LHC Data Science

Tilman Plehn

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ML examples

Anomalies

Symbolic re

# LHC Theory as Fun Data Science

Tilman Plehn

Universität Heidelberg

Dortmund, May 2022



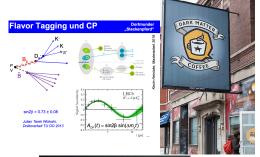
Tilman Plehn

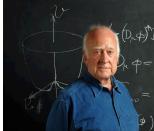
#### Modern LHC physics Science

#### LHC physics

#### Classic motivation

- · dark matter
- · baryogenesis
- · Higgs VEV







#### LHC physics

ML examp

Anomalie

Symbolic

#### Classic motivation

- dark matter
- · baryogenesis
- · Higgs VEV

#### LHC physics

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



# Modern LHC physics

#### LHC physics

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Anomali

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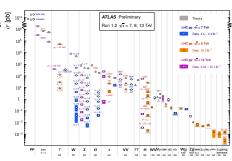
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#### Traditional methods

- · discover in rates
- · unveil little black holes
- · find supersymmetry
- · travel through extra dimensions
- · beat Bochum





#### LHC physics

ML exampl

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#### LHC physics

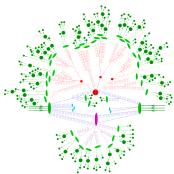
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### First-principle simulations

- · start with Lagrangian
- · calculate scattering using QFT
- · simulate events [theory]
- · simulate detectors [experiment]
- ightarrow LHC events in virtual worlds





# Modern LHC physics

#### LHC physics

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scattering

decay

QCD

beat Bochum

# First-principle simulations

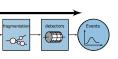
- · start with Lagrangian
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- · simulate detectors [experiment]
- → LHC events in virtual worlds

# Searching for BSM physics

shower

- · compare simulations and data
- · analyze data systematically
- · understand LHC dataset [SM or BSM]
- → With a little help from data science...





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LHC physics

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# Ask a data scientist

# LHC questions

 $\cdot$  How to get from 3  $\cdot$  10  $^{15}$  Bytes/s to 300  $\cdot$  10  $^{6}$  Bytes/s?



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Anomalies

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# Ask a data scientist

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Anomalies

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ML example

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   Graph neural networks



# LHC physics

ML examples

Uncertaintie

Symbolic

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- · How to combine tracker and calorimeter?



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   Super-resolution networks



### LHC physics

ML example:

Anomalies

Symbolic

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 Graph neural networks

How to combine tracker and calorimeter?
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How to remove pile-up?
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· How to look for BSM physics?



### LHC physics

ML example

Anomalies

Symbolic re

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· How to look for BSM physics?

Autoencoders

· How to compare measured with data?



#### LHC physics

LHC questions

How to get

ML example

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**Autoencoders** 

· How to compare measured with data?

Simulation-based inference



LHC physics

# LHC questions

Ask a data scientist

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LHC physics

LHC questions

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Simulation-based inference

What's in there for theory?



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# Shortest ML-intro ever

### Fit-like approximation

- · approximate known f(x) using  $f_{\theta}(x)$
- $\cdot$  no parametrization, just very many values  $\theta$
- $\cdot$   $\theta$ -space the fun space [latent space]

#### Construction and contol

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

#### LHC applications

- regression
- · classification
- · generation
- conditional generation
- . . . .
- → Transforming numerical science



#### Generative networks

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GANGogh [2017]

· create new pieces of art

· generation  $r \to p_{\theta}(r)$  sampled  $r \sim \mathcal{N}$ 

· train on 80,000 pictures

· generate flowers





#### LHC Data Science

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LHC physics

### Generative networks

### GANGogh [2017]

- · create new pieces of art
- $r o p_{ heta}(r)$  sampled  $r \sim \mathcal{N}$ generation
- · train on 80,000 pictures
- generate portraits
- $\rightarrow$  LHC?





#### LHC Data Science

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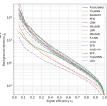
Anomalies

Symbolic

# ML-applications for analysis

#### Top tagging [supervised classification]

- · 'hello world' of LHC-ML
- · different NN-architectures
- → Just do it right...



#### out Physics

The Machine Learning Landscape of Top Taggers

G. Karlevska (ed)<sup>1</sup>, T. Feder (ed)<sup>2</sup>, A. Butter<sup>3</sup>, K. Crameer<sup>3</sup>, D. Debautt<sup>4</sup>, B. M. Dilou<sup>5</sup>, M. Birkskin<sup>5</sup>, D. A. Brenghy<sup>5</sup>, W. Federich<sup>5</sup>, C. Gey<sup>7</sup>, L. Geschier<sup>5</sup>, J.F. Kameik<sup>5,5</sup>, P. T. Kemisk<sup>5,6</sup>, S. Leis<sup>1</sup>, A. Lister<sup>5</sup>, S. Meschon<sup>5</sup>, E. M. Metches<sup>1</sup>, L. Morcel<sup>1</sup>, B. Norlman, <sup>3,1,5</sup>, K. Neufstrien<sup>1,1,5</sup>, J. Penishe<sup>5</sup>, H. Qu<sup>5</sup>, Y. Ruhi<sup>5</sup>, M. Keger<sup>5</sup>, D. Shh<sup>5</sup>, J. Temporot<sup>5</sup>, and S. Vorme<sup>5</sup>

Institut für Experimentajdyydk, Universität Hurzburg, Germany
 Institut für Timoettische Physik, Universität Heidelberg, Germany
 Gemier Se Connelog und Particle Physics and Genter Se Data Science, NYU, USA:
 NHECT, Dept. of Physics and Astronous, Retgers, The State University of NJ, USA
 Siand Studies Lantitute, Ijalikan, Stooreia.

6 Theoretical Particle Physics and Astronomy, Springer, Springer College London, United Kingdom 7 Department of Physics and Astronomy, The University of British Columbia, Canada 8 Department of Physics, University of Colorins, Santa Berlara, USA 9 Passity of Mathematics and Physics, University of Liphipan, Liphipan, Storeda 10 Contro for Theoretical Physics, Math. Control, 2016.

31 CPS, Universibitis Calcibility of Lorenta, Lorenta-la-Nevro, Belgium 11 CPS, Universibites Calcibility of Lorenta, Lorenta-la-Nevro, Belgium 21 Physics Division, Lorenta-Berbelly, National Laboratory, Berbelly, USA 13 Stences Inch. for the Throey of Congusting, University of Collidation, Berbelly, USA 14 National Institute for Substonic Physics (NIKREF), Austrelains, Netherlands 15-17 THE, CNIS & Substance (NIKREF), Austrelains, Netherlands





Tilman P

#### LHC physic

ML examples

Uncertain

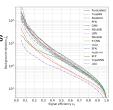
#### Anomalies

Symbolic

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#### it Physics

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M. Fatrisch\*, D. A. Farregir\*, W. Pecker\*, C. Gar', L. Conisot\*, J. R. Knemida\*,
P. T. Knishe\*, S. Lein\*, A. Lister\*, S. Machino\*\*, E. M. Mitches\*, L. Moccel,
B. Noltzana, 2014. N. Neutrick\*, P. P. Passiof\*, H. Q. Y. Palls\*, M. Riggers\*, D. Shift,
N. Noltzana, 2014.

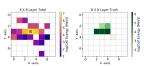
Institut für Enperimentalphysik, Universität Hamburg, Germany
 Institut für Theoretische Physik, Universität Heidelberg, Germany
 Center for Cossoliupy and Particle Physics and Center for Data Science, NYU, USA:
 A NIBCTI, Dept. of Physics and Astronomy, Ratgers, The State University of NJ, USA:

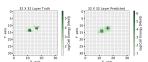
6 Theoretical Particle Physics and Councilogy, Kingle College Leaden, United Kingdom 7 Department of Physics and Astronomy, The University of British Columbia, Canada 8 Department of Physics, University of Calebraia, Saxia Barbara, USA 9 Family of Mathematics and Physics, University of Liphipan, Liphipan, Storeia 10 Council and Council and Physics, University of Liphipan, Liphipan, Storeia

 UPS, Universitées Cathelique de Lever de Levende Neiver, Belgium J. Physics Debriec, Levence Berheley States all hoberatery Berkeley, 184
 Stanes Inst. for the Theory of Computing, University of California, Berleiny, USA
 Montan Inst. for the Theory of Computing, University of California, Berleiny, USA
 Montania Institute for Scharcher Physics (NIGISE), Australeus, Netherlands
 IS LPTIEC, CNIS & Surbonne University, Paris, Prazee
 III. Physics Institutes A, WATH Adacher University, Germany

# Particle flow [classification, super-resolution]

- · mother of jet tools
- · combined detector channels
- → Seriously impressive





#### Towards a Computer Vision Particle Flow \*

Francesco Armando Di Bello<sup>1,1</sup>, Sanmay Ganguly<sup>3,1</sup>, Ellam Gross<sup>1</sup>, Marumi Kado<sup>3,4</sup>, Michael Pitt<sup>2</sup>, Lorenzo Santi <sup>3</sup>, Jonathan Shlomi<sup>1</sup>

<sup>1</sup>Weizrum Institut of Science, Robert 76100, Innel

\*\*CERN, CH 1211, Geneva 23, Switzerland

\*\*Università di Roma Sapienza, Piazza Aldo Moro, 2, 0035 Roma, Italy e INFN, Italy

\*\*Università di Paris-Sacloy, CNES/INDP3, IECLab, 91405, Ossay, France

Fig. 7. An event display of total energy shower (within topocluster), as captured by a calorimeter layer of  $8 \times 8$  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  $32 \times 32$  granularity (middle). The bottom right panel shows the corresponding event predicted by the NN. The figure shows that the shower originating from a  $\pi^0 \to \gamma \gamma$  is resolved by a  $32 \times 32$  granularity layer.

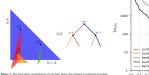


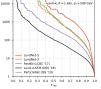
ML examples

#### Lund plane representation [input preprocessing]

- · QCD-inspired input with cutting-edge networks
- · angular separation vs transverse momentum OCD rejection v. Top tagging efficiency
- → Understanding data helps

The thick blue line represents the primary sequence of tuples  $\mathcal{L}_{primary}$ 





Pythia 8.223 simulation at pp → tf, background: pp → // PROPRIED FOR SURRESPONDS TO JOSEP

OUTF-29-15P

#### Jet tagging in the Lund plane with graph networks

#### Frédéric A. Drover," Huilin Qu<sup>b</sup> \*Rodolf Prioris Contro for Theoretical Physics, Clarendon Laboratory, Parks Road, Oxford OX1

\*CERN, EP Department, CH-1211 Genera 23, Systocriend

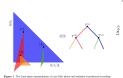
ARTHACT: The identification of boosted heavy particles such as top quarks or vector bosons is one of the key problems arising in experimental studies at the Large Hadron Collider. In this article, we introduce LundNet, a novel let tagging method which relies on graph neural networks and an efficient 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 releastness of the LandNet turners to non-nerturbative and detector effects, and show how kinematic cuts in the Land plane can mitigate overfitting of the nound 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.

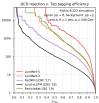


# QCD and symmetries

#### Lund plane representation [input preprocessing]

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#### Self-supervised training [contrastive learning, transformer network]

- · rotations, translations, permutations, soft splittings, collinear splittings
- · learn symmetries/augmentations
- → Symmetry-aware latent space





#### Symmetries, Safety, and Self-Supervision

Barry M. Dillon<sup>1</sup>, Gregor Kasiocaka<sup>2</sup>, Hans Olischlager<sup>1</sup>, Tilman Pietzi<sup>1</sup>

1 Institut für Theoretische Physik, Universität Heidelberg, German-2 Institut für Experimentalphysik, Universität Hamburg, German 3 Heidelberg Collaboratory for Iraque Processing, Universität Heidelberg, Germans

August 11, 2021

Abstract

Collider searches face the challenge of defining a representation of high-dimensional dat such that physical symmetries are manifest, the discriminating features are retained, and the choice of representation is new-physics againstic. We introduce JetCLR to solve the mapping from low-level data to optimized observables though self-supervised contrastive using a permutation-invariant transformer-encoder network and visualize its evaporate reporties. We compare the JetCLR representation with alternative representations using linear classifier tests and find it to work quite well



#### LHC Data Science

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ML examples

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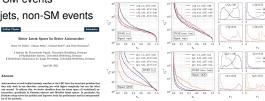
Anomalies

Symbolic

# Non-QCD and parton densities

#### Anomaly searches [unsupervised training]

- · train on QCD-jets, SM-events
- · look for non-QCD jets, non-SM events
- → Discussed later



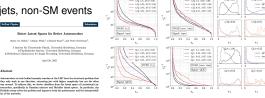


ML examples

# Non-QCD and parton densities

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#### NNPDF/N3PDF parton densities

· starting point: pdfs without functional ansatz

Abstract

- · moving on: cutting-edge ML everywhere
- → Leaders in ML-theory



A data-based parametrization of parton distribution functions Stelans Currana <sup>1,2,3</sup>, Jana Crus-Martines<sup>1</sup>, and Boy Stepman TIF Lab, Diparticuento di Fisica, Univenità degli Studi di Milano and INFN Seriose di Milano

Abstract. Since the first determination of a structure function many decades ago, all methodologies of







ML examples

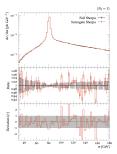
#### Speeding up Sherpa [sampling]

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

	$gg \rightarrow t\bar{t}ggg$	ug → třggu	$uu \to t\bar{t}guu$	$w\bar{u} \to t\bar{t}gd\bar{d}$
feat	1.1e-2	7.3e-3	6.8e-3	6.6e-4
Chicago	6.7e-3	5.8e-3	4.7e-3	3.6c-4
(fast)/(fase)	39312	2417	199	64
20.00	52.03	32.52	63.76	326.19
Park.	2.40-2	3.8e-2	2.1e-2	5.6e-3
opm.	0.0069	0.9984	0.9994	0.9951
for.	2.21	4.89	1.47	0.29
yord	30.40	19.14	27.78	25.34
e mod	4.3e-2	6.4e-2	5.1e-2	7.1e-2
o <sup>med</sup>	0.9983	0.9966	0.9943	0.5021
CV <sup>4</sup>	3.50	8.26	3.91	2.22



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





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ML examples

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# Events and amplitudes

#### Speeding up Sherpa [sampling]

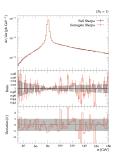
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feat	1.1e-2	7.3e-3	6.8e-3	6.6e-4
Chilaran	8.7e-3	5.8e-3	4.7e-3	3.6e-4
(feat)/(fear)	39312	2417	199	64
20.00	52.03	32.52	63.76	326.19
Ontary	2.40-2	3.8e-2	2.1e-2	5.6e-3
opm.	0.9969	0.9984	0.9994	0.9951
for.	2.21	4.89	1.47	0.29
yout	30.40	19.14	27.78	25.34
e mod	4.3e-2	6.4e-2	5.1e-2	7.1e-2
ormed	0.9983	0.9966	0.9943	0.5021
COTA .	3.50	8.26	3.91	2.22



# Abstract The generation of unit-weight events for complex scattering processes presents a severe challenge to modern Mente Carlo event generators. Even when using so-philicated phose-space sampling tecinizations adopted to the underlying trendition samples can be concess a limiting factor in practical applications. Here we present

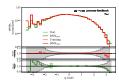
native discrete, the efficiency for generating unit-voidal events from weights combon complication becomes a limiting float is protected applications. Here we present a need to-votaged nareally discrete that a new part of the state of the



#### Speeding up amplitudes [precision regression]

- · loop-amplitudes expensive
- · interpolation standard
- → Network amplitudes





PREPARED FOR SUBMISSION TO JHEP

IPPP/20/116

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

Joseph Aylett-Bullock\*\* Simon Badger\* Ryan Moodie\*

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ABSTRACT Medical searring referedacy has the potential to demandable politics consists. We confirm to integrate the end of some describe to approximate and sinchmine. We confirm to integrate the end of some describes to approximate matrix demands for high analyzinder scattering prosone. We force on the case of the procession of the p



LHC Data Science

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LHC physic

ML examples

Uncertaintie

Anomalies

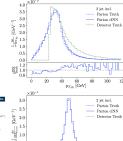
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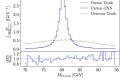
# Invertible event generation and errors

#### Unfolding and inversion [conditional normalizing flows]

- $\cdot$  shower/hadronization unfolded by jet algorithm
- · detector/decays unfolded e.g. in tops
- · calibrated inverse sampling
- → Backwards generation









ML examples

# Invertible event generation and errors

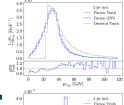
#### Unfolding and inversion [conditional normalizing flows]

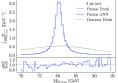
- shower/hadronization unfolded by jet algorithm
- · detector/decays unfolded e.g. in tops
- calibrated inverse sampling Backwards generation





ible neural networks are expecially useful. A conditional INN can invert a detector simulation in terms of high-level observables, specifically for ZW production at the LHC. It allows for a per-room statistical interpretation. Next, we allow for a variable number of QCD jets.
We unfold detector effects and QCD radiation to a per-defined hard process, again with a per-event probabilistic interpretation over parton-level phase space.





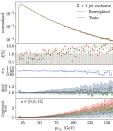
#### Generative networks with uncertainties [Bavesian discriminator-flows]

training data.

- · control through discriminator [GAN-like]
- · uncertainties through Bayesian networks
- → Discussed later



improves the generation. Our joint training relies on a novel counling of the two networks which does not require a Nash equilibrium. We then estimate the generation uncertainties through a Boyosian notwork setup and through conditional data sugmentation, while the discriminator ensures that there are no systematic incombination compared to the





Tilman Plehn

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ML examples

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Anomalies

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# String landscape and learned formulas

### Navigating string landscape [reinforcement learning]

- · searching for viable vacua
- · high dimensions, unknown global structure
- $\rightarrow \ \text{Model space sampling}$

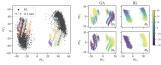


Figure 1: Left: Cluster structure in dimensionally reduced flux samples for RL and 25 GA runs (PCA on all samples of GA and RL). The colors indicate individual GA runs. Right: Dependence on flux (inpat) values (N<sub>2</sub> and N<sub>3</sub> respectively) in relation to principal components for a PCA fit of the individual output of GA and RL.

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

Alex Cole

Swen Krippendari

Amada Sommerida Lamendari

Amada Sommerida Color in Theoretical Physics

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Centre in Mathematical Somers

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Abstract

Identifying string theory vacua with desired physical properties at low energies

requires succiding through high-dimensional solution spaces - collectively relateral to a the string influency. We highligh that this search problem is mensible to minimize many and a president properties of the context of this vacuum, we are able to reveal source functions (angested approximate angested of symmetries in the able to reveal source) furnishing the problem of the problem of the context of the total context of the context of the context of the context of the which we are also it importants for endosting sampling blass.



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# String landscape and learned formulas

#### Navigating string landscape [reinforcement learning]

- · searching for viable vacua
- high dimensions, unknown global structure
- → Model space sampling

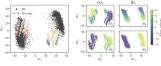


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#### Probing the Structure of String Theory Vacua with Genetic Algorithms and Reinforcement Learning

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#### Abstract

Identifying utring theory vocan with desired physical properties at low energies requires meating forced high-demonstrate alwakes spaces—collectively referred to as the string landscape. We highlight that this essent problem is amonable to redeferencement insuring and protein algorithms. In the content of the vacane, we are able to reveal novel features (engagesting proviously unidentified symmetries) in the string theory solutions required for proteiners such as the tring content, to feet to identify these features solvanity, we combine results from both search methods, which we supple in imperative for redecing sampling bias.

#### Learning formulas [genetic algorithm, symbolic regression]

- · approximate numerical function through formula
- · example: score/optimal observables
- → Discussed later



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

#### Back to the Formula — LHC Edition

Anja Butter<sup>2</sup>, Tilman Pishn<sup>2</sup>, Nathalio Soyhelman<sup>2</sup>, and Johann Brohmser<sup>2</sup>

1. Institut für Theoretische Physik, Universität Heidelberg, Germany
2 Center for Data Science, New York University, New York, United States
nothalis/forty-relama.

November 16, 2

#### Abstract

SciPost Physics

With neural networks offer an attractive up to manerically recode functions, actual formula remain the inguage of the excelled parties. We supposed to suppose the precise points of the possible regression trained on mattic-bearoni inferension to extract, for instance, optional IIIC observables. This was inverted to make simulation paragraphs and extract easily interpretable formulas from complex districted data. We interrube the neutron of the other of a districted series complex districted that we have been a supposed to the properties of the pr



# Controlled precision generator

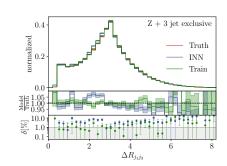
.HC physics

# ML-event generators

Uncertainties

 speed up generation ship events train on MC plus data useful ML-playground detector simulation next

 $\cdot$   $Z_{\mu\mu}+\{$  1, 2, 3 $\}$  jets  $_{[Z ext{-peak, variable jet number, jet-jet topology]}}$ 





...

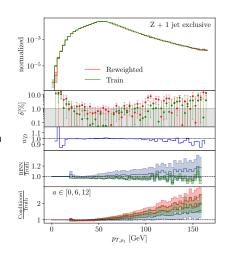
#### ML-event generators

IL examples S
ncertainties tr

- speed up generation ship events train on MC plus data useful ML-playground detector simulation next
- $\cdot \ \textit{Z}_{\mu\mu} + \{\text{1},\text{2},\text{3}\} \text{ jets}$

#### Control through discriminator

- · classification easier than generation
- · output D = 0(generator), 1(truth)
- · decent generator training  $D \approx 0.5$
- · additional event weight  $w_D = \frac{D}{1-D}$
- → Control & reweight

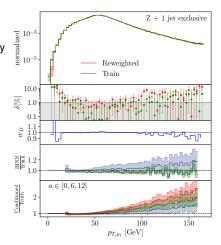




### Uncertain precision generator

#### Uncertainties from Bayesian INN

- learned phase space density plus uncertainty over phase space
- · useful after control step
- · low statistics means large uncertainty
- $\rightarrow \mbox{ Training-related error bars}$





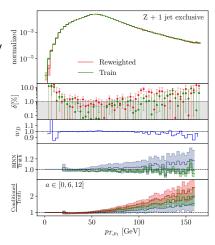
- · learned phase space density plus uncertainty over phase space
  - · useful after control step
- low statistics means large uncertainty
- → Training-related error bars

#### Systematic uncertainties

data augmentation

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

- training conditional on a uncertainty from sampling a
- · correlation to all of phase space
- Network for LHC standards





#### LHC Data Science

Tilman Plehn

### Learning background only

### Unsupervised classification

Unsupervised classification

 anomaly searches [autoencoder] train on background only extract unknown signal

- · reconstruct typical QCD jet
- · non-QCD jets hard to describe

⇒ Problem with complexity





Anomalies

#### Learning background only

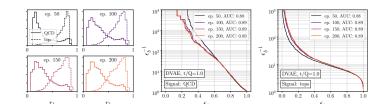
# 1@40x40 10@40x40 10@20x20 5@20x20 400 100 100 400 5@20x20 5@40x40 10@40x40 10@40x40 10@40x40

#### Unsupervised classification

- anomaly searches [autoencoder] train on background only extract unknown signal
- · reconstruct typical QCD jet
- · non-QCD jets hard to describe
- ⇒ Problem with complexity

#### Autoencoder magic

- anything goes@LHC
- · symmetric performance  $S \leftrightarrow B$ ?
- · identify BSM in latent space
- ⇒ LHC solutions needed...





## LHC Data

Unsupervised classification

Learning background only

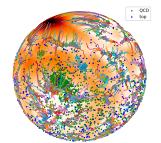
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#### Autoencoder magic

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- · symmetric performance  $S \leftrightarrow B$ ?
- · identify BSM in latent space
- ⇒ LHC solutions needed...







Symbolic rea

### Optimal observables

#### Measure model parameter $\theta$ optimally

· single-event likelihood

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

· expanded in  $\theta$  around  $\theta_0$ , define score

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

· leading order parton level

$$p(x|\theta) \approx |\mathcal{M}|_0^2 + \theta |\mathcal{M}|_{\text{int}}^2 \qquad \Rightarrow \qquad t(x|\theta_0) \sim \frac{|\mathcal{M}|_{\text{int}}^2}{|\mathcal{M}|_2^2}$$



#### Optimal observables

Tilman Plehn

Measure model parameter  $\theta$  optimally

ML example

Symbolic rea

· single-event likelihood

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

Uncertainties

Anomalies

· expanded in  $\theta$  around  $\theta_0$ , define score

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

leading order parton level

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

#### **CP-violating Higgs production**

· unique CP-observable

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

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





Symbolic rea

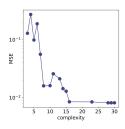
#### Analytic formula for score

- · function to approximate  $t(x|\theta)$
- · phase space parameters  $x_{p}=p_{T}/m_{H},\Delta\eta,\Delta\phi$  [node]
- $\cdot \ \, \text{operators} \quad \sin x, x^2, x^3, x+y, x-y, x*y, x/y \quad \text{\tiny [node]}$
- · represent formula as tree [complexity = number of nodes]
- ⇒ Figures of merit

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

#### Score around Standard Model

compl	dof	function	MSE
3	1	$ a \Delta \phi $	$1.30\cdot 10^{-1}$
4	1	$\sin(a\Delta\phi)$	$2.75 \cdot 10^{-1}$
5	1	$a\Delta\phi x_{p,1}$	$9.93\cdot10^{-2}$
6	1	$-x_{p,1}\sin(\Delta\phi+a)$	$1.90 \cdot 10^{-1}$
7	1	$(-x_{p,1}-a)\sin(\sin(\Delta\phi))$	$5.63\cdot10^{-2}$
8	1	$(a-x_{p,1})x_{p,2}\sin(\Delta\phi)$	$1.61 \cdot 10^{-2}$
14	2	$x_{p,1}(a\Delta\phi - \sin(\sin(\Delta\phi)))(x_{p,2} + b)$	$1.44\cdot 10^{-2}$
15	3	$-(x_{p,2}(a\Delta\eta^2 + x_{p,1}) + b)\sin(\Delta\phi + c)$	$1.30\cdot 10^{-2}$
16	4	$-x_{p,1}(a-b\Delta\eta)(x_{p,2}+c)\sin(\Delta\phi+d)$	$8.50\cdot 10^{-3}$
28	7	$\begin{vmatrix} (x_{p,2} + a)(bx_{p,1}(c - \Delta\phi) \\ -x_{p,1}(d\Delta\eta + ex_{p,2} + f)\sin(\Delta\phi + g) \end{vmatrix}$	$8.18\cdot 10^{-3}$





Symbolic rea

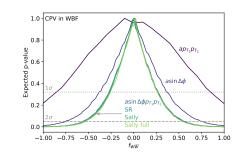
#### Analytic formula for score

- · function to approximate  $t(x|\theta)$
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- · operators  $\sin x, x^2, x^3, x + y, x y, x * y, x/y$  [node]
- · represent formula as tree [complexity = number of nodes]
- ⇒ Figures of merit

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

#### Score around Standard Model

- · expected limits:
  - very wrong formula wrong formula right formula MadMiner
- · same within statistical limitation
- ⇒ New optimal observables next





### LHC Data

Tilman Pl

MI ovamr

Uncertain

Anomalies

Symbolic

## ML for LHC Theory

#### ML-applications in LHC physics

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

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22

23

24

25

· goals are...

Contents

- ...improve established tasks
- ...develop new tools for established tasks
- ...transform through new ideas
- → Turn HL-LHC into fun!

4.3 Unfolding to parton level

5 Synergies, transparency and reproducibility

4.5 Matrix element method

4.4 MadMiner

6 Outlook

References

#### 1 Introduction 2 Machine Learning in event generators 2.1 Phase space sampling 2.2 Scattering Amplitudes 2.3 Loon integrals 2.4 Parton shower 2.5 Parton distribution functions 2.6 Fragmentation functions 3 End-to-end ML-generators 12 3.1 Fast generative networks 3.2 Control and precision 4 Inverse simulations and inference 4.1 Particle reconstruction 4.2 Detector unfolding 17

#### Machine Learning and LHC Event Generation

Asja Butter<sup>1</sup>, Tilman Felm<sup>1</sup>, Steffen Schumann' (Editora), Simon Badjer<sup>1</sup>, Asada Carra<sup>2</sup>, <sup>1</sup>Ng Lennari<sup>2</sup>, <sup>1</sup>Finaces Arma<sup>2</sup>, <sup>1</sup>Ng Lennari<sup>2</sup>, <sup>1</sup>Finaces Carra<sup>2</sup>, <sup>1</sup>Ng Lennari<sup>2</sup>, <sup>1</sup>Finaces Carra<sup>2</sup>, <sup>1</sup>Ng Lennari<sup>2</sup>, <sup>1</sup>Finaces Carra<sup>2</sup>, <sup>1</sup>Ng Lennari<sup>2</sup>, <sup>1</sup>Ng Lennari<sup>2</sup>

Roy Stegeman<sup>11</sup>, Bob Stienen<sup>5</sup>, Jesse Thaler<sup>37</sup>, Rob Verheyen<sup>38</sup>, Daniel Whiteson<sup>18</sup>, Ramon Winterhalder<sup>28</sup>, and Jure Zupan<sup>19</sup>

#### Abstract

Fire-principle simulations are at the heart of the high-energy physics research programs. They link the vat data output of multi-purpose detectors with undamental theory predictions and interpretation. This review illustrates a wide range of applications of modorized machine in the properties of the properties o

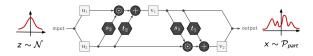
> Submitted to the Proceedings of the US Community Study on the Puture of Particle Physics (Snowmass)

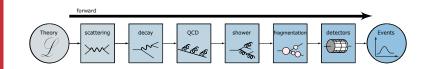


### Modern generative networks

#### Normalizing flows — INN

- Gaussian latent space
- · bijective mapping
- · known Jacobian
- · log-likelihood loss
- $\rightarrow$  Better than VAEs and GANs







LHC Data

Tilman Pleh

Symbolic rea

# Modern generative networks

Normalizing flows — INN

· Gaussian latent space

· bijective mapping

· known Jacobian

· log-likelihood loss

→ Better than VAEs and GANs

#### Bayesian INNs

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



