Modern Machine Learning for Jets

Tilman Plehn

Universität Heidelberg

JetMET, Brussels, May 2023



LHC physics vs data scientist

LHC questions

• How to trigger from 3 PB/s to 300 MB/s?



LHC physics vs data scientist

- · How to trigger from 3 PB/s to 300 MB/s?
 - Data compression [Netflix]



LHC physics vs data scientist

- · How to trigger from 3 PB/s to 300 MB/s?
 - Data compression [Netflix]
- · How to analyze ntuples?



LHC physics vs data scientist

- How to trigger from 3 PB/s to 300 MB/s?
 Data compression [Nettlix]
- How to analyze ntuples?
 Graph neural networks [Car cameras]



LHC physics vs data scientist

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- · How to incorporate symmetries?



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- · How to combine tracker and calorimeter?



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 Super-resolution [Gaming]



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- How to analyse LHC data?
 Simulation-based inference [LHC leading?]
- · But how about uncertatinties?



Shortest ML-intro ever

Fit-like approximation [ask NNPDF]

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

Construction and contol

- $\cdot \,$ minimize loss to find best θ
- $\cdot\,$ typically, likelihood generalizing fit χ^2
- · compare $x o f_{ heta}(x)$ for training/test data

LHC applications

. . . .

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



Analysis

Jet tagging [supervised classification]

- · 'hello world' of LHC-ML
- · end of QCD-taggers
- · powerful NN-architectures
- → ParticleNet & Co established





The Machine Learning Landscape of Top Taggers

 Kasicaia (ed)¹, T. Fisha (ed)², A. Borne², K. Cramer², D. Dobasti⁵, B. M. Dillou¹, M. Birisham⁵, D. A. Foroughy⁵, W. Federich⁵, C. Gay², L. Goniko⁴, J. F. Kanesh^{5,5}, P. T. Koniko⁴, S. Lissi A. Luter⁶, S. Matolaudh, E. M. Mitodire¹, L. Mozel¹, B. Mozel¹, B. Matolaudh^{5,6}, L. Mozel¹, J. Mozel¹, J. Mozel¹, J. Mozel¹, J. Mozel¹, J. Mozel¹, J. Mozel¹, D. Shit⁴, J. W. Tompson¹, and S. Varas¹

Laterate for Dependenciphers, Marcella, Bardong, Corener Bardon C. Honester, Bruck, Yanesh Sankar, Bornes Martin, C. Honester, Bruck, Yanesh Sankar, S



Modern ML ML examples

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 Institut für Experimentalphysik, Universität Hamburg, Germany
 Institut für Theoretische Physik, Universität Heidelberr, Germany 2 Center for Cosmology and Particle Physics and Center for Data Science, NYU, USJ 4 NHECT, Dept. of Physics and Astronomy, Butarra, The State University of NJ, USA 6 Theoretical Particle Physics and Cosmology, King's College London, United Kingdom 10 Center for Theoretical Physics, MIT, Cambridge, USA 11 CP3, Universiteter Cathelique de Louvain, Louvain-le-Neuve, Belgiar 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 LPTHE, CNR5 & Sorbonne Université, Paris, France

16 III. Physics Institute A, IDWTH Aachen University, Germany

Particle flow [classification, super-resolution]

- mother of jet tools
- combined detector channels
- similar studies in CMS
- \rightarrow Seriously impressive





Towards a Computer Vision Particle Flow *

Francesco Armando Di Bello^{6,3}, Sanmay Gangaly^{5,1}, Eilam Gross¹, Marumi Kado^{3,4}, Michael Pitt², Lorenzo Santi³, Jonathan Shlomi

Weizmann Institute of Science, Rohavot 76100, Ismel ²CERN, CH 1211, Geneva 23, Switzerland *CERN, CH 1211, Geneva 23, Switzerland ¹Università di Roma Sapienza, Piazza Aldo Moro, 2, 60185 Roma, Italy e INFN, Italy ⁴Università Paris-Saclav, CNRS/INIP3, IJCLab, 91405, Osav, 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 $\pi^0 \rightarrow \gamma \gamma$ is resolved by a 32×32 granularity layer.



Symmetries

Learning symmetries [representation, visualization]

- · (particle) physics is all symmetries
- · identify symmetries in 2D systems [paintings]
- \rightarrow NN-identified symmetries



Symmetry meets A

Galaxiek Barenheim", Julaanses Birn", and Versinius $\operatorname{Ham}^{n,k}$.

Department de Plaise Televis and IPE, Determint de Talewis-OSE, K.(120), Berjasol, Apain and

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Nature. The discovery of a symmetry signifies the rule, wave of a bandworld principle and manifests irod' in the laws of physical laws and polytom as to divised from heaves bandworld laws of Popolyton ran to divised from recoupling in the state of the state of the symmetry of recoupling in the state of the state of the state of the recoupling in the state of the state of the state of the relationship of the state of the state of the state of the relationship of the state of the st



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Symmetry



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Symmetry i

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s $\operatorname{Sam}^{n,1}$

Department de Flaiss Teiries and IFE, Determint de Talbacis.COE, K.(138), Berjasol, Spain and

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Symmetric networks [contrastive learning, transformer network]

- · rotations, translations, permutations, soft splittings, collinear splittings
- · learn symmetries/augmentations
- → Symmetric latent representation







Symmetries, Safety, and Self-Supervision

Barry M. Dillon¹, Gregor Kasieczka², Hans Olsehlager¹, Tikman Pieka¹, Peter Sorrenson³, and Lorenz Vogel¹

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

August 11, 2021

Abstract

Califies another from the duffunge of duffung a regressration of high-dimensional data, such that high-duff assumeria are assumed in the discriminating informs are vertained, and the duffe of representation in an exploying squarkit. We intersisten ACCLR is only the manying from low-duff of alta to spitzbin discrimination through of dufferentiation of the low dufferentiation in the dufferentiation of the duffer



Anomalous jets and parton densities

Anomaly searches [unsupervised training]

- · train on QCD-jets, SM-events
- · look for non-QCD jets, non-SM events
- \rightarrow LHC spirit, more later

Better Latent Spaces for Better Autoencoders

Barry M. Dillos¹, Tilman Picho², Christol Sauer², and Peter Sorrease²,

1 Institut für Theoretische Physik, Universität Beideberg, Germany 2 Physikalisches Institut, Universität Beideberg, Germany 2 Beideberg Collaboratory für Image Processing, Universität Beideberg, Germany

April 20, 2021

Abstrac

Autoencoders as tools behind assumily sourches as the LBC have the structural problem half by endy work is an effective, arternizing just with higher complexity just and the other way arrends. To address this, we derive chasilien from the hietent space of (matrixed) as consorders, specifically is Gaussian and interior and Dirichlet hietent appendix the Dirichlet structure. The Dirichlet structure.





Modern ML ML examples

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ada Recent Dehendes Documents - For the public

NNPDF/N3PDF parton densities [full blast]

· starting point: pdfs without functional ansatz

Abstract

April 20, 2021

Astarmoulers as tools helped anomaly searches at the LHC have the structural medden th they only work in one direction, extracting jots with higher complexity but not the other

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

A data-based parametrization of parton distribution functions

Stefano Carrama^{12,0}, Jana Cran-Martinez¹, and Boy Stepman TIF Lab, Diparticuento di Finica, Università degli Studi di Milano and INFN Sectore di Milano

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

PACS. 12.38-1 Quantum chromodynamics - 12.39-n Phenomenological cands models - 85.35.+1 Neural





Faster event generators

Tilman Plehn

ML motivation
ML examples
Regression
Classification
Inference
Resilience

Speeding up Sherpa and MadNIS [phase space sampling]

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

→ ML-Multichannel-Vegas



			Submission
IRMP-013-22-56	MONET 22-2	D, FERMEN	a 158-22-915

MadNIS - Neural Multi-Channel Importance Sampling

Theo Heimel¹, Ramon Winnerhalder², Anja Burne^{1,3}, Joshun Isaacon⁶, Chrafius Krause¹, Johio Mahoni^{2,5}, Olivier Marrelae², and Tilman Piehn¹

1 Institut für Theoremischer Physik, Universitä Heidelberg, Germany 2 GPG, Universitä ethologies de Loravin, Loussie holtener, Reighims 3 199485, Sorthonou Universitä, Universitä Paris Cala, CNSS(NSPA), Paris, Parase Honorical Physics Iolisios, Fenni Statistad Accelerator, Lidossang Inatusia, II, US Stipartinessa of Pacias a Auranoemis, Universitä di Bulogas, Italy ramon adventuballer gluciaryunis ho Pacias and Pacias and

Abstract

Theory predictions for the UIC require protein mumerical phase-space integration and premerisor of unweighted worms, the combine matchine-laward multi-charado unighted with a neuralizing flow for importance sampling, as improve disastical methods for an methcal integration. We develop an efficient bi-directual steep hand on an inverteble network, combining ealine and buffred training for potentially separative integrateds. We illustrate our methch for the Direct-Ray process with an addisional neuron measance.

Post Physics	Submissic

SciPost Phy MCNET-2

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

K. Dassiger¹, T. Jasfen², S. Schumann³, F. Siegert¹

Institut für Keen- und Teikhenphysik, TU Dossien, Dossien, Germany
 Institut für Theoretische Physik, Georg-August-Universit
 Güttigen, Gättigen, Germany

September 27, 2001

Ubstract

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ML examples Regression Classification Inference Resilience

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	IBMP-0P3-02-56, MONET-02-02, FERMEAR-PUB-02-91
MadNIS	- Neural Multi-Channel Importance Sampling
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1 Instit 2 CP3, 2 LPNHH, Sor 4 Theoretical Ph 5 Dipa	at für Theoretische Physik, Universität Heidelberg, Germany Inivertifiel cathodique de Louvain, Louvain-le-Neures, Belgium hone Universitä, Universitä Partis Cala, CMS(20127), Breit, Prance picz Kristice, Fermi National Accelerator Laboratorg, Buzuria, IL, ES- rimento d'Fucie a Arznoncia, Università d'Rueloga, Italy
	ramon winterhalder@ucloavain.be
Abstract	

presentante or unrecipited works, we contrast machine-sourced musti-mannel weights with a neuralizing flow for importance sampling, so improve disadial methods for mimerical integration. We devolop an efficient hi-directional strap based on an invertible network, combining soliton and buffered training for potentially expansive integrands. We illustrate our method for the brell-bap precess with an additional narrow resenance.

Speeding up amplitudes [phase space regression]

- · loop-amplitudes expensive
- · interpolation standard
- → Precision NN-regression, more later





SciPost Physics Subsc

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Abstract

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PREPARED FOR SUBMISSION TO JHEP

IPPP/20/135

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

Joseph Aylott-Bullock^{1,2} Simon Badger' Ryan Moodie'

¹Institute for Particle Physics Phenomenology, Department of Physics, Darhum University, Darhum, DHI 2021, United Kingdom ¹Institute for Data Science, Darhum University, Darhum, DHI 2021, United Kingdom

¹Institute for Data Science, Darham University, Dorbam, DNI IEE, United Eingdom Dipartiments de Fasico and Areadé-Regge Contor, Université de Torino, and DIPN, Sections de Torino, Via P. Gurría 1, I-INDS Torino, Baly

E-well j.p. bulleck8durham.sc.uk, minendavid.badger@mite.it, ryam.i.meedie@durham.ar.uk

Attracts: Madras learning technology has the potential to demandially optimise course prevation and singularity. We consist a bigging the test of anomy structure gravitory and structure by prevation and singularity prevation and singularity and the structure by the prevation of the structure by the structure b



Forward and inverse simulation

Precision NN-generators [INN + Bayesian discriminator]

- · control through discriminator [GAN-like]
- · uncertainties through Bayesian networks
- · phase space prototypical
- → Precision & control



Generative answerks are opening new meanse in fast event ponentiats for the LHC. We show here ponentiates free waterakes can sends porceatively precision for Manamit distributions, here they can be include platicly with distributions, and been the distribution of the the distribution in the system of the strategies of the distribution of the through a hypothesis between the distribution of the the distribution of the the distribution of the





Modern ML ML examples

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Unfolding and inversion [conditional normalizing flows]

shower/hadronization unfolded by jet algorithm

Abstract

per-event probabilistic interpretation over parton-level phase space

- detector/decays unfolded e.g. in tops
- calibrated inverse sampling
- \rightarrow Inverse generation





Modern ML Tilman Plehn ML motivation ML examples Regression

Inference

Resilience

Targeting 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 (N₃ and N₅ 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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Alex Cale University of Amsterdam Arnold a.e.cole@sys.nl syes.3	Sven Krippendorf Sommerfeld Center for Theoretical Physics LMU Munich trippendorf Ophysik . uni-maenchen . de	
Andreas Schachner Centre for Mathematical Sciences University of Cambridge an/28730cam.at.uk	Gary Shia University of Wiscensin-Madison ahts#physics.wisc.edu	
Abr	stract	
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		

Identifying uring theory scans with denied physical properties at low energies requires searching through high-fitnessimal solution squeer - collectively referent to as the wring hardwaye. We highlight that this search problem is amenable to referencement learning and gunited applications. It the context of flaw scans, year as able to result aware frazense (suggesting previously understifted symmetries) in the string theory solvings may end of the strength scanse of the scans, year to identify these features (suggesting previously understifted symmetries) and which we argue its imparative for modeling sampling bias.

Learning formulas [genetic algorithm, symbolic regression]

- · approximate numerical function through formula
- · example: score/optimal observables
- → Useful approximate formulas







Back to the Formula — LHC Edition

Anja Butter¹, Tilman Piehn¹, Nathalio Soybelman¹, and Johann Beehmer²

1 Institut für Theoretische Physik, Universitilt Heidelberg, Germany Center for Data Science, New York University, New York, United States nathalis@acybelman.de

November 16, 2021

Abstract

While neared activates offer an attractive way to numerically exceed functions, actual formation has remain the language of theoretical patricle arrows: we use symbolic regressions trained on matrix-beauced information to extract, for instance, optimal LHC observables. This way we invert the usual similaritor pareling and extract analy historectable formation frame comsentences of the symbol strategies and the symbol strategies and the symbol compared and the symbol strategies and the symbol strategies and the symbol compared and the symbol strategies and the symbol strategies and the symbol symbol strategies and the symbol strategies and the symbol strategies and weak-boom fourism Higgs productions. We then weak not it for the known case of CP-violation in weak-boom fourism Higgs productions.



Modern ML Tilman Plehn ML motivation ML examples Regression Classification

Resilience

Precision regression

Regression as in jet calibration?

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

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

· pull Gaussian?

$$\frac{\textit{A}_{j}(\omega)-\textit{A}_{j}^{\text{truth}}}{\sigma_{j}(\omega)}$$

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





Modern ML Tilman Plehn ML motivation ML examples Regression

Regression Classification Inference

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Precision

· quality of NN-amplitudes

$$\Delta_j = rac{\langle A
angle_j - A_j^{ ext{truth}}}{A_j^{ ext{truth}}}$$

 \rightarrow Beyond fit-like regression





Modern ML Tilman Plehn ML motivation ML examples Regression

- Inference
- Resilience

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m truth}}$$

 \rightarrow Beyond fit-like regression





ML motivation ML examples Regression Classification Inference Resilience

Training on QCD only



Unsupervised classification

- train on background only extract unknown signal from reconstruction error
- \cdot reconstruct QCD jets \rightarrow top jets hard to describe reconstruct top jets \rightarrow QCD jets just simple top-like jet
- · dark-jets complexity: mass drop vs semivisible constituents
- \rightarrow Symmetric performance $S \leftrightarrow B$?



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1/m40x40

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Anomaly score from latent space

 $\begin{array}{rrrr} \cdot \mbox{ VAE } \rightarrow \mbox{ does not work} \\ \mbox{ GMVAE } \rightarrow \mbox{ does not work} \\ \mbox{ density estimation } \rightarrow \mbox{ does not work} \\ \mbox{ Dirichlet VAE } \rightarrow \mbox{ works okay} \end{array}$



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

5@20x20 5@40x40 10@40x40 1@40x40



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Normalized autoencoder [penalize missing features]

- normalized probability loss
- · Boltzmann mapping $[E_{\theta} = MSE]$

$$p_{\theta}(x) = \frac{e^{-E_{\theta}(x)}}{Z_{\theta}}$$
$$L = -\langle \log p_{\theta}(x) \rangle = \langle E_{\theta}(x) + \log Z_{\theta} \rangle$$

- inducing background metric
- $\cdot\,$ small MSE for data, large MSE for model
- · Z_{θ} from (Langevin) Markov Chain
- \rightarrow Proper autoencoder, at last...







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ML motivation ML examples Regression Classification Inference Resilience

Measuring QCD splitting

Conditional INN for inference

 $\begin{array}{lll} & \mbox{ condition } jets \mbox{ with QCD parameters} \\ train & \mbox{ model parameters} \rightarrow \mbox{ Gaussian latent space} \\ test & \mbox{ Gaussian sampling} \rightarrow \mbox{ parameter measurement} \end{array}$

· beyond C_A vs C_F [Kluth etal]

$$\begin{split} P_{qq} &= C_F \left[D_{qq} \frac{2z(1-y)}{1-z(1-y)} + F_{qq}(1-z) + C_{qq}yz(1-z) \right] \\ P_{gg} &= 2C_A \left[D_{gg} \left(\frac{z(1-y)}{1-z(1-y)} + \frac{(1-z)(1-y)}{1-(1-z)(1-y)} \right) + F_{gg}z(1-z) + C_{gg}yz(1-z) \right] \\ P_{gq} &= T_B \left[F_{qq} \left(z^2 + (1-z)^2 \right) + C_{gq}yz(1-z) \right] \end{split}$$

Training

Inference





ML motivation ML examples Regression Classification Inference Resilience

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





ML motivation ML examples Regression Classification Inference Resilience

ML for the LHC

ML-applications

- · just another numerical tool for a numerical field
- $\cdot\,$ 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

 \rightarrow Fun with good old QCD problems

Modern Machine Learning for LHC Physicists

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November 2, 2022

Abstract

Moders mechanic learning in transforming particle physics, faster than we can follow, and bullying its way into our mortical tool lock. Two your essentherm is to reach to use put op tool his development, which mean applying entitying edge methods, and tools in the full array of LLP physics problems. These lecture noise are meant to last allowed with possible. They native that ILLP-specific mortizing and a structure of the physics problem. The top term with the lLP-specific mortizing and a structure of the physics and the



ML motivation ML examples Regression Classification Inference Resilience

Resilient training

Training on simulation, testing on data

- assume a simulation vs data difference [generalization gap] plus, different simulation datasets
- · simple question: how train on several datasets?
- adversarial training? nuisance parameter?
- → Uncertain feature same as main discriminator??

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





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- · lowest uncertainty for Herwig training
- · best calibration for Herwig





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- · lowest uncertainty for Herwig training
- · best calibration for Herwig
- · continuous approach to calibration?
- \rightarrow A hammer looking for nails...

