

Machine Learning for Madgraph

Tilman Plehn

Universität Heidelberg

Madgraph Workshop, September 2023



Shortest ML-intro ever

Fit-like approximation

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

Construction and control

- minimize loss to find θ
- sample θ -distributions [Bayesian networks]
- compare independent test data

LHC applications

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

→ Transforming numerical science

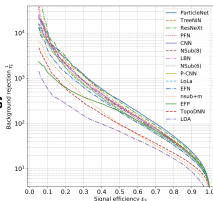


ML-applications in experiment

Top tagging

- 'hello world' of LHC-ML
- end of QCD-taggers
- different NN-architectures

→ Non-NN left in the dust...



SciPost Physics

Submission

The Machine Learning Landscape of Top Taggers

G. Kasieczko^{1(a)}, T. Plehn^(a), A. Butter², K. Craner³, D. DeLauter⁴, B. M. Ertel⁵,
M. Fairhead⁶, D. A. Faroughy⁷, W. Finkbeiner⁸, C. Gay⁹, L. Gornow⁹, J. F. Kerner^{10,11},
P. T. Komodo¹², S. Loefer¹³, A. Lister¹³, S. Maciunas¹⁴, E. M. Metodiev¹⁵, L. Moore¹⁶,
B. Nusslein^{1,11}, K. Nusslein^{1,11}, J. Puckert¹⁶, H. Qiu¹⁷, R. Ratt¹⁸, M. Rieger¹⁸, D. Scharf¹,
J. M. Thompson¹⁹, and S. Varron²⁰

- 1 Institut für Experimentelle Physik, Universität Hamburg, Germany
- 2 Institut für Theoretische Physik, Universität Heidelberg, Germany
- 3 Center for Cosmology and Particle Physics and Center for Data Science, NYU, USA
- 4 NHETC, Dept. of Physics and Astronomy, Rutgers, The State University of NJ, USA
- 5 Joint Institute for Nuclear Research, JINP, Dubna, Russia
- 6 Theoretical Particle Physics and Cosmology, King's College London, United Kingdom
- 7 Department of Physics and Astronomy, The University of British Columbia, Canada
- 8 Department of Physics, University of California, Santa Barbara, USA
- 9 Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia
- 10 Center for Theoretical Physics, MIT, Cambridge, USA
- 11 CPJ, Universitat de València, Valencia, Spain
- 12 Physics Division, Lawrence Berkeley National Laboratory, Berkeley, USA
- 13 SLAC, for the Theory of Computing, University of California, Berkeley, USA
- 14 National Institute for Subatomic Physics (Nikhef), Amsterdam, Netherlands
- 15 LPTHE, CNRS & Sorbonne Université, Paris, France
- 16 III. Physikalisches Institut A, RWTH Aachen University, Germany

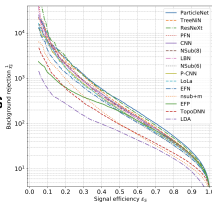


ML-applications in experiment

Top tagging

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

→ Non-NN left in the dust...



SciPost Physics

Submission

The Machine Learning Landscape of Top Taggers

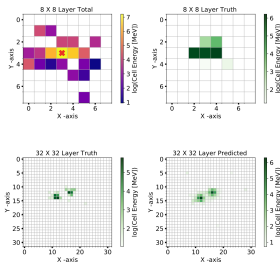
G. Kasieczko (ed.), T. Plehn (ed.), K. Craner², D. DeLoraine¹, B. M. Ellert³, M. Fairhead⁴, D. A. Farrelly⁵, W. Fickel⁶, C. Gay¹, L. Goushe⁷, J. F. Kerner^{8,9}, P. T. Komoda¹⁰, S. Liao¹¹, A. Lister¹², S. Maciuch¹³, E. M. Metcalfe¹⁴, L. Moore¹⁵, B. Naudus^{1,11}, K. Nandorini^{1,11}, J. Puck¹⁶, H. Qiu¹, Y. Ruan¹⁶, M. Sauer¹⁶, D. Shih¹, J. M. Thompson¹, and S. Varma⁸

- 1 Institut für Experimentelle Physik, Universität Hamburg, Germany
- 2 Institut für Theoretische Physik, Universität Heidelberg, Germany
- 3 Center for Cosmology and Particle Physics and Center for Data Science, NYU, USA
- 4 NHETC, Dept. of Physics and Astronomy, Rutgers, The State University of NJ, USA
- 5 Joint Institute for Nuclear Physics, Ljubljana, Slovenia
- 6 Theoretical Particle Physics and Cosmology, King's College London, United Kingdom
- 7 Department of Physics and Astronomy, The University of British Columbia, Canada
- 8 Department of Physics, University of California, Santa Barbara, USA
- 9 Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia
- 10 Center for Theoretical Physics, MIT, Cambridge, USA
- 11 CPJ, Universitat Catòlica de Leuven, Leuven-la-Neuve, Belgium
- 12 Physics Division, Lawrence Berkeley National Laboratory, Berkeley, USA
- 13 Simons Institute for the Theory of Computing, University of California, Berkeley, USA
- 14 National Institute for Subatomic Physics (NINHEP), Amsterdam, Netherlands
- 15 LPTHE, CNRS & Sorbonne Université, Paris, France
- 16 III. Physikalisches Institut A, RWTH Aachen University, Germany

Particle flow

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

→ Beyond just concepts



Towards a Computer Vision Particle Flow *

Francesco Armando Di Belle^{1,1}, Sammy Ganguly^{1,1}, Eliam Gross¹, Marumi Kado^{1,1}, Michael Pitt¹, Lorenzo Santi¹, Jonathan Shlomo¹

¹Wissmann Institute of Science, Rehovot 76100, Israel

²CERN, CH 1211, Geneva 23, Switzerland

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

⁴Université Paris-Saclay, CNRS/IN2P3, UCLab, 91105, Orsay, France

Fig. 7: An event display of total energy shower (within topecluster), 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 $p^0 \rightarrow \gamma\gamma$ is resolved by a 32×32 granularity layer.



Jets and parton densities

Anomaly searches

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

→ Autoencoders

arXiv:2304.08111 [hep-ph]

Better Latent Spaces for Better Autoencoders

Harry M. Dickinson¹, Tilman Plehn¹, Christian Bauer², and Peter Schwenn²

¹ Institut für Theoretische Physik, Universität Heidelberg, Germany

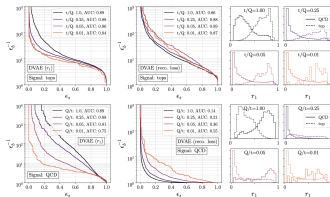
² Physikalisches Institut, Universität Heidelberg, Germany

² Heidelberg Collaboratory for Large Accelerators, Universität Heidelberg, Germany

April 26, 2023

Abstract

Autoencoders as tools behind anomaly searches at the LHC have 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 networks.



Jets and parton densities

Anomaly searches

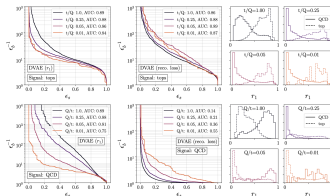
- train on QCD-jets, SM-events
- look for non-QCD jets, non-SM events

→ Autoencoders



Abstract

Autoencoders as tools to detect anomaly events at the LHC have 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 space. In particular, the Dirichlet setup solves the problem and improves both the performance and the interpretability of the networks.



NNPDF/N3PDF parton densities [full blast]

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

→ Leaders in ML-theory

N3PDF
Machine Learning - PDFs - QCD

Home

About

Team

Jobs

Publications

Deliverables

Documents

For the public

A data-based parametrization of parton distribution functions

Stefano Caronni^{1,2,*}, Juan Cruz-Martinez¹, and Ryo Suganuma³

¹ INFN, Dipartimento di Fisica, Università degli Studi di Milano and INFN Sezione di Milano.

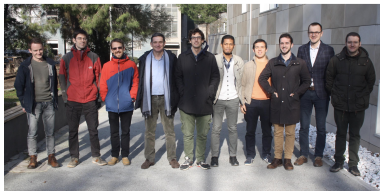
² INFN, Teorietica Fisica Department, CNAI-11, Genova, 16, Italy

³ Quantum Research Center, Technology Innovation Institute, Abu Dhabi, U.A.E.

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 procedure 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 procedure as a preprocessing. Over the years various, increasingly sophisticated, techniques have been introduced to consider the effect of the prior on the PDF determination. In this paper we present a methodology to ensure the posterior stability, thereby significantly simplifying the methodology, without a loss of efficiency and finding good agreement with previous results.

PACS. 22.20.+g Quantum chromodynamics · 12.20.+g Phenomenological quark models · 81.20.+g Neural Networks

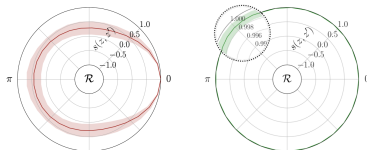


Symmetries

Symmetric networks [contrastive learning, transformer network]

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

→ Symmetric latent representation



SelfPost Physics

Symmetries

Symmetries, Safety, and Self-Supervision

Barry M. D'Eka¹, Grigor Kasieczko², Hans Gieseler¹, Tilman Plehn²,
Peter Sorensen³, and Lorenz Vogt¹

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, 2023

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-polygenic 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 validate its symmetry properties. We compare the JetCLR representation with alternative representations using linear classifier tests and find it to work quite well.

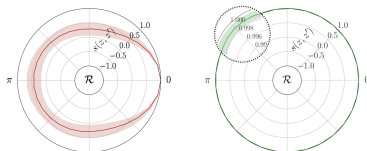


Symmetries

Symmetric networks [contrastive learning, transformer network]

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

→ Symmetric latent representation



Self-Poetry

Symmetries

Symmetries, Safety, and Self-Supervision

Barry M. Dikar¹, Gregor Kasieczka¹, Hans Gieseler¹, Thomas Plehn²,
Peter Sorensen¹, and Lorenz Vogt¹

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, 2023

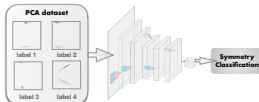
Abstract

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-arbitrary. 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.

Learning symmetries [representation, visualization]

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

→ Networks representing structure



Symmetry invariance AI

Gabriella Baranidou¹, Johannes Bore², and Vitoriano Romo³

¹ Department de Física Teòrica and IFIC, Universitat de València-CMCC, E-46100, Burjassot, Spain and

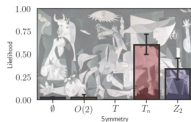
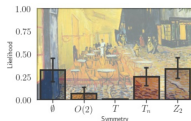
² Department of Physics and Astronomy, University of Texas, Arlington 76019, TX

1. INTRODUCTION

We explore whether Neural Networks (NN) can discover the presence of symmetries in their own input data. For this, we train feedforward NNs using a self-supervised learning framework, where the objective is to maximize the invariance of the NN output to the action of a symmetry group. We show that NNs can indeed learn to identify symmetries in their input data, and we discuss the implications of this for the discovery of new symmetries in particle physics.

of symmetries¹. From this simple representation of the data, these NNs were able to discover the laws of physics, which include a central symmetry, the laws of conservation, and the laws of conservation of energy. These NNs were able to discover the laws of conservation of energy, which include a central symmetry, the laws of conservation, and the laws of conservation of energy.

We also show that NNs can indeed learn to identify symmetries in their input data, and we discuss the implications of this for the discovery of new symmetries in particle physics.



Integrals

Learning integrands and integrals [differentiable activations]

- learn integrand through differentiable network
- evaluate integral as primitive

→ **Novel ML-integrator**

In practice, analytically, we would compute the primitive F ,

$$\frac{d^2 F(x, y)}{dx_1 dx_2} = f(x, y), \quad (3.88)$$

and then the integral by evaluating the integration boundaries

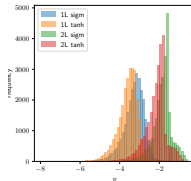
$$\begin{aligned} F(x) &= \int_{x_1=0}^1 dx_1 \int_{x_2=0}^1 dx_2 \frac{d^2 F(x, y)}{dx_1 dx_2} \bigg|_{y=0}^{y=1} \\ &= \int_{x_1=0}^1 dx_1 \int_{x_2=0}^1 dx_2 \frac{d^2 F(x, y)}{dx_1 dx_2} \bigg|_{y=0}^{y=1} \\ &= \sum_{i=1}^N \int_{x_1=0}^1 dx_1 \int_{x_2=0}^1 dx_2 f(x, y). \end{aligned} \quad (3.89)$$

In particle physics we really never know the primitive of a phase space integrand, but we can try to construct it and encode it in a neural network,

$$F_N(x, y) \approx F(x, y). \quad (3.90)$$

On the other hand, we do not have data to train a regression network for F directly. The idea is to instead train on integrated integrands, such that its 1D-th derivative matches f ,

$$\mathcal{L}_{\text{int}} \left(F_N(x, y) \frac{d^2 F_N(x, y)}{dx_1 dx_2} \right). \quad (3.91)$$



PUBLISHED FOR SISSA BY SPRINGER

RECEIVED: December 6, 2022

ACCEPTED: March 14, 2023

PUBLISHED: March 28, 2023

Multi-variable integration with a neural network

D. Maître^{a,1} and R. Santos-Mateos^b

^a*Institute for Particle Physics Phenomenology, Physics Department, Durham University, Durham DH1 1TA, U.K.*

^b*Department of Electronics and Computing, University of Santiago de Compostela, Santiago de Compostela, Spain*

E-mail: daniel.maître@durham.ac.uk, roi.santos@usc.es

ABSTRACT: In this article we present a method for automatic integration of parametric integrals over the unit hypercube using a neural network. The method fits a neural network to the primitive of the integrand using a loss function designed to minimize the difference between multiple derivatives of the network and the function to be integrated. We apply the method to two example integrals resulting from the sector decomposition of a one-loop and two-loop scalar integrals. Our method can achieve per-mille and percent accuracy for these integrals over a range of invariant values. Once the neural network is fitted, the evaluation of the integral is between 40 and 125 times faster than the usual numerical integration method for our examples, and we expect the speed gain to increase with the complexity of the integrand.



Integrals

Learning integrands and integrals [differentiable activations]

- learn integrand through differentiable network
- evaluate integral as primitive

→ Novel ML-integrator

boundaries. Analytically, we would compute the primitive F ,

$$\frac{\partial^2 F(x, y)}{\partial x_1 \partial x_2} = f(x, y), \quad (2.80)$$

and then the integral by evaluating the integration boundaries,

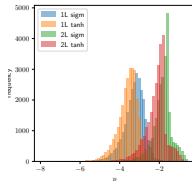
$$F(x) = \int_{x_1}^x dx_1 \int_{x_2}^x dx_2 \frac{\partial^2 F(x, y)}{\partial x_1 \partial x_2} = \int_{x_1}^x dx_1 \int_{x_2}^x dx_2 f(x, y) \Big|_{x_1=x_2}^{x_1=x_2} = \sum_{i=1}^n \int_{x_i}^x dx_1 \int_{x_i}^x dx_2 f(x, y). \quad (2.81)$$

In particle physics we really never know the primitive of a phase space integrated, but we can try to construct it and encode it in a neural network,

$$F_{\text{NN}}(x, y) \approx F(x, y). \quad (2.82)$$

On the other hand, we do not have data to train a surrogate network for F directly. The idea is to instead train on integrated integrands, such that its 1D-like derivative matches f ,

$$\mathcal{L}_{\text{int}} \left(f(x, y) \frac{\partial F_{\text{NN}}(x, y)}{\partial x_1} \right). \quad (2.83)$$



PUBLISHED FOR SISSA BY SPRINGER

RECEIVED: December 6, 2022

ACCEPTED: March 14, 2023

PUBLISHED: March 26, 2023

Multi-variable integration with a neural network

D. Maître^{a,1} and R. Santos-Mateos^a^aInstitute for Particle Physics Phenomenology, Physics Department, Durham University,

Durham DH1 1TA, U.K.

^bDepartment of Electronics and Computing, University of Santiago de Compostela,

Santiago de Compostela, Spain

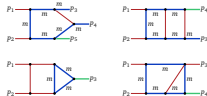
E-mail: daniel.maître@durham.ac.uk, roberto.santos-mateos@usc.es

ABSTRACT: In this article we present a method for automatic integration of parametric integrals over the unit hypercube using a neural network. The method fits a neural network to the primitive of the integrand using a loss function designed to minimize the difference between multiple derivatives of the network and the function to be integrated. We apply the method to two example integrals resulting from the sector decomposition of a one-loop and two-loop scalar integrals. Our method can achieve per-mille and percent accuracy for these integrals over a range of invariant values. Once the neural network is fitted, the evaluation of the integral is between 40 and 125 times faster than the usual numerical integration method for one example, and we expect the speed gain to increase with the complexity of the integrand.

Learning integration paths [invertible networks]

- find optimal integration paths
- learn variable transformation

→ Theory-integrator



SciPost

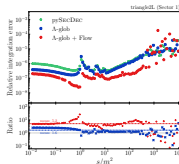
SciPost Phys. 12, 129 (2022)

Targeting multi-loop integrals with neural networks

Ramon Winterhalder^{1,2,3}, Vinay Mogerya⁴, Emilio Villa⁴, Stephen E. Jones⁵, Matthias Kerner^{4,b}, Anja Butter^{1,2}, Gudrun Heinrich^{4,c} and Tilman Plehn^{1,2}¹ Institut für Theoretische Physik, Universität Heidelberg, Germany² HEiG – Heidelberg Karlsruhe Strategic Partnership, Heidelberg University, Karlsruhe Institute of Technology (KIT), Germany³ Centre for Cosmology, Particle Physics and Phenomenology (CP3), Université catholique de Louvain, Belgium⁴ Institut für Theoretische Physik, Karlsruher Institut für Technologie, Germany⁵ Institute for Particle Physics Phenomenology, Durham University, UK⁶ Institute for Astrophysics, Karlsruher Institut für Technologie, Germany

Abstract

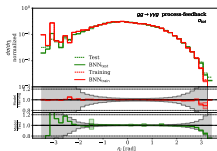
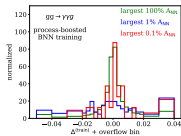
Numerical evaluations of Feynman integrals often proceed via a deformation of the integration contour into the complex plane. While valid contours are easy to construct, the numerical precision for a multi-loop integral can depend critically on the chosen contour. We present methods to optimize this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



Speeding up amplitudes [precision regression]

- loop-amplitudes expensive
- training up to interpolation

→ Precision NN-amplitudes



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

Joseph Ayres-Bullock^{a,b}, Simon Badger^a, Ryan Mandle^a

^a*Institute for Particle Physics Phenomenology, Department of Physics, Durham University, Durham, DH1 1TA, United Kingdom*

^b*Institute for Data Science, Durham University, Durham, DH1 1TA, United Kingdom*

^c*Dipartimento di Fisica e Astronomia Galileo Galilei, 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@durham.ac.uk, ryan.1.mandle@durham.ac.uk

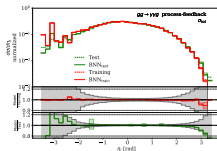
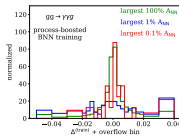
ABSTRACT: Machine learning technology has the potential to dramatically optimise event generation and simulations. We continue to investigate the use of neural networks to approximate matrix elements for high-multiplicity scattering processes. We focus on the case of loop-induced diphoton production through gluon fusion, and develop a modular simulation method that can be applied to hadron collider observables. Neural networks are trained using the one-loop amplitudes implemented in the *KKMC*++ 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.



Speeding up amplitudes [precision regression]

- loop-amplitudes expensive
- training up to interpolation

→ Precision NN-amplitudes



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

Joseph Ayres-Buckley^{a,b}, Simon Badger^a, Ryan Moadel^a^a*Institute for Particle Physics Phenomenology, Department of Physics, Durham University, Durham, DH1 1TA, United Kingdom*^b*Institute for Data Science, Durham University, Durham, DH1 1TA, United Kingdom*^c*Department of Physics and Arnold-Regge Center, University of Torino, 10125, Torino, Italy*E-mail: j.buckley@durham.ac.uk, simonbadger@durham.ac.uk, ryan.moadel@durham.ac.uk

ABSTRACT: Machine learning technology has the potential to dramatically optimise event generation and simulation. 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 `infix` C++ library, and interfaced to the Sherpa Monte Carlo event generator, where we perform a detailed study for $2 \rightarrow 3$ and $2 \rightarrow 4$ scattering problems. 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.

Unfolding and inversion [conditional normalizing flows]

- detector/decays/QCD unfolded
- calibrated inverse sampling

→ Publishing analysis results

Software Physics

Simulation

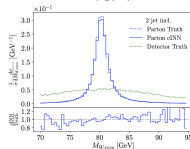
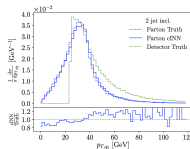
Invertible Networks or Partons to Detector and Back Again

Marco Bellaguardo¹, Anja Bhatta², George Katsoulis³, Thomas Plehn¹, Arseniy Romanenko^{1,2}, Razvan Watanabara², Lynne Aschmann², and Ulrich Kiese²¹*Institut für Theoretische Physik, Universität Heidelberg, Germany*²*Heidelberg Collaboratory for Image Processing, Universität Heidelberg, Germany*³*Institut für Experimentelle Physik, Universität Heidelberg, Germany*invertiblephys.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 to issues of high-level observables, specifically for $2N$ production at the LHC. It allows for a per-event statistical interpretation. Next, we show for a variable number of QCD jets. We switch detector effects and QCD radiation to a pre-defined level, produce, apply with a per-event probabilistic interpretation over parton-level phase space.



Proper theory

Navigating string landscape [reinforcement learning]

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

→ **Model space sampling**

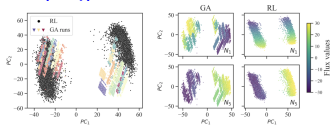


Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_3 and N_5 respectively) in relation to principal components for a PCA fit of the individual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

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

Alex Cate
University of Amsterdam
a.s.cate@uva.nl

Sven Krippendorf
Arnold Sommerfeld Center for Theoretical Physics
LMU Munich
sven.krippendorf@physik.uni-muenchen.de

Andreas Schachner
Centre for Mathematical Sciences
University of Cambridge
as2873@cam.ac.uk

Gary Shiu
University of Wisconsin-Madison
shiug@physics.wisc.edu

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.



Proper theory

Navigating string landscape [reinforcement learning]

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

→ Model space sampling

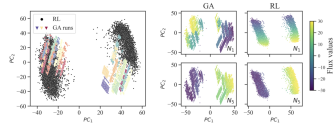


Figure 1: *Left:* Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. *Right:* Dependence on flux (input) values (N_1 and N_2 respectively) in relation to principal components for a PCA fit of the individual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

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

Alex Cule
University of Amsterdam
a.c.cule@uva.nl

Sven Krippendorff
Arnold Sommerfeld Center for Theoretical Physics
LMU Munich
sven.krippendorff@physik.uni-muenchen.de

Andreas Schachner
Centre for Mathematical Sciences
University of Cambridge
as2073@cam.ac.uk

Gary Shiu
University of Wisconsin-Madison
shiug@physics.wisc.edu

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 inducing sampling bias.

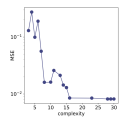
Learning formulas [genetic algorithm, symbolic regression]

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

→ Understanding numerics through formulas

compil	dxdf/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 $a \Delta \phi \mp_{p,1}$	$9.50 \cdot 10^{-2}$
6	1 $-x_{p,1} \sin(\Delta \phi + a)$	$1.90 \cdot 10^{-1}$
7	1 $(-x_{p,1} - a) \sin(\sin(\Delta \phi))$	$5.63 \cdot 10^{-2}$
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 $-(x_{p,2} (a \Delta \phi^2 + x_{p,1}) + b) \sin(\Delta \phi + c)$	$1.30 \cdot 10^{-2}$
16	4 $-x_{p,1} (a - b \Delta \phi) (x_{p,2} + c) \sin(\Delta \phi + d)$	$8.50 \cdot 10^{-3}$
28	7 $(x_{p,2} + a) ((x_{p,1} (c - \Delta \phi) - x_{p,1} (b \Delta \phi + x_{p,2} + f) \sin(\Delta \phi + g)))$	$8.18 \cdot 10^{-3}$

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



Back to the Formula — LHC Edition

Arja Bratter¹, 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.seydoux@desy.de
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-8 coefficient on associated ZH production. We then validate it for the known case of CP-violation in weak-boson-fusion Higgs production, including interference effects.



Bayesian network loss

Deriving the loss

- energy measurement for jet j

$$\langle E \rangle = \int dE \ E \ p(E)$$

- weighted by reproduced training data $p(\theta|T)$

$$p(E) = \int d\theta \ p(E|\theta) \ p(\theta|T)$$

→ θ -distributions means BNN



Bayesian network loss

Deriving the loss

- energy measurement for jet j

$$\langle E \rangle = \int dE E p(E)$$

- weighted by reproduced training data $p(\theta|T)$

$$p(E) = \int d\theta p(E|\theta) p(\theta|T)$$

→ θ -distributions means BNN

Variational approximation

- definition of training [think $q(\theta)$ as Gaussian with mean and width]

$$p(E) = \int d\theta p(E|\theta) p(\theta|T) \approx \int d\theta p(E|\theta) q(\theta)$$

- similarity through minimal KL-divergence [Bayes' theorem to remove unknown posterior]

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



Bayesian network loss

Deriving the loss

- energy measurement for jet j

$$\langle E \rangle = \int dE E p(E)$$

- weighted by reproduced training data $p(\theta|T)$

$$p(E) = \int d\theta p(E|\theta) p(\theta|T)$$

→ θ -distributions means BNN

Variational approximation

- definition of training [think $q(\theta)$ as Gaussian with mean and width]

$$p(E) = \int d\theta p(E|\theta) p(\theta|T) \approx \int d\theta p(E|\theta) q(\theta)$$

- similarity through minimal KL-divergence [Bayes' theorem to remove unknown posterior]

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



Bayesian network loss

Deriving the loss

- energy measurement for jet j

$$\langle E \rangle = \int dE E p(E)$$

- weighted by reproduced training data $p(\theta|T)$

$$p(E) = \int d\theta p(E|\theta) p(\theta|T)$$

→ θ -distributions means BNN

Variational approximation

- definition of training [think $q(\theta)$ as Gaussian with mean and width]

$$p(E) = \int d\theta p(E|\theta) p(\theta|T) \approx \int d\theta p(E|\theta) q(\theta)$$

- similarity through minimal KL-divergence [Bayes' theorem to remove unknown posterior]

$$\begin{aligned} D_{\text{KL}}[q(\theta), p(\theta|T)] &= \int d\theta q(\theta) \log \frac{q(\theta)}{p(\theta|T)} \\ &= \int d\theta q(\theta) \log \frac{q(\theta)p(T)}{p(T|\theta)p(\theta)} \\ &\approx D_{\text{KL}}[q(\theta), p(\theta)] - \int d\theta q(\theta) \log p(T|\theta) \equiv \mathcal{L} \end{aligned}$$

→ Two-term loss: likelihood + prior



Relation to deterministic networks

Regularization

- BNN loss

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



Relation to deterministic networks

Regularization

- Gaussian prior

$$\mathcal{L} = - \int d\theta \, q(\theta) \log p(T|\theta) + \frac{\sigma_q^2 - \sigma_p^2 + (\mu_q - \mu_p)^2}{2\sigma_p^2} + \dots$$

- deterministic network

$$q(\theta) = \delta(\theta - \theta_0) \quad \Rightarrow \quad \mathcal{L} \approx -\log p(T|\theta_0) + \frac{(\theta_0 - \mu_p)^2}{2\sigma_p^2}$$

→ Likelihood with L2-regularization



Relation to deterministic networks

Regularization

- Gaussian prior

$$\mathcal{L} = - \int d\theta \, q(\theta) \log p(T|\theta) + \frac{\sigma_q^2 - \sigma_p^2 + (\mu_q - \mu_p)^2}{2\sigma_p^2} + \dots$$

- deterministic network

$$q(\theta) = \delta(\theta - \theta_0) \quad \Rightarrow \quad \mathcal{L} \approx -\log p(T|\theta_0) + \frac{(\theta_0 - \mu_p)^2}{2\sigma_p^2}$$

→ Likelihood with L2-regularization

Dropout

- Bernoulli weights

$$q(\theta) \rightarrow q(x) = \rho^x (1 - \rho)^{1-x} \Big|_{x=0,1} \quad \text{with} \quad \theta = x\theta_0$$

- likelihood loss

$$\mathcal{L} = - \sum_{x=0,1} \left[\rho^x (1 - \rho)^{1-x} \right] \log p(T|x\theta_0) = -\rho \log p(T|\theta_0)$$

- likelihood Gaussian or whatever else...

→ Regularized likelihood with dropout



Generative-network revolution

Generative networks

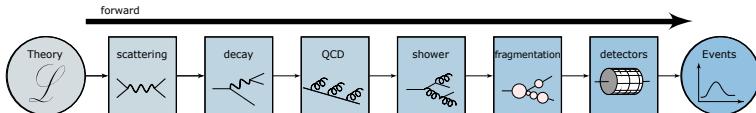
- generate **new** images, text blocks, LHC events
- encode density in target space
sample from Gaussian into target space
- reproduce training data, statistically independently
- include uncertainty on estimated density [Bayesian NN]



Generative-network revolution

Generative networks

- generate **new** images, text blocks, LHC events
 - encode density in target space
sample from Gaussian into target space
 - reproduce training data, statistically independently
 - include uncertainty on estimated density [Bayesian NN]
 - Variational Autoencoder
→ low-dimensional physics, high-dimensional representation
 - Generative Adversarial Network
→ generator trained by discriminator
 - Normalizing Flow/Diffusion Model
→ stable (bijective) mapping
 - Generative Transformer [JetGPT]
→ learning correlations successively
- **Pick model for purpose**



Transformers

Extracting correlations

- Start with (compact) query representation

$$x_i \longrightarrow q = \frac{x_i}{|x|}$$

- Orthonormal values basis [related to q through scalar product]

$$q = \sum_j (q \cdot v_j) v_j$$

- Simpler orthogonal keys basis

$$q = \sum_j (q \cdot k_j) v_j \quad \text{with} \quad k_j = \frac{v_j}{v^2}$$

→ Self-attention representation

$$x_i \longrightarrow z_i = \sum_j (q \cdot k_j) v_j$$



Transformers

Extracting correlations

- Start with (compact) query representation

$$x_i \longrightarrow q = \frac{x_i}{|x|}$$

- Orthonormal values basis [related to q through scalar product]

$$q = \sum_j (q \cdot v_j) v_j$$

- Simpler orthogonal keys basis

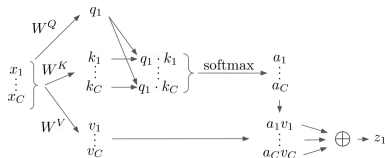
$$q = \sum_j (q \cdot k_j) v_j \quad \text{with} \quad k_j = \frac{v_j}{v^2}$$

→ Self-attention representation

$$x_i \longrightarrow z_i = \sum_j (q \cdot k_j) v_j$$

LHC phase space

- learn bin-bin relation $x_i \leftrightarrow x_j$
- latent query representation $q = W^Q x$
latent key representation $k = W^K x$
correlation $A_{ij} = q_i \cdot k_j$
- latent value representation $v = W^V x$
constructed representation $z = A v$



JetGPT

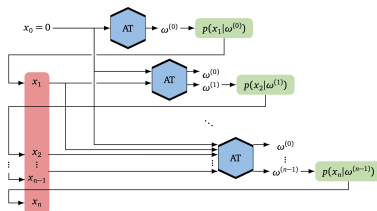
Autoregressive transformer

- factorized density

$$p_{\text{model}}(x|\theta) = \prod_i p(x_i | x_1, \dots, x_{i-1})$$

- bins \rightarrow Gaussian mixture model
- autoregressive $A_{ij} = 0$ for $j > i$

\rightarrow Bayesian version for uncertainties



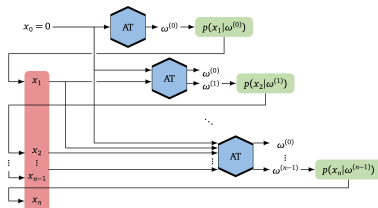
JetGPT

Autoregressive transformer

- factorized density

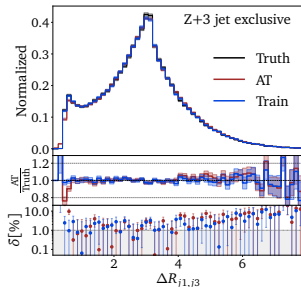
$$p_{\text{model}}(x|\theta) = \prod_i p(x_i | x_1, \dots, x_{i-1})$$

- bins \rightarrow Gaussian mixture model
 - autoregressive $A_{ij} = 0$ for $j > i$
- \rightarrow Bayesian version for uncertainties



Bayesian JetGPT

- sometimes you win...



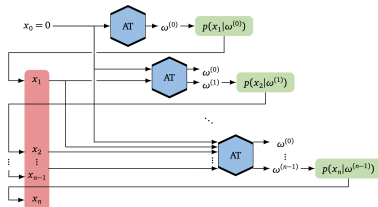
JetGPT

Autoregressive transformer

- factorized density

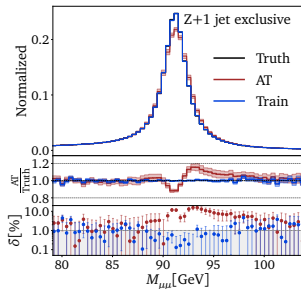
$$p_{\text{model}}(x|\theta) = \prod_i p(x_i | x_1, \dots, x_{i-1})$$

- bins \rightarrow Gaussian mixture model
 - autoregressive $A_{ij} = 0$ for $j > i$
- \rightarrow Bayesian version for uncertainties



Bayesian JetGPT

- sometimes you win...
- ...and sometimes there is work to do...



ML for LHC Theory

ML-applications

- just another numerical tool for a numerical field
- driven by money from data science and medical research
- goals are...
 - ...improve established tasks
 - ...develop new tools for established tasks
 - ...transform through new ideas
- xAI through...
 - ...precision control
 - ...uncertainties
 - ...symmetries
 - ...formulas

→ Lots of fun with hard LHC problems

Modern Machine Learning for LHC Physicists

Tilman Plehn^a; Anja Butter^{a,b}, Barry Dillon^a, Claudius Krause^{a,c}, and Ramon Winterhalder^d

^a Institut für Theoretische Physik, Universität Heidelberg, Germany

^b LPNHE, Sorbonne Université, Université Paris Cité, CNRS/IN2P3, Paris, France

^c NHEC, Dept. of Physics and Astronomy, Rutgers University, Piscataway, USA

^d CP3, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

July 21, 2023

Abstract

Modern machine learning is transforming particle physics, faster than we can follow, and bullying its way into our numerical tool box. For young researchers it is crucial to stay on top of this development, which means applying cutting-edge methods and tools to the full range of LHC physics problems. These lecture notes are meant to lead students with basic knowledge of particle physics and significant enthusiasm for machine learning to relevant applications as fast as possible. They start with an LHC-specific motivation and a non-standard introduction to neural networks and then cover classification, unsupervised classification, generative networks, and inverse problems. Two themes defining much of the discussion are well-defined loss functions reflecting the problem at hand and uncertainty-aware networks. As part of the applications, the notes include some aspects of theoretical LHC physics. All examples are chosen from particle physics publications of the last few years. Given that these notes will be outdated already at the time of submission, the week of ML4lets 2022, they will be updated frequently.

