Machine Learning for the LHC

Tilman Plehn

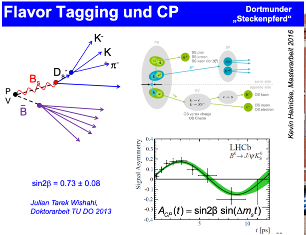
Universität Heidelberg

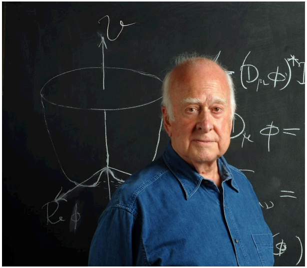
Stuttgart 7/2022

Modern LHC physics

Classic motivation

- dark matter
- baryogenesis
- Higgs VEV





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LHC physics

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

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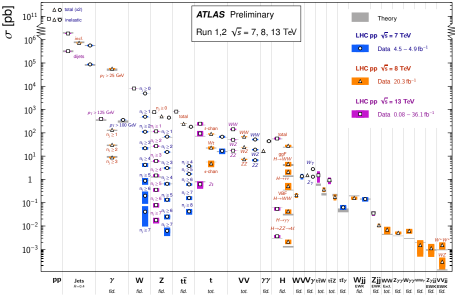
Traditional methods

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



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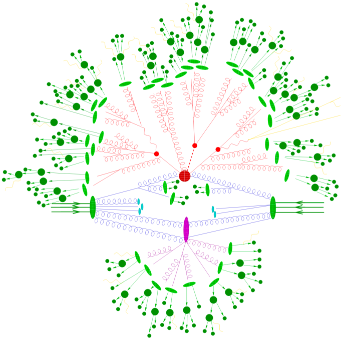
First-principle simulations

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

$\rightarrow$ LHC events in virtual worlds



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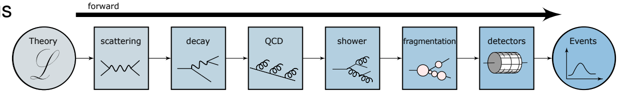
New physics searches

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

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



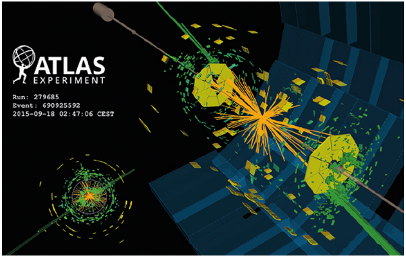
LHC data

Data from ATLAS & CMS

- protons on protons at $E \approx 13000 \times m_p \rightarrow$ relativistic kinematics
- crossing every 25 ns, 40 MHz, 1.6 MB per event $\rightarrow$ 1 PB/s
- frequency vs size

$$\frac{10\ \text{m}}{3 \times 10^8\ \text{m/s}} \approx 3 \times 10^{-8}\ \text{s} = 30\ \text{ns}$$

$\rightarrow$ Big and fast data



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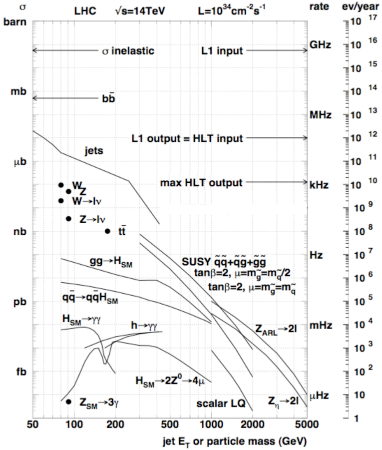
$\to$ Big and fast data

Triggering

- 10^{-6} suppression physics-loss-less
- L1 hardware   40 MHz $\to$ 100 kHz
- L2/HL software $\to$ 3 kHz
- L3 software $\to$ 200 Hz, 320 MB/s



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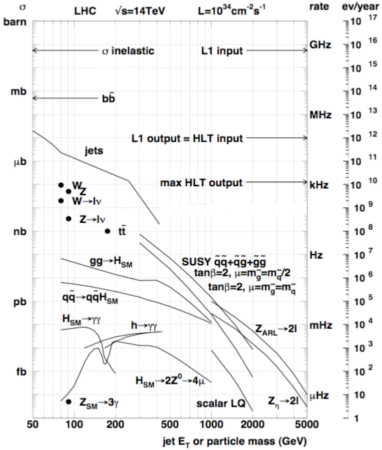

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Strategies

- classic trigger cuts
- probabilistic prescale trigger
- downsized data scouting

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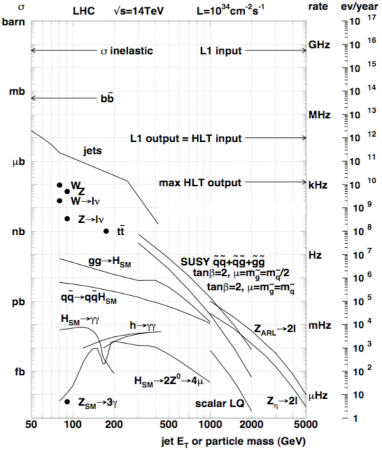
ML-questions

- identification of interesting events?
- identification unexpected events?
- data compression for analyses?

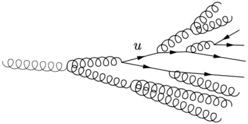


Jets

Partons as QCD jets

- most interactions $q\bar{q}, gg \to q\bar{q}, gg$

$$\sigma_{pp\to jj} \times \mathcal{L} \approx 10^8\,\text{fb} \times \frac{80}{\text{fb}} \approx 10^{10}\ \text{events}$$



- quarks/gluon visible as jets
  splittings described by QCD
  hadronization and hadron decays in jets
- jets as decay products
  67% $W \to jj$ 70% $Z \to jj$ 60% $H \to jj$ 67% $t \to jjj$ 60% $\tau \to j$ ...
- new physics in 'dark jets'
- typical process $pp \to t\bar{t}H + \text{jets} \to bjj\ \bar{b}jj\ b\bar{b} + \text{jets}$

$\to$ Everywhere in LHC physics

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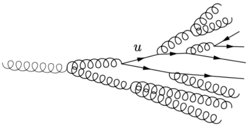

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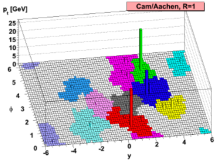
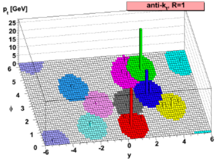


Dealing with jets

- 50-200 constituents per jet
  40 pile-up events on top
- calorimeter + tracking = particle-flow
- jet algorithms returning parton 4-momentum
- sub-jet physics new for LHC



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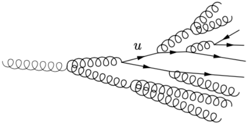

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ML-questions

- fast particle/parton identification?
- data denoising against jet radiation and pileup?
- combination of calorimeter and tracking resolution?
- combination of low-level and high-level observables?

ML-tagging: nothing is ever new

LHC visionaries

- 1991: NN-based quark-gluon tagger

USING NEURAL NETWORKS TO IDENTIFY JETS

Leif LÖNNBLAD*, Carsten PETERSON** and Thorsteinn RÖGNVALDSSON***

Department of Theoretical Physics, University of Lund, Sölvegatan 14A, S-22362 Lund, Sweden

Received 29 June 1990

A neural network method for identifying the ancestor of a hadron jet is presented. The idea is to find an efficient mapping between certain observed hadronic kinematical variables and the quark-gluon identity. This is done with a neuronic expansion in terms of a network of sigmoidal functions using a gradient descent procedure, where the errors are back-propagated through the network. With this method we are able to separate gluon from quark jets originating from Monte Carlo generated e^+e^- events with $\sim 85\%$ approach. The result is independent of the MC model used. This approach for isolating the gluon jet is then used to study the so-called string effect.

In addition, heavy quarks (b and c) in e^+e^- reactions can be identified on the 50% level by just observing the hadrons. In particular we are able to separate b-quarks with an efficiency and purity, which is comparable with what is expected from vertex detectors. We also speculate on how the neural network method can be used to disentangle different hadronization schemes by compressing the dimensionality of the state space of hadrons.

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- 1994: jet-algorithm W/top-tagger

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Searches for new particles using cone and cluster jet algorithms: a comparative study

Michael H. Seymour

Department of Theoretical Physics, University of Lund, Sölvegatan 14A, S-22362 Lund, Sweden

Received 18 June 1993; in revised form 16 September 1993

Abstract. We discuss the reconstruction of the hadronic decays of heavy particles using jet algorithms. The ability to reconstruct the mass of the decaying particle is compared between a traditional cone-type algorithm and a recently proposed cluster-type algorithm. The specific examples considered are the semileptonic decays of a heavy Higgs boson at $\sqrt{s} = 16$ TeV, and of top quark–antiquark pairs at $\sqrt{s} = 1.8$ TeV. We find that the cluster algorithm offers considerable advantages in the former case, and a slight advantage in the latter. We briefly discuss the effects of calorimeter energy resolution, and show that a typical resolution dilutes these advantages, but does not remove them entirely.

except that the invariant mass of a pair is replaced by the transverse momentum of the softer particle relative to the other.

More recently, this algorithm was extended to collisions with incoming hadrons [5], and a longitudinally-invariant $k_\perp$-clustering algorithm for hadron-hadron collisions was proposed [6]. This algorithm has been compared with the more commonly used cone algorithm from the viewpoints of a parton-shower Monte Carlo program [6, 7], and a fixed-order matrix-element calculation [8], and advantages of the cluster algorithm were reported in both cases. This paper is concerned with a comparison between the algorithms for the task of reconstructing the hadronic decays of heavy particles, which was also studied in a preliminary way in [9].

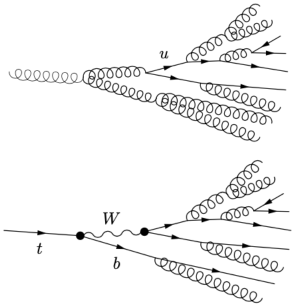
The only as-yet unobserved particles of the minimal Standard Model are the top quark and Higgs boson. The search for, and study of, these particles are among the most important goals of current and planned hadron-

QCD jet representation

Jet constituents

- historically

  only hard parton 4-momentum interesting
  parton content from ‘tagging’
  QCD tests from theory observables



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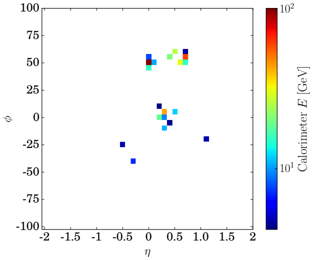
- ML-excitement phase [since 2015]

  data-driven jet analyses
  include as much data as possible
  avoid intermediate high-level variables
  calorimeter output as image



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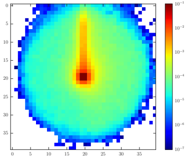
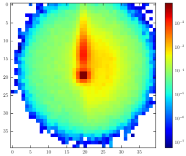
$\rightarrow$ Deep learning = modern networks on low-level observables





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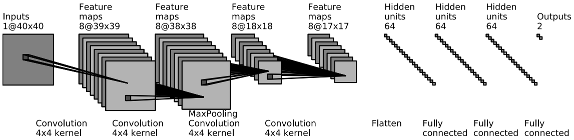
Convolutional network

- image recognition standard ML task
- top tagging on 2D jet images
- 40×40 bins with calorimeter resolution



Physics representation

Networks with 4-vector input

- sparsely filled picture: graph CNN
- physics objects from calorimeter and tracker
- distance measure known from e&m

ML-jet algorithm — combination layer

- input 4-vectors

$$(k_{\mu,i}) = \begin{pmatrix} k_{0,1} & k_{0,2} & \cdots & k_{0,N} \\ k_{1,1} & k_{1,2} & \cdots & k_{1,N} \\ k_{2,1} & k_{2,2} & \cdots & k_{2,N} \\ k_{3,1} & k_{3,2} & \cdots & k_{3,N} \end{pmatrix}$$

- combining them

$$k_{\mu,i} \xrightarrow{\text{CoLa}} \widetilde{k}_{\mu,j} = k_{\mu,i}\; C_{ij} \qquad C = \begin{pmatrix} 1 & 0 & \cdots & 0 & C_{1,N+2} & \cdots & C_{1,M} \\ 0 & 1 & & \vdots & C_{2,N+2} & \cdots & C_{2,M} \\ \vdots & \vdots & \ddots & 0 & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 & C_{N,N+2} & \cdots & C_{N,M} \end{pmatrix}$$

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- combining them $k_{\mu,i} \xrightarrow{\text{CoLa}} \widetilde{k}_{\mu,j} = k_{\mu,i}\, C_{ij}$

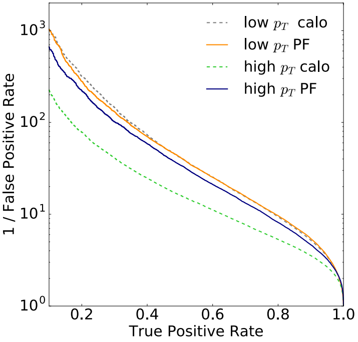
Invariants — Lorentz layer

- DNN on Lorentz scalars

$$\tilde{k}_j \xrightarrow{\text{LoLa}} \hat{k}_j = \begin{pmatrix} m^2(\tilde{k}_j) \\ p_T(\tilde{k}_j) \\ \vdots \end{pmatrix}$$

$\rightarrow$ Learn Minkowski metric

$g = \text{diag}(0.99 \pm 0.02,$
$-1.01 \pm 0.01, -1.01 \pm 0.02, -0.99 \pm 0.02)$



Meet the professionals

A brief history of achievement

- 2014/15: first jet image papers
- 2017: first (working) ML top tagger
- ML4Jets 2017: What architecture works best?
- ML4Jets 2018: Lots of architectures work

→ Jet classification understood and done

SciPost Physics Submission

The Machine Learning Landscape of Top Taggers

G. Kasieczka (ed)[1], T. Plehn (ed)[2], A. Butter[2], K. Cranmer[3], D. Debnath[4], M. Fairbairn[5], W. Fedorko[6], C. Gay[6], L. Gouskos[7], P. T. Komiske[8], S. Leiss[1], A. Lister[6], S. Macaluso[3,4], E. M. Metodiev[8], L. Moore[9], B. Nachman,[10,11], K. Nordström[12,13], J. Pearkes[6], H. Qu[7], Y. Rath[14], M. Rieger[14], D. Shih[4], J. M. Thompson[2], and S. Varma[5]

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April 12, 2019

Abstract

Based on the established task of identifying boosted, hadronically decaying top quarks, we compare a wide range of modern machine learning approaches. We find that they are extremely powerful and great fun.

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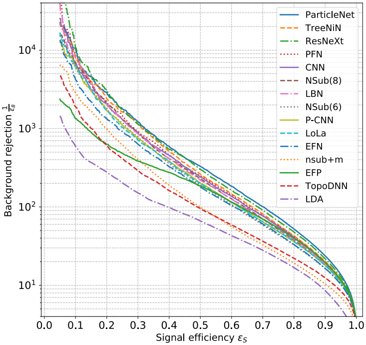

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Path to LHC reality

- application in analyses?
- beyond top and QCD jets?
- uncertainties?
- resilience in experimental reality?
- beyond fully supervised learning?
- from jets to events?
- analyses only ML will allow us to do?

etc

LHC

Tilman Plehn

Motivation

Data

Jets

Simulation

Inference

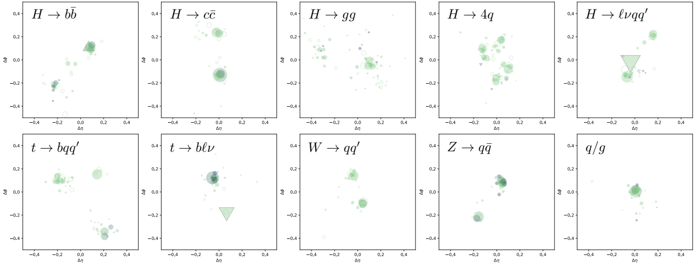
State of the art [Huilin Qu, CMS]

THE NEED FOR A LARGE DATASET

H. Qu, C. Li, S. Qian, arXiv:2202.03772, https://github.com/jet-universe/particle_transformer/

- **JetClass**: a new large-scale public jet dataset
  - 100M jets for training: ~ two orders of magnitude larger than existing public datasets
  - 10 classes: several unexplored scenarios, e.g., H->WW*->4q, H->WW*->ℓvqq, etc.
  - comprehensive information per particle: kinematics, particle ID, track displacement

Simulated w/ MadGraph + Pythia + Delphes



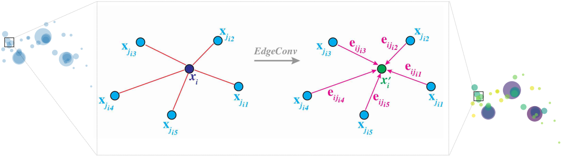
Jet Tagging in the Era of Deep Learning - June 9, 2022 - Huilin Qu (CERN)

State of the art [Huilin Qu, CMS]

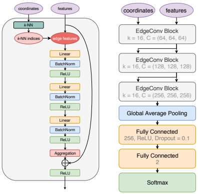
PARTICLENET

H. Qu and L. Gouskos
Phys.Rev.D 101 (2020) 5, 056019

- ParticleNet: jet tagging via particle clouds
  - treating a jet as an **unordered set of particles**, distributed in the $\eta - \phi$ space
  - **graph neural network architecture**, adapted from Dynamic Graph CNN [arXiv:1801.07829]
    - treating a point cloud as a graph: each point is a vertex
      - for each point, a local patch is defined by finding its k-nearest neighbors
    - designing a permutation-invariant "convolution" function
      - define "edge feature" for each center-neighbor pair: $e_{ij} = h_\Theta(x_i, x_j)$
      - aggregate the edge features in a symmetric way: $x_i' = \mathrm{mean}_j\, e_{ij}$



ParticleNet architecture



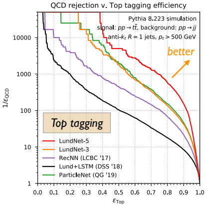
cf. P.T. Komiske, E. M. Metodiev and J. Thaler, *JHEP 01 (2019) 121*;
V. Mikuni and F. Canelli, *Eur. Phys. J. Plus 135, 463 (2020)*; *Mach.Learn.Sci.Tech. 2 (2021) 3, 035027*.

State of the art [Huilin Qu, CMS]

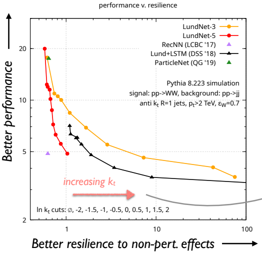
LundNet: Performance

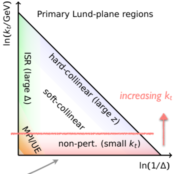
F. Dreyer and H. Qu, JHEP 03 (2021) 052

- LundNet achieves very high performance at significant lower computational cost than ParticleNet
  - due to fewer number of neighbors in a binary tree & static graph structure
- Moreover, LundNet provides a systematic way to control the robustness of the tagger
  - the non-perturbative region can be effectively rejected by applying a k_t cut on the Lund plane



	Number of parameters	Training time [ms/sample/epoch]	Inference time [ms/sample]
LundNet	395k	0.472	0.117
ParticleNet	369k	3.488	1.036
Lund+LSTM	67k	0.424	0.131





* Resilience assessed by applying the model trained on hadron-level samples to parton-level samples and compare the difference

State of the art [Huilin Qu, CMS]

PARTICLE TRANSFORMER

H. Qu, C. Li, S. Qian, arXiv:2202.03772, https://github.com/jet-universe/particle_transformer/

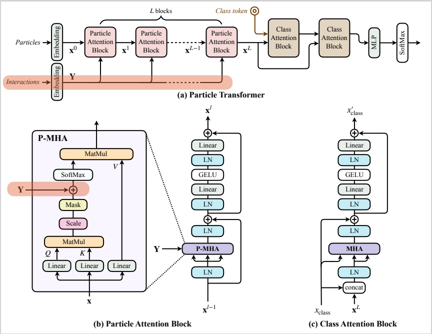
- **Attention mechanism and Transformers**: the new state-of-the-art architecture in ML
  - Large Language Models: BERT, GPT-3, ...
  - Computer Vision: ViT, Swin-T, ...
  - AlphaFold2 for protein structure prediction
- **Particle Transformer (ParT)**
  - Transformer-based architecture for jet tagging
  - injecting physics-inspired pairwise features to "bias" the dot-product self-attention

$$\text{P-MHA}(Q,K,V) = \text{SoftMax}(QK^T/\sqrt{d_k} + \mathbf{Y})V,$$

"Interaction" features

$$\begin{aligned}\Delta &= \sqrt{(y_a - y_b)^2 + (\phi_a - \phi_b)^2},\\ k_\mathrm{T} &= \min(p_{\mathrm{T},a}, p_{\mathrm{T},b})\Delta,\\ z &= \min(p_{\mathrm{T},a}, p_{\mathrm{T},b})/(p_{\mathrm{T},a} + p_{\mathrm{T},b}),\\ m^2 &= (E_a + E_b)^2 - \|\mathbf{p}_a + \mathbf{p}_b\|^2,\end{aligned}$$

and more...



Simulation

Event generation

- start from Lagrangian

$$\mathcal{L} = \sum_q \overline{\psi}_q \left(i\gamma^\mu \partial_\mu - m - gG_\mu \right) \psi_q - \frac{1}{4} G_{\mu\nu} G^{\mu\nu} + \ldots - \mu^2 |\phi|^2 - \lambda |\phi|^4$$

- total rate for proton-proton collisions

$$\sigma_{\text{tot}} = \int_0^1 dx_1 \int_0^1 dx_2 \sum_{\text{partons } ij} f_i(x_1)\, f_j(x_2)\, \hat{\sigma}_{ij}(x_1 x_2 E^2)$$

- simulation factorized by energy
- Monte Carlo generation, LO or NLO in QCD
- production process particle decays
  QCD jet radiation
  QCD showering
  fragmentation/hadronization

$\rightarrow$ Theory task
Pythia, Madgraph, Sherpa, Herwig

Machine Learning and LHC Event Generation

Anja Butter[1,2], Tilman Plehn[1], Steffen Schumann[3] (Editors),
Simon Badger[4], Sascha Caron[5, 6] Kyle Cranmer[7,8], Francesco Armando Di Bello[9],
Etienne Dreyer[10], Stefano Forte[11], Sanmay Ganguly[12], Dorival Gonçalves[13], Eilam Gross[10],
Theo Heimel[1], Gudrun Heinrich[14], Lukas Heinrich[15], Alexander Held[16], Stefan Höche[17],
Jessica N. Howard[18], Philip Ilten[19], Joshua Isaacson[17], Timo Janßen[3], Stephen Jones[20],
Marumi Kado[9,21], Michael Kagan[22], Gregor Kasieczka[23], Felix Kling[24], Sabine Kraml[25],
Claudius Krause[26], Frank Krauss[20], Kevin Kröninger[27], Rahool Kumar Barman[13],
Michel Luchmann[1], Vitaly Magerya[14], Daniel Maitre[20], Bogdan Malaescu[2],
Fabio Maltoni[28,29], Till Martini[30], Olivier Mattelaer[28], Benjamin Nachman[31,32],
Sebastian Pitz[1], Juan Rojo[33,34], Matthew Schwartz[35], David Shih[25], Frank Siegert[36],
Roy Stegeman[11], Bob Stienen[5], Jesse Thaler[37], Rob Verheyen[38], Daniel Whiteson[18],
Ramon Winterhalder[28], and Jure Zupan[19]

Abstract

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

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

Simulation

Event generation

- start from Lagrangian

$$\mathcal{L} = \sum_q \overline{\psi}_q \left(i\gamma^\mu \partial_\mu - m - gG_\mu \right) \psi_q - \frac{1}{4} G_{\mu\nu} G^{\mu\nu} + \dots - \mu^2 |\phi|^2 - \lambda |\phi|^4$$

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Contents

Simulation

Detector simulation

- process-independent response function
  millions of output channels
- full MC simulation Geant4
  lepton/pion/photon shower in matter
  built from detector plans
- fast detector simulation
  Gaussian approximation of response

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Detector simulation

- process-independent response function
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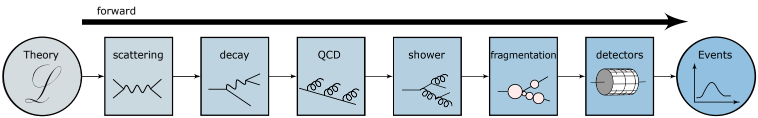
ML-questions

- fast and precise surrogates for individual steps?
- full phase space coverage?
- full feature mapping?
- variable-dimensional and high-dimensional phase spaces?
- improved data- and theory-driven models?



Likelihood-based inference

Unlabeled likelihood ratio [CWoLa]

- Neyman-Pearson lemma: LR optimal discriminator
- likelihood ratio for event samples

$$\text{LR}(x) = \frac{p(x|H_{S+B})}{p(x|H_B)} = \frac{\text{Pois}(n|s+b)\ \Pi_{j=1}^n f_{S+B}(x_j)}{\text{Pois}(n|b)\ \Pi_{j=1}^n f_B(x_j)} = e^{-s} \left(\frac{s+b}{b} \right)^n \frac{\Pi_j f_{S+B}(x_j)}{\Pi_j f_B(x_j)}$$

- additive log-likelihood ratio

$$\text{LLR}(x) = -s + \sum_j \log \left(1 + \frac{s f_S(x_j)}{b f_B(x_j)} \right)$$

- LLR from simulation and/or classifier

Likelihood-based inference

Unlabeled likelihood ratio [CWoLa]

- Neyman-Pearson lemma: LR optimal discriminator
- problem no signal and background samples to train on
  instead samples p_j with signal fractions f_j and background fractions $1 - f_j$
- phase space densities

$$\begin{pmatrix} p_1(x) \\ p_2(x) \end{pmatrix} = \begin{pmatrix} f_1 & 1 - f_1 \\ f_2 & 1 - f_2 \end{pmatrix} \begin{pmatrix} p_S(x) \\ p_B(x) \end{pmatrix}$$

$$\Leftrightarrow \qquad \begin{pmatrix} p_S(x) \\ p_B(x) \end{pmatrix} = \frac{1}{f_1 - f_2} \begin{pmatrix} 1 - f_2 & f_1 - 1 \\ -f_2 & f_1 \end{pmatrix} \begin{pmatrix} p_1(x) \\ p_2(x) \end{pmatrix}$$

- goal: train classifier to extract

$$\frac{p_S(x)}{p_B(x)} = \frac{(1 - f_2)p_1(x) + (f_1 - 1)p_2(x)}{-f_2 p_1(x) + f_1 p_2(x)}$$

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- trick: train classifier for

$$\frac{p_1(x)}{p_2(x)} = \frac{f_1 p_S(x) + (1-f_1)p_B(x)}{f_2 p_S(x) + (1-f_2)p_B(x)} = \frac{f_1 \dfrac{p_S(x)}{p_B(x)} + 1 - f_1}{f_2 \dfrac{p_S(x)}{p_B(x)} + 1 - f_2}$$

$$\frac{d}{d(p_S/p_B)} \frac{p_1(x)}{p_2(x)} = \frac{f_1 \left[f_2 \dfrac{p_S(x)}{p_B(x)} + 1 - f_2 \right] - f_2 \left[f_1 \dfrac{p_S(x)}{p_B(x)} + 1 - f_1 \right]}{\left[f_2 \dfrac{p_S(x)}{p_B(x)} + 1 - f_2 \right]^2} = \frac{f_1 - f_2}{\left[f_2 \dfrac{p_S(x)}{p_B(x)} + 1 - f_2 \right]^2}$$

$\rightarrow$ Apply mixed instead of pure classifier

Likelihood-based inference

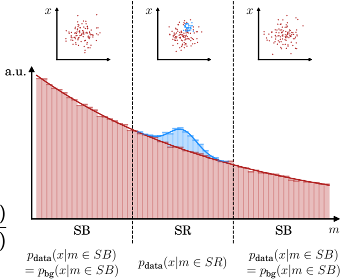
Impoved bump hunts [CWoLa, Anode, Cathode]

- bump hunt in m
  orthogonal information in x

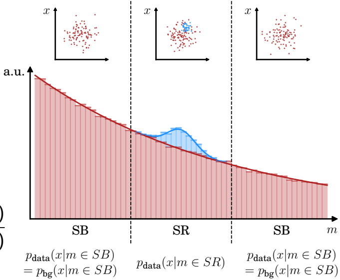
1. CWola on SB and SR samples

$$\frac{x \sim p_\text{data}(x|m \in SR)}{x \sim p_\text{data}(x|m \in SB)} \xrightarrow{\text{class}} \frac{p_{S+B}(x)}{p_B(x)} \to \frac{p_S(x)}{p_B(x)}$$

- but problem with correlations in m and x



Likelihood-based inference



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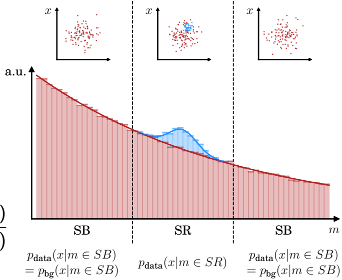
2. density estimation through normalizing flow

$$p_\text{model}(x|m \in SB) \xrightarrow{\text{interpol}} p_\text{model}(x|m \in SR)$$

- computable LR in signal regions

$$\text{LR}(x) = \frac{p_\text{data}(x|m \in SR)}{p_\text{model}(x|m \in SR)} \sim \frac{p_{S+B}(x)}{p_B(x)}$$

Likelihood-based inference



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3. background generation using normalizing flow

$$p_{\text{model}}(x|m \in SB) \xrightarrow{\text{sample}} x \sim p_{\text{model}}(x|m \in SR)$$

- classifier on event samples

$$\frac{x \sim p_{\text{model}}(x|m \in SR)}{x \sim p_{\text{model}}(x|m \in SB)} \xrightarrow{\text{class}} \frac{p_{S+B}(x)}{p_B(x)}$$

$\to$ Guess which works best?

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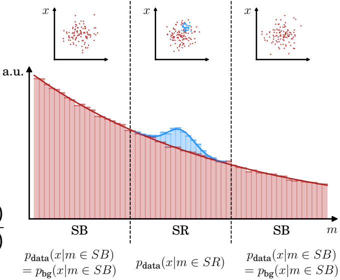

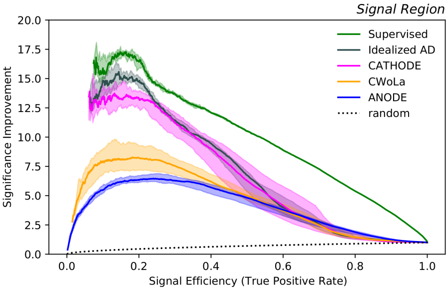

ML-Parton densities

Dirty LHC secret

- proton-proton collisions from parton-parton predictions $[x = E_{\text{parton}} / E_{\text{proton}}]$

$$\sigma_{\text{tot}} = \int_0^1 dx_1 \int_0^1 dx_2 \sum_{\text{partons } ij} f_i(x_1)\, f_j(x_2)\, \hat{\sigma}_{ij}(x_1 x_2 E^2)$$

- DGLAP equation, including factorization scale μ

$$\frac{df_i(x,\mu)}{d\log\mu^2} = \sum_{\text{partons} j} \int_x^1 \frac{dz}{z} \frac{\alpha_s}{2\pi} P_{i\leftarrow j}(z)\, f_j\left(\frac{x}{z},\mu\right) = \frac{\alpha_s}{2\pi} \sum_j \left(P_{i\leftarrow j} \otimes f_j\right)(x,\mu)$$

- historic parametrization

$$f_i(x,\mu_0) = a_0 x^{a_1} (1-x)^{a_2} e^{a_3 x + a_4 x^2}$$

$\to$ WTF... $\to$ lattice gauge theory?

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Non-parametric network fit

- parametrizations not useful
- bias problematic

$\to$ NNPDF

hep-ph/0204232
GeF/TH/3-02
RM3-TH/02-01

Neural Network Parametrization of Deep–Inelastic Structure Functions

Stefano Forte[a], Lluís Garrido[b], José I. Latorre[b] and Andrea Piccione[c]

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Via della Vasca Navale 84, I-00146 Rome, Italy

[b]Departament d'Estructura i Constituents de la Matèria, Universitat de Barcelona,
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[c]INFN sezione di Genova and Dipartimento di Fisica, Università di Genova,
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Abstract

We construct a parametrization of deep–inelastic structure functions which retains information on experimental errors and correlations, and which does not introduce any theoretical bias while interpolating between existing data points. We generate a Monte Carlo sample of pseudo–data configurations and we train an ensemble of neural networks on them. This effectively provides us with a probability measure in the space of structure functions, within the whole kinematic region where data are available. This measure can then be used to determine the value of the structure function, its error, point–to–point correlations and generally the value and uncertainty of any function of the structure function itself. We apply this technique to the determination of the structure function F_2 of the proton and deuteron, and a precision determination of the isotriplet combination F_2[p-d]. We discuss in detail these results, check their stability and accuracy, and make them available in various formats for applications.

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$\to$ WTF... $\to$ lattice gauge theory?

Non-parametric network fit

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- bias problematic

$\to$ NNPDF

6 Summary

We have presented a determination of the probability density in the space of structure functions for the structure function F_2 for proton, deuteron and nonsinglet, as determined from experimental data of the NMC and BCDMS collaborations. Our results, for each of the three structure functions, take the form of a set of 1000 neural nets, each of which gives a determination of F_2 for given x and Q^2. The distribution of these functions is a Monte Carlo sampling of the probability density. This Monte Carlo sampling has been obtained by first, producing a sampling of the space of data points based on the available experimental information through a set of Monte Carlo replicas of the original data, and then, training each neural net to one of these replicas.

In practice, all functions are given by a FORTRAN routine which reproduces a feed–forward neural network (described in Section 3) entirely determined by a set of 47 real parameters. Each function is then specified by the set of values for these parameters. Our results are available at the web page `http://sophia.ecm.ub.es/f2neural/`. The full set of FORTRAN routines and parameters can be downloaded from this page. On–line plotting and computation facilities for

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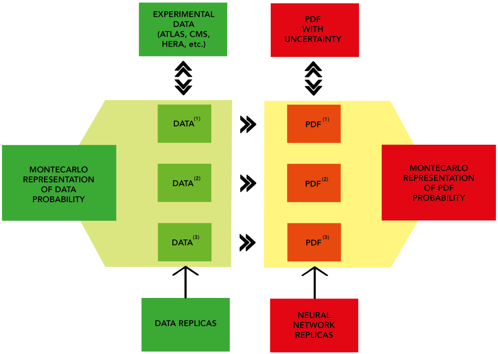
State of the art [Stefano Forte, NNPDF]

THE FUNCTIONAL MONTE CARLO

REPLICA SAMPLE OF FUNCTIONS ⇔ PROBABILITY DENSITY IN FUNCTION SPACE
KNOWLEDGE OF LIKELIHHOD SHAPE (FUNCTIONAL FORM) NOT NECESSARY



FINAL PDF SET: $f_i^{(a)}(x,\mu)$;
i =up, antiup, down, antidown, strange, antistrange, charm, gluon; $j = 1, 2, \ldots N_{\text{rep}}$

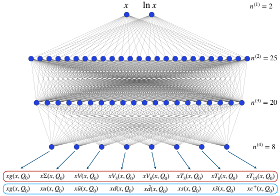
State of the art [Stefano Forte, NNPDF]

THE ML METHODOLOGY

HYPEROPTIMIZED PARAMETERS

Parameter	NNPDF4.0	L as in Eq. (3.21)	Flavour basis Eq. (3.2)
Architecture	25-20-8	70-50-8	7-26-27-8
Activation function	hyperbolic tangent	hyperbolic tangent	sigmoid
Initializer	glorot_normal	glorot_uniform	glorot_normal
Optimizer	Nadam	Adadelta	Nadam
Clipnorm	6.0×10^{-6}	5.2×10^{-2}	2.3×10^{-5}
Learning rate	2.6×10^{-3}	2.5×10^{-1}	2.6×10^{-3}
Maximum # epochs	17×10^{3}	45×10^{3}	45×10^{3}
Stopping patience	10% of max epochs	12% of max epochs	16% of max epochs
Initial positivity $\Lambda^{(\mathrm{pos})}$	185	106	2
Initial integrability $\Lambda^{(\mathrm{int})}$	10	10	10

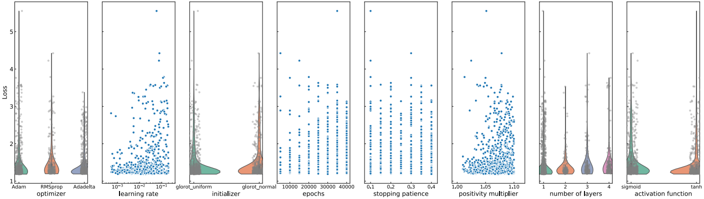
NN ARCHITECTURE



- HYPEROPT ADAPTS TO EXTERNAL CHOICES (E.G. PARAMETRIZATION BASIS)
- SIMILAR RESULTS CAN BE OBTAINED WITH RATHER DIFFERENT SETTINGS
- ~ 800 FREE PARAMETERS

State of the art [Stefano Forte, NNPDF]

FITTING THE METHODOLOGY
HYPEROPTIMIZATION SCANS



HYPEROPT PARAMETERS

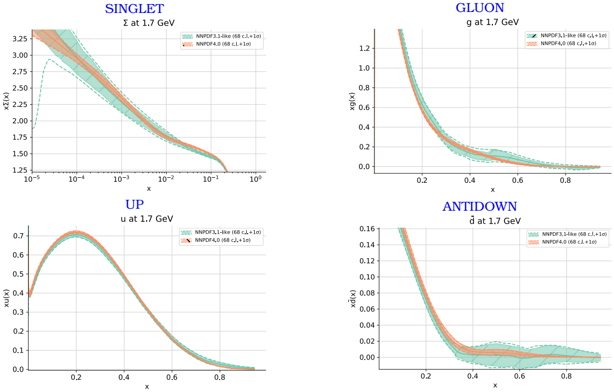
Neural Network	Fit options
Number of layers (*)	Optimizer (*)
Size of each layer	Initial learning rate (*)
Dropout	Maximum number of epochs (*)
Activation functions (*)	Stopping Patience (*)
Initialization functions (*)	Positivity multiplier (*)

- SCAN PARAMETER SPACE
- OPTIMIZE FIGURE OF MERIT: VALIDATION χ^2
- BAYESIAN UPDATING

State of the art [Stefano Forte, NNPDF]

NNPDF4.0 vs. NNPDF3.1

- FULL BACKWARD COMPATIBILITY
- SUBSTANTIAL REDUCTION IN UNCERTAINTY



ML-LHC introduction

Summary

- particle physics has questions
- LHC is big and fast data
- data needs regression and classification
- knowledge comes through theory and simulation
- stochastic data and uncertainty craziness

Outlook

1. introduction (done)
2. uncertainties and Bayesian networks [TP]
3. generation and inversion [AB]
4. tutorial/hands-on fun [AB]
5. favorite cool ideas [AB,TP]