



LHC simulations

LHC

Some ML...

GAN

GANplification

Statistical gains

VAE

Calomplification

INN

Uncertainties

Inverting

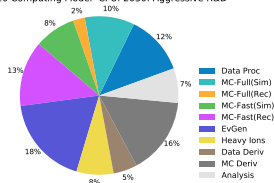
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HL-LHC: preparing for 25-fold data set

- simulated event numbers \sim expected events
- statistics requiring 1%-2% uncertainty
- flexible signal hypotheses [time-dependent]
- low-rate high-multiplicity backgrounds

ATLAS Preliminary
2020 Computing Model -CPU: 2030: Aggressive R&D



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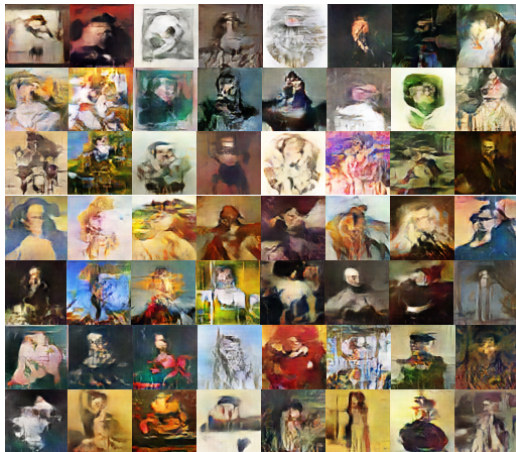
Three ways to use ML

- improve current tools
- new ML-tools
- conceptually new ideas



GANGogh [Bonafilia, Jones, Danyluk (2017)]

- can networks create **new pieces of art?**
map random numbers to image pixels
- train on 80,000 pictures [organized by style and genre]
- generate portraits



Generative neural networks

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Edmond de Belamy [Caselles-Dupre, Fautrel, Vernier (2018)]

- trained on 15,000 portraits
 - sold for \$432.500
- ⇒ **ML all marketing and sales**



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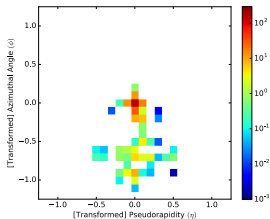
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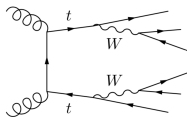
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Jet portraits [de Oliveira, Paganini, Nachman (2017)]

- calorimeter or jet images
 - reproduce valid jet images from training data
 - organize them by QCD vs W -decay jets
- ⇒ **Generative networks useful for particle physics**

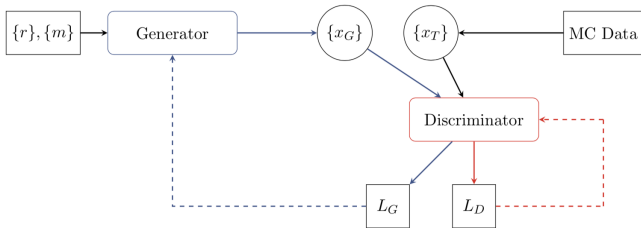


How to GAN



Adversarial training

- training: true events $\{x_T\}$
output: generated events $\{r\} \rightarrow \{x_G\}$
 - **discriminator** classifier function $D(x)$ from minimizing $[D(x) = 1(T), 0(G)]$
$$L_D = \langle -\log D(x) \rangle_{x_T} + \langle -\log(1 - D(x)) \rangle_{x_G}$$
 - **generator** mapping $r \rightarrow x_G$ by minimizing $[D \text{ needed}]$
$$L_G = \langle -\log D(x) \rangle_{x_G}$$
 - Nash equilibrium $D = 0.5$
- ⇒ statistically independent copy of training events



How to GAN

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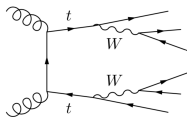
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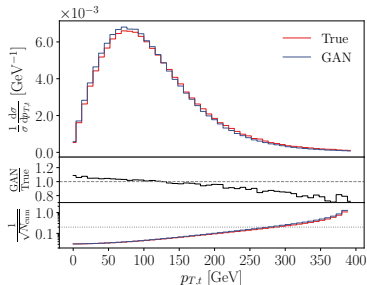
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- Nash equilibrium $D = 0.5$
- ⇒ statistically independent copy of training events



GAN LHC events

- typical process $t\bar{t} \rightarrow 6$ quarks [18D final state]
 - observables with tails
- ⇒ two big LHC questions:
- How **precisely** can we GAN?
- What is their **uncertainty**?



Chemistry of loss functions

Pointing GANs to specific features

- low-dimensional sharp features

phase space boundaries

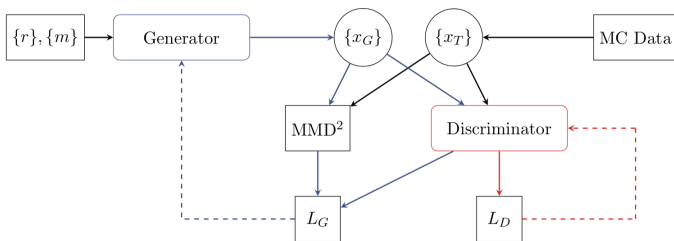
kinematic cuts

invariant masses

- batch-wise comparison of distributions, MMD loss with kernel k

$$\text{MMD}^2(P_T, P_G) = \langle k(x, x') \rangle_{x_T, x'_T} + \langle k(y, y') \rangle_{y_G, y'_G} - 2\langle k(x, y) \rangle_{x_T, y_G}$$

$$L_G \rightarrow L_G + \lambda_G \text{MMD}^2$$



Pointing GANs to specific features

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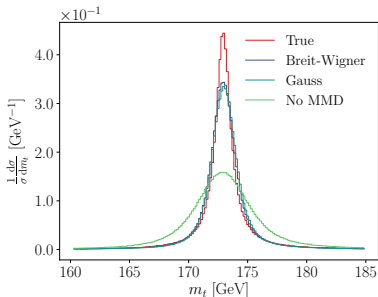
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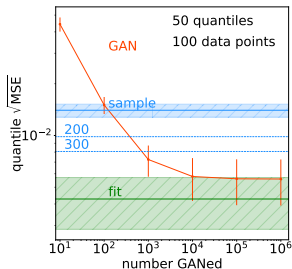
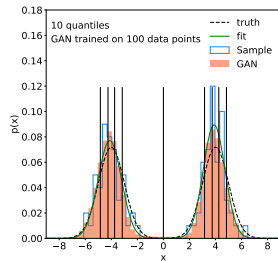
⇒ It works...



GANplification

Gain beyond training data

- true function known
compare **sampling** vs **GAN** vs **fit**
 - quantiles with χ^2 -values
 - start with 100 sampled points
fit like 700 sampled points
GAN like 500 sampled points ...
... but requiring 10,000 GANned events
 - interpolation and resolution key [implicit bias]
- ⇒ **Generative networks beyond training data**



Statistical bonus: unweighting

Gaining beyond GANplification

- phase space sampling: PS weight $\times |\mathcal{M}|^2$
density information in weights [for uniform grid]
 - experiment: observed configurations
density information in density
- ⇒ information in mix of density and weights

LHC

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- ⇒ information in mix of density and weights
- weak spot: hit-and-miss unweighting
relative event weights $w_j/w_{\max} \in [0, 1]$
random number $r \in [0, 1] < w_j/w_{\max}$ means keep event

LHC

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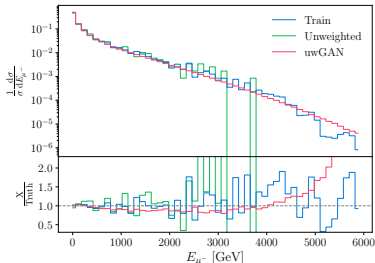
Gaining beyond GANplification

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- weak spot: hit-and-miss unweighting
relative event weights $w_j/w_{\max} \in [0, 1]$
random number $r \in [0, 1] < w_j/w_{\max}$ means keep event
 - learn from weighted, generate unweighted events

$$L_D = \frac{\langle -w(x) \log D(x) \rangle_{x_T}}{\langle w(x) \rangle_{x_T}} + \langle -\log(1 - D(x)) \rangle_{x_G}$$

$$L_G = \langle -\log D(x) \rangle_{x_G}$$

⇒ GANs can unweight



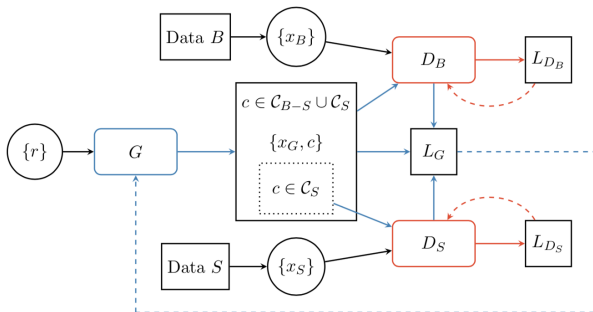
Statistical bonus: subtraction

Subtract samples without binning

- statistical uncertainty

$$\Delta_{B-S} = \sqrt{\Delta_B^2 + \Delta_S^2} > \max(\Delta_B, \Delta_S)$$

- GAN setup: differential class label, sample normalization



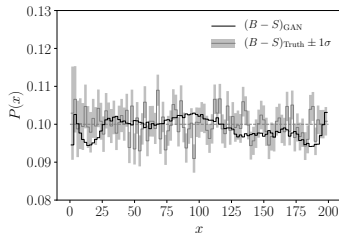
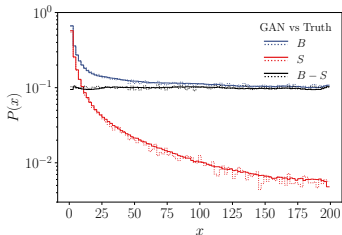
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- toy example

$$P_B(x) = \frac{1}{x} + 0.1 \quad P_S(x) = \frac{1}{x} \quad \Rightarrow \quad P_{B-S} = 0.1$$



Subtract samples without binning

- statistical uncertainty

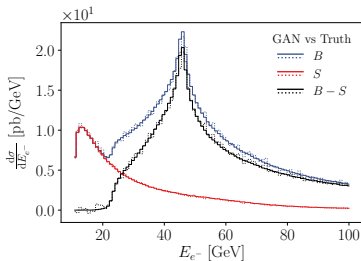
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- event-based background subtraction [weird notation, sorry]

$$pp \rightarrow e^+ e^- \quad (B) \quad pp \rightarrow \gamma \rightarrow e^+ e^- \quad (S) \quad \Rightarrow \quad pp \rightarrow Z \rightarrow e^+ e^- \quad (B-S)$$



Subtract samples without binning

- statistical uncertainty

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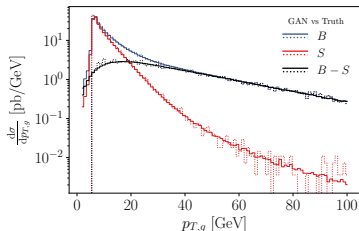
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- collinear subtraction [assumed non-local]

$$pp \rightarrow Zg \quad (B: \text{matrix element}, S: \text{collinear approximation})$$

\Rightarrow GANs can subtract samples



Alternative generative architecture

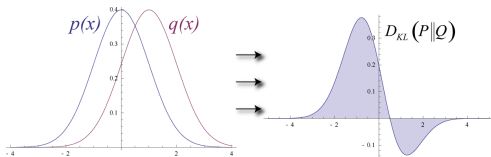
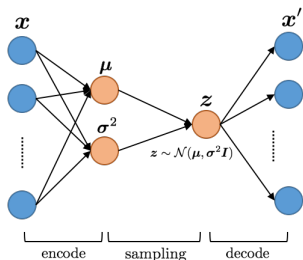
- reconstruction loss [like autoencoder]

$$L_{VAE} = \sum |x - x'|^2 + \beta D_{KL}$$

- Gaussian latent space via KL-divergence

$$D_{KL}(p; q) = \int dx p(x) \log \frac{p(x)}{q(x)}$$

$$D_{KL}(\mathcal{N}_{\mu, \sigma}; \mathcal{N}_{0, 1}) = \frac{1 + \log \sigma^2 - \mu^2 - \sigma^2}{2}$$



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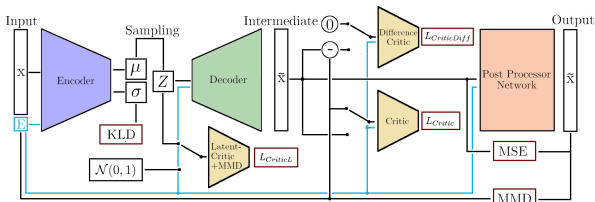
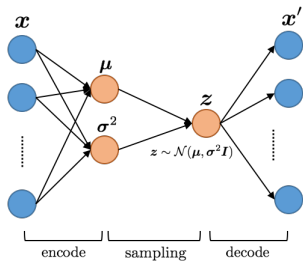
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- VAE-GAN replacing reconstruction loss

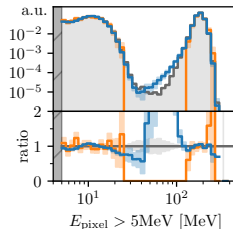
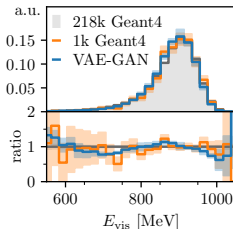
$$L_{\text{VAE-GAN}} = L_{\text{GAN}} + \beta D_{\text{KL}}$$

- application to detector simulations [ask Gregor]



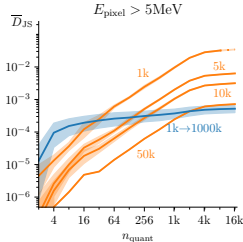
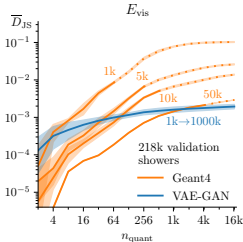
Gain for fast detector simulation

- photon shower in 3D-calorimeter
energy deposition in 30^3 cells
1k showers for training, 218k showers as truth
downsized VAE-GAN architecture
- ⇒ how many generated events make sense?



Gain for fast detector simulation

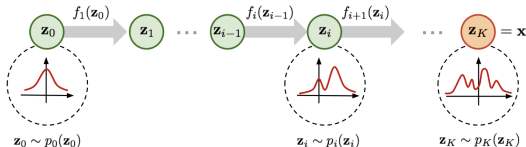
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- 1k showers for training, 218k showers as truth
downsized VAE-GAN architecture
- ⇒ how many generated events make sense?
- benchmarking as function of quantiles [bin resolution]
comparison using $D_{JS}(p; q) = D_{KL}(p; q) + D_{KL}(q; p)$
- ⇒ **Generative networks really amplify data sets**



Looking for stable networks

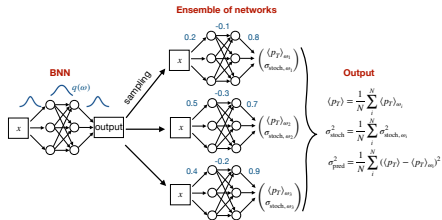
- mapping physics space \longleftrightarrow latent space
- INN: bijective mapping
symmetric training and evaluation
Gaussian latent space
- structural element: coupling block [affine, spline]
- log-likelihood loss [moved into Gaussian latent space]

$$\begin{aligned}
 L_{\text{INN}} &= - \left\langle \log \frac{P_G(x)}{P_T(x)} \right\rangle_{x_T} \\
 &= - \left\langle \frac{\psi(x)^2}{2} - \log J(x) - \log P_T(x) \right\rangle_{x_T}
 \end{aligned}$$



Bayesian generative network

- data: event sample [points in 2D space]
- learn phase space density
- Gaussian in latent space
- mapping bijective
- sample from latent space
- Bayesian version
- allow weight distributions
- learn uncertainty map



Generative networks with error bars

Bayesian generative network

- data: event sample [points in 2D space]

learn phase space density

Gaussian in latent space

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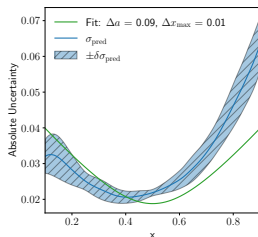
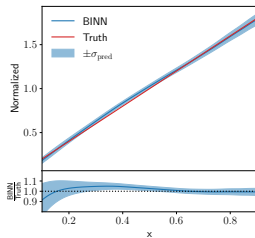
learn uncertainty map

- 2D wedge ramp

$$p(x) = ax + b = ax + \frac{1 - \frac{a}{2}(x_{\max}^2 - x_{\min}^2)}{x_{\max} - x_{\min}}$$

$$(\Delta p)^2 = \left(x - \frac{1}{2}\right)^2 (\Delta a)^2 + \left(1 + \frac{a}{2}\right)^2 (\Delta x_{\max})^2 + \left(1 - \frac{a}{2}\right)^2 (\Delta x_{\min})^2$$

explaining minimum in $\sigma_{\text{pred}}(x)$



Generative networks with error bars

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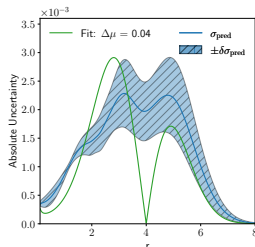
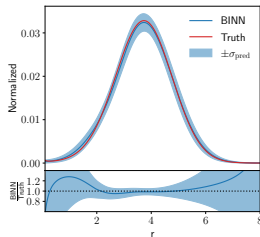
learn uncertainty map

- Gaussian ring [$\mu = 4, w = 1$]

$$\Delta p = \left| \frac{G(r)}{r} \frac{\mu - r}{w^2} \right|^2 (\Delta\mu)^2 + \left| \frac{(r - \mu)^2}{w^3} - \frac{1}{w} \right|^2 (\Delta w)^2$$

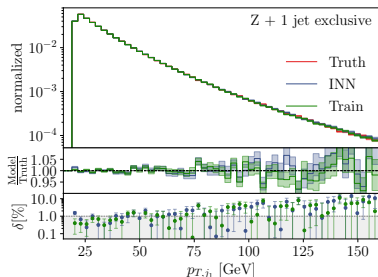
explaining dip in $\sigma_{\text{pred}}(x)$

⇒ Generative networks just (non-parametric) fits



Challenging an INN-generator

- $Z_{\mu\mu} + \{1, 2, 3\}$ jets [Z-peak, variable jet number, jet-jet topology]
- training on 5.4M Z+jets events
truth defined as high-stats training data
goal: 1% precision relative to truth



Challenging an INN-generator

- $Z_{\mu\mu} + \{1, 2, 3\}$ jets [Z-peak, variable jet number, jet-jet topology]
- training on 5.4M Z+jets events
truth defined as high-stats training data
goal: 1% precision relative to truth
- holes in geometric distance ΔR_{jj} [QFT problem :)]
- magic transformation
monotonous function with weights [opposite of importance sampling]

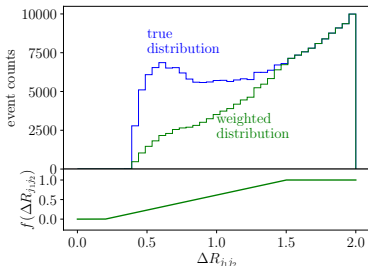
$$w^{(1\text{-jet})} = 1$$

$$w^{(2\text{-jet})} = f(\Delta R_{j_1, j_2})$$

$$w^{(3\text{-jet})} = f(\Delta R_{j_1, j_2})f(\Delta R_{j_2, j_3})f(\Delta R_{j_1, j_3})$$

with

$$f(\Delta R) = \begin{cases} 0 & \text{for } \Delta R < R_- \\ \frac{\Delta R - R_-}{R_+ - R_-} & \text{for } \Delta R \in [R_-, R_+] \\ 1 & \text{for } \Delta R > R_+ \end{cases}$$



Challenging an INN-generator

- $Z_{\mu\mu} + \{1, 2, 3\}$ jets [Z-peak, variable jet number, jet-jet topology]
- training on 5.4M Z +jets events
truth defined as high-stats training data
goal: 1% precision relative to truth
- holes in geometric distance ΔR_{ij} [QFT problem :)]
- magic transformation
monotuous function with weights [opposite of importance sampling]

$$w^{(1\text{-jet})} = 1$$

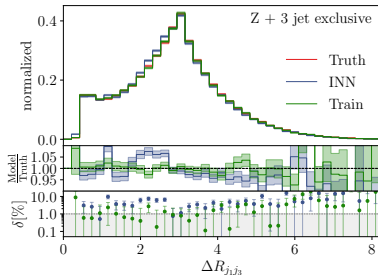
$$w^{(2\text{-jet})} = f(\Delta R_{j_1, j_2})$$

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⇒ Per-cent precision possible

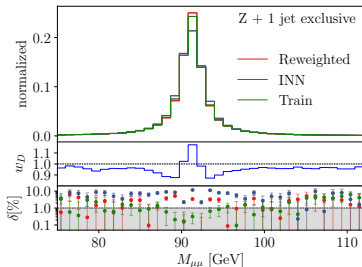


Additional discriminator: training vs generated

- input $\{p_T, \eta, \phi, M, M_{\mu\mu}, \Delta R\}$
- output $D = 0(G), 1(T) \rightarrow 0.5$
- decent generator training $D \approx 0.5$
- additional event weight

$$w_D(x) = \frac{D(x)}{1 - D(x)}$$

⇒ 1. control and 2. reweight



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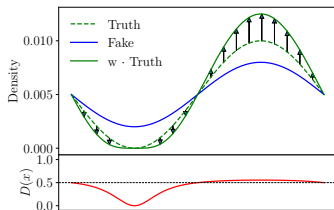
⇒ 1. control and 2. reweight

Joint DiscFlow training [GAN-inspired]

- GAN-like training unstable [Nash equilibrium?]
- coupling through weights

$$L_{\text{DiscFlow}} = - \sum_{i=1}^B w_D(x_i)^\alpha \log \frac{P(x_i)}{P_{\text{ref}}(x_i)}$$

$$\approx - \int dx \frac{P_{\text{ref}}^{\alpha+1}(x)}{P^\alpha(x)} \log \frac{P(x)}{P_{\text{ref}}(x)}$$



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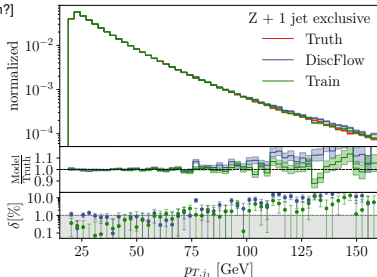
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⇒ Controlled unweighted events



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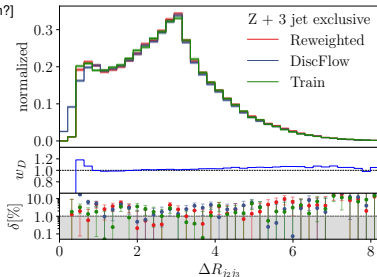
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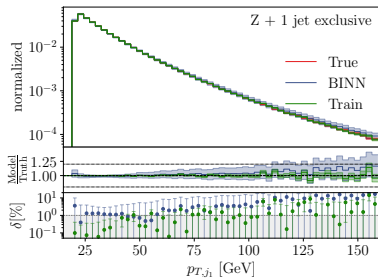
⇒ Reweighted precision events



Uncertainties

Bayesian INN generator

- uncertainty over phase space
 - training statistics leading source
- ⇒ Training-related error bars



Uncertainties

Bayesian INN generator

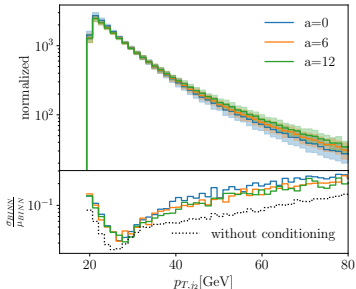
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Theory uncertainties

- BNN regression/classification: systematics from data augmentation
- systematic uncertainties in tails

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

- augment training data $[a = 0 \dots 30]$
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Uncertainties

Bayesian INN generator

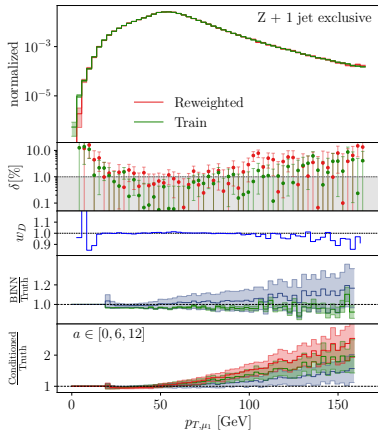
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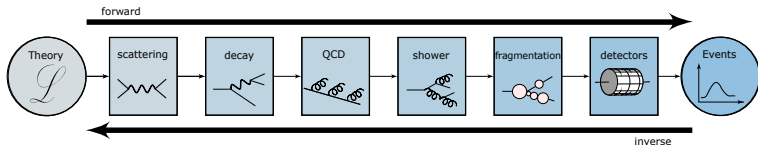
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Inverting event simulations

Inverting LHC simulations

- unfolding QCD-shower to hard parton standard [jet algorithm]
 - unfolding detector common
 - unfolding top-quark decays useful
 - matrix element method complete unfolding
- ⇒ systematic approach through generative network



Conditional GAN

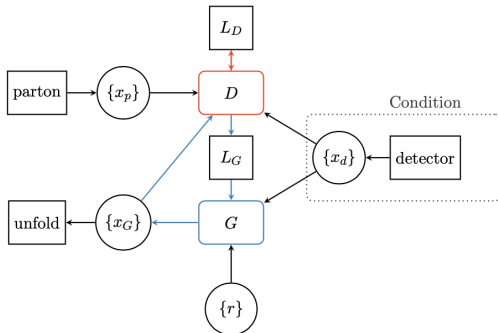
Goal: invert standard simulation

- detector simulation typical Monte Carlo, random-number-driven
- inversion possible, in principle [but entangled convolutions]
- **generative network task**

$$\text{partons} \xrightarrow{\text{DELPHES}} \text{detector} \xrightarrow{\text{GAN}} \text{partons}$$

Conditional generative networks

- random numbers to parton level
hadron level as condition
training on matched event pairs
- FCGAN the first example



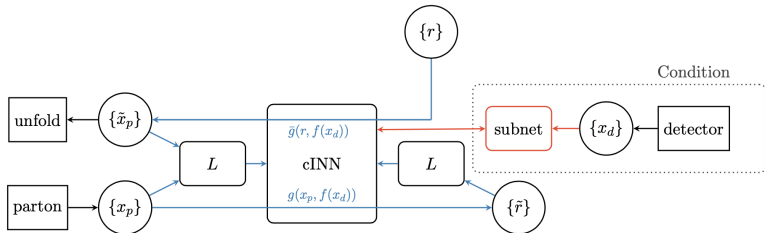
Statistical inversion

– task: construct parton-level pdf for (single) detector-level event

1- generative network: parton-level events from $\{r\}$

2- maximum likelihood loss

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



Conditional INN

Statistical inversion

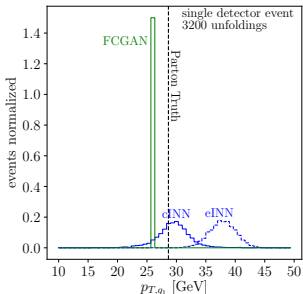
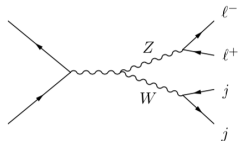
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This time $pp \rightarrow ZW \rightarrow (\ell\ell)(jj)$

– distribution: single pair (x_p, x_d) , 3200 unfoldings



Conditional INN

Statistical inversion

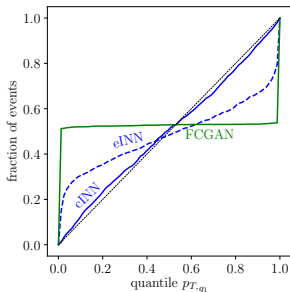
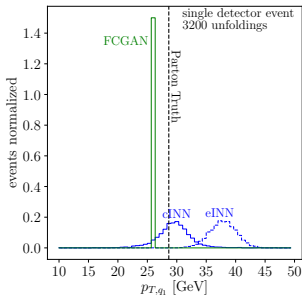
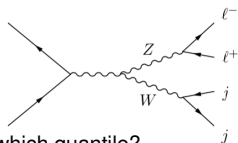
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This time $pp \rightarrow ZW \rightarrow (\ell\ell)(jj)$

- distribution: single pair (x_p, x_d) , 3200 unfoldings
- calibration: 1500 pairs (x_p, x_d) , 60 unfoldings, truth in which quantile?

⇒ **Conditional INNs solve inverse problems statistically**



Machine learning for LHC theory

Machine learning for the LHC

- Classification/regression standard
uncertainties?
symmetries?
experimental realities?
- GANs the cool kid
generator producing best events
discriminator checking generator
limited in precision and uncertainty control
- INNs my work horse
flow networks for control and precision
Bayesian for error bars
condition for inversion
- All results from 3 years, clearly a field for young people!

LHC

Some ML...

GAN

GANplification

Statistical gains

VAE

Calomplification

INN

Uncertainties

Inverting

