KNO-scaling of charged hadron multiplicities within a Machine Learning based approach

Universidad Nacional Autónoma de México Instituto de Ciencias Nucleares - Seminar

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arXiv:2111.15655 arXiv:2210.10548 arXiv:2303.05422







1950: Alan Turing creates the "Turing Test"

1957: Frank Rosenblatt: the first neural network for computers (the **perceptron**), which simulate the thought processes of the human brain.

1959: Arthur Samuel, IBM: Machine Learning

1967: The first general, working learning algorithm for supervised, deep, feedforward, multilayer perceptrons by A. G. Ivakhnenko and V. G. Lapa

1986: First mention of Deep Learning by Rina Dechter (Learning While Searching in Constraint-Satisfaction Problems)

1989: Yann LeCun et al: standard backpropagation algorithm for recognizing handwritten ZIP codes on mail

1997: "A computer program is said to learn from experience **E** with respect to some class of tasks **T** and performance measure **P** if its performance at tasks in **T**, as measured by **P**, improves with experience **E**." - Tom M. Mitchell: Machine Learning

1997: IBM's Deep Blue beats Garri Kaszparov (the world champion at chess). Computing capacity: 11.38 GFLOPS, TOP500: 259th (comparison: Nvidia RTX 4090: 82.6 TFLOPS)





https://researcher.watson.ibm.com/researcher/view_page.php?id=6814





2009: ImageNet by prof. Fei-Fei Li a database of 14 million labeled images in 2009

- 2011: IBM's Watson: winner of game show Jeopardy!
- 2011: Google Brain: cats in Youtube videos
- 2012: AlexNet by Alex Krizhevsky: first CNN
- 2013: Word2vec algorithms: foundations for language models
- 2014: DeepFace by Facebook
- 2014: Generative adversarial networks (GAN) by Ian Goodfellow
- 2016: AlphaGo by Deepmind
- 2016: Face2Face (baseline for 'DeepFake')
- 2017: Waymo: first self-driving car company to operate without human intervention
- 2018: AlphaFold by Deepmind

2020: GPT-3 by OpenAI to generate human-like text. Trainable parameters: **175 billion**











CNN (image classification, object detection, recommender systems)...

Recurrent/recursive neural networks (RNNs): Sequence modeling, next word prediction, translating sounds to words, human language translation...

Generative models: anomaly detection, pattern recognition, reinforced learning



Various frameworks for training and inference:



Motivaton - data, data, more data

Autonomous driving Medical imaging Predictive maintenance Anomaly detection, fake news detection Search of BSM physics Stock price prediction Natural Language Processing Virtual Assistants Virtual reality Colorization of Black and White Images Content generation, examples:

https://infiniteconversation.com/ https://huggingface.co/spaces/stabilityai/stable-diffusion Robotics

Expression Encodin

Noise $\epsilon \mu + \epsilon \cdot \sigma$

-

Expressi Code



Motivaton - data, data, more data



Worldwide LHC Computing Grid



2016

128 GB

Micron

1TB ## V30

2006

128 MB

2020

1 TB

LHC in numbers: 2013 and now:

| ata: | 15 PB/year | VS | 200+ PB/year |
|-------|------------|----|--------------|
| ape: | 180 PB | VS | 740+ PB |
| isk: | 200 PB | VS | 570+ PB |
| IS06: | 2M | VS | 100+ B |

Storing and distributing the data is only one side of the challange

\rightarrow analysis, simulations







Approaches



Main ingredients

Perceptrons:

- Input value(s) ٠
- Weight: the connection between the units •
- Bias: the intercept added in a linear equation ٠

Softplus

 $y = ln(1+e^{x})$

Mish

Activation Function





Other important components: pooling layers, regularization and normalization, recurrent layers...

https://sefiks.com/2020/02/02/dance-moves-of-deep-learning-activation-functions/

Main ingredients



Main ingredients

The *learning* part: optimizing "somehow" the weights (Curse of dimensionality)

Loss function:

$$\mathcal{L} = \frac{1}{n} \sum_{i} (y_i - f(x_i))^2 := \frac{1}{n} \sum_{i} (y_i - (mx_i + b))^2$$

The gradient descent method:

- 1) Start with random weights
- 2) Evaluate the loss
- 3) Figure out which direction the loss function steeps downward the most (with respect to changing the parameters)

4) Repeat from 2)

Gradient of the loss function with respect to all of the parameters

$$\frac{\partial \mathcal{L}}{\partial m} = \frac{2}{n} \sum_{i} x_{i} \cdot (y_{i} - (mx_{i} + b)) \qquad \qquad m := m - \alpha \cdot \frac{\partial \mathcal{L}}{\partial m}$$
$$\frac{\partial \mathcal{L}}{\partial b} = \frac{2}{n} \sum_{i} (y_{i} - (mx_{i} + b)) \qquad \qquad b := b - \alpha \cdot \frac{\partial \mathcal{L}}{\partial b}$$





Input

Stacking more layers: solve complex problems more efficiently, get highly accurate results **BUT**:

Vanishing/exploding gradients

ResNet: Residual blocks with "skip connections" (SOTA image classifier of 2015)

3x3 conv. N⊧ Batch norm. ReLU 3x3 conv. N⊧ Batch norm. ReLU



A Living Review of Machine Learning for Particle Physics

https://iml-wg.github.io/HEPML-LivingReview/

Matthew Feickert, Benjamin Nachman, arXiv:2102.02770

2021 May: 417 references 2021 November: 568 references 2022 October: 724 references

Today: **759** references

- Track reconstruction
- Quark/gluon jet separation
- Jet reconstruction
- Tuning Monte Carlo event generators
- GAN of detectors

- Particle Track Reconstruction using Geometric Deep Learning Jet tending in the Lund plane with graph petworks (DOI).
- Vertex and Energy Reconstruction in UNO with Machine Learning Methods
- Accelerated Charned Particle Tracking with Graph Neural Networks on EPGA MLPE: Efficient machine-learned particle-flow reconstruction using graph neural pr
- 25th International Conference on Computing in High-Energy and Nuclear Physics emational Conference on Computing in High-Energy and Nuclear Physic
- Graph Neural Network for Otherst Reconstruction in Liquid Argon Time Projection
- Instance Segmentation GNNs for One-Shot Conformal Tracking at the LHC
- Charged particle tracking via edge-classifying interaction networks tation in Heavy Ion Collisions by QCD-Aware Graph N
- Granh Generative Models for Fast Detector Simulations in High Energy Physics
- Segmentation of EM showers for neutrino experiments with deep graph neural networks
- Sets (point clouds)
- Energy Flow Networks: Deep Sets for Particle Jets (DOI)
- ParticleNet: Jet Tagging via Particle Clouds [DOI]
- Secondary Vertex Einding in Jets with Neural Networks
- Equivariant Energy Flow Networks for Jet Tagging Permutationless Many-Jet Event Reconstruction with Sym
- Learning to Isolate Muons
- Point Cloud Transformers applied to Collider Physic
- Physics-Inspired basis
- Automating the Construction of Jet Observables with Machine Learning [DOI] How Much Information is in a Jet? [DOI]
- Novel Jet Observables from Machine Learning (DOI)
- Energy flow polynomials: A complete linear basis for jet substructure [DOI] Deep-learned Top Tagging with a Lorentz Laver (DOI)
- Resurrection \$b/bar/b/b\$ with kinematic abanes

SW/ZS tanging

- Jet-images deep learning edition [DOI]
- Parton Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks [DOI]
- OCD-Aware Recursive Neural Networks for Jet Physics (DOI) Identification of heavy energetic, hartronically decaying particles using a
- Boosted SWS and SZS tagging with let charge and deep learning [DOI]
- Supervised Jet Clustering with Graph Neural Networks for Lorentz Boosted Bosons (DOI)
- Jet tagging in the Lund plane with graph networks [DOI] A \$W^opm\$ polarization analyzer from Deep Neural Network

- Shippinghtarrows hithards (1)

- Automating the Construction of let Obsequables with Machine Learning (DOI)
- Boosting \$H\to b\bar b\$ with Machine Learning [DOI]
- Interaction networks for the identification of boosted \$H vight
- Interpretable deep learning for two-prong jet classification with jet spectra [DOI] Identification of heavy enemetic hadronically decaying particles using machine-lea
- Disentangling Boosted Higgs Boson Production Modes with Machine Learning
- Benchmarking Machine Learning Techniques with Di-Higgs Production at the LH
- The Boosted Higgs Jet Reconstruction via Graph Neural Network
- Extracting Signals of Higgs Boson From Background Noise Using Deep Neural Networks Learning to increase matching efficiency in identifying additional b-jets in the \$\text{(})\bar
- guarks and gluons
- Quark versus Gluon Jet Tagging Using Jet Images with the ATLAS Detector
- Deep learning in color: towards automated guark/gluon [DOI] Recursive Neural Networks in Quark/Gluon Tension (DOI)
- DeepJet: Generic physics object based jet multiclass classification for LHC exp
- · Probing heavy ion collisions using guark and gluon jet substructure
- JEDI-net: a jet identification algorithm based on interaction
- Quark-Gluon Tagging: Machine Learning vs Detector [DOI] Towards Machine Learning Analytics for Jet Substructure [DOI]

Classification

- Parameterized classifiers
- Parameterized neural networks for high-energy physics (DO) Approximating Likelihood Ratios with Calibrated Discriminative Class
- E Pluribus Unum Ex Machina: Learning from Many Collider Events at Once Jet images
- How to tell quark jets from gluon jets Jet-Images: Computer Vision Inspired Techniques for Jet Tagging (DOI)
- Playing Tag with ANN: Boosted Top Identification with Pattern Recognition (DOI)
- Jet-images deep learning edition [DOI]
- Quark versus Gluon Jet Tagging Using Jet Images with the ATLAS Detector
- Boosting \$Hito b\bar b\$ with Machine Learning (DOI)
- Learning to classify from impure samples with high-dimensional data [DOI] Parton Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks [DOI]
- Deep learning in color: towards automated quark/oluon (DOI).
- Deep-learning Top Taggers or The End of QCD? (DOI)
- Ruting Out All the Tons with Computer Vision and Deep Learning (DOI)
- Reconstructing boosted blogs lets from event image segmentation
- An Attention Based Neural Network for Jet Tagging
- Quark-Gluon Jet Discrimination Using Convolutional Neural Networks (DOI)
- Learning to Isolate Muons
- Deep learning jet modifications in heavy-ion collision

Event images

- Topology classification with deep learning to improve real-time event selection at the LHC [DOI]
- Convolutional Neural Networks with Event Images for Pileup Mitigation with the ATLAS Detector Boosting \$Hito b\bar b\$ with Machine Learning [DOI]
- End-to-End Physics Event Classification with the CMS Open I
- Data to Directly Classify Collision Events at the LHC IDOI
- Disentangling Boosted Higgs Boson Production Modes with Machine Learning
- Identifying the nature of the QCD transition in relativistic collision of heavy nuclei with deep learning [DOI]

- 200000000

- Jet Flavor Classification in High-Energy Physics with Deep Neural Networks (DOI)
- Topology classification with deep learning to improve real-time event selection at the LHC [DOI]
- Jet Flavour Classification Using DeepJet [DOI]
- Development of a Vertex Finding Algorithm using Recurrent Neural Network Sequence-based Machine Learning Models in Jet Physics

Trees

(DOI)

- OCD-Aware Recursive Neural Networks for Jet Physics (DOI) Recursive Neural Networks in Quark/Gluon Tagging (DOI)

Graphs

- Neural Message Passing for let Physics
- Granh Neural Networks for Particle Reconstruction in High Energy Physics de
- Probing stop pair production at the LHC with graph neural networks [DOI]

Probing triple Higgs coupling with machine learning at the LHC.

Casting a graph net to catch dark showers [DOI]

Graph neural networks in particle physics [DOI]

- Pileup mitigation at the Large Hadron Collider with graph neural networks [DOI]
- Unveiling CP property of top-Higgs coupling with graph neural networks at the LHC [DOI] JEDI-net: a jet identification algorithm based on interaction networks [DOI]

Supervised Jet Clustering with Graph Neural Networks for Lorentz Boosted Bosons (DOI)

Graph neural network for 3D classification of ambiguities and optical crosstalk in scinti

Neural Network-based Top Tagger with Two-Point Energy Correlations and Geometry of Soft Emissions [DOI

Distance-Weighted Graph Neural Networks on FPGAs for Real-Time Particle Reconstruction in High Energy Pl

- Learning representations of irregular particle-detector geometry with distant Interpretable deep learning for two-prong jet classification with jet spectra [DOI]

Track Seeding and Labelling with Embedded-space Graph Neural Networks

Parton shower and hadronization



Hadronization

Partons → hadrons Non-perturbative process

Lund-fragmentation (Comput.Phys.Commun. 27 (1982) 243)

$$f(z) = \frac{1}{z}(1-z)^a e^{\frac{-bm_T^2}{z}}$$



Inspiration

J.W. Monk: Deep Learning as a Parton Shower (arXiv:1807.03685)

Dataset: 500 000 QCD pp event @ 7 TeV, generated by Sherpa

| parameter | model k_2 | model k_3 |
|---------------------------------|-------------------|-------------------|
| Kernel size, k | 2 | 3 |
| Input image size, N | 64 | 81 |
| Size of filter bank, F | 9 | 7 |
| Levels of decomposition | 5 | 3 |
| Regularisation, λ | 500 | 300 |
| Learning rate | $5 	imes 10^{-5}$ | $1 	imes 10^{-5}$ |
| Loss weight w_1 | 5 | 4 |
| Loss weight w_2 | 2 | 2 |
| Loss weight w_3 | 1 | 1 |
| Total number of trained weights | 72 | 126 |





Inspiration



Train and validation sets

Monte Carlo data: Pythia 8.303

Monash tune Rescattering and decays turned off ISR, FSR, MPI: turned on **(*)**

Selection:

- All final particles with $|y| < \pi$
- At least 2 jets
 - Anti- k_{τ}
 - R=0.4
 - p_T>40 GeV

Event number:

- Train: 750 000, **√s = 7 TeV**
- Validation and test: 100 000
- ~20 GB raw data





S=3/4 A=0

S=1 A=1/2

Input:

Parton level Discretized in the (y, ϕ) plane: p_T, m, multiplicity $\times \sqrt{s}/1GeV$ $y \in [\pi, \pi]$ 32 bins $\phi \in [0, 2\pi]$, 32 bins

Hadron level output:

(Charged) event multiplicity, (tr-)sphericity, mean jet p_T , -mass, -width, -multiplicity

$$M_{xyz} = \sum_{i} \begin{pmatrix} p_{xi}^{2} & p_{xi}p_{yi} & p_{xi}p_{zi} \\ p_{yi}p_{xi} & p_{yi}^{2} & p_{yi}p_{zi} \\ p_{zi}p_{xi} & p_{zi}p_{yi} & p_{zi}^{2} \end{pmatrix}$$

 $\lambda_1 > \lambda_2 > \lambda_3 \qquad \sum_i \lambda_i = 1$

Sphericity:

Eigenvalues:

Transverse sphericity:

Models

Stacking more layers: solve complex problems more efficiently, get highly accurate results **BUT:**

Vanishing/exploding gradients

ResNet:

Residual blocks with "skip connections"



Used hardwares: Nvidia Tesla T4, GeForce GTX 1080 @ Wigner Scientific Computing Laboratory

Framework: Tensorflow 2.4.1, Keras 2.4.0





Results



Charged hadron multiplicity at various rapidity windows Comparison to reference MC model Good agreement for both models





The smaller model performs better



Jets:

- Mean p_T ≤ 400 GeV
- Mean mass p_T ≤ 400 GeV
- Mean multiplicity
- Mean width
- The smaller model performs better









(*) What about the partonic processes?







Qualitative agreement \rightarrow the models adopted the hadronization properties

Proton-proton @ 0.9-13 TeV, Predictions





 10^{2}

- So far: everything at $\sqrt{s} = 7 \text{ TeV} \rightarrow \text{the ONLY}$ energy, where the models were trained
 - Good agreement for all observable quantities as predictions for other LHC energies
- Multiplicity scaling?

 p_T (GeV)

KNO-scaling

The collapse of multiplicity distributions P_n onto a universal scaling curve:

$$P_n = \frac{1}{\langle n \rangle} \Psi\left(\frac{n}{\langle n \rangle}\right)$$

The scale parameters governed by leading particle effects and the growth of average multiplicity

Violation of the scaling at high CM energies: not fully understood (relation to MPI?)



Nuclear Physics B 40 (1972), 317–334.

(Nucl. Phys. B Proc. Suppl. 92 (2001). 122–129) 25

Test of KNO-scaling for the predictions



Heavy Ion Jet INteraction Generator (C++ version)

(C++ version) even 京易经 Req

A NEW GENERATION OF HEAVY-ION MONTE CARLO

"Nuclear change theory"; Book of Changes, "Originally a divination manual in the Western Zhou period (1000–750 BC)"

First, FORTRAN version: 1991, X.N. Wang, M. Gyulassy, Phys. Rev. D 44, (1991) 3501.

Computational challenge: more than 600 million collision in each second \rightarrow HiLumiLHC: even more

Requirements for a new version: multithreaded mode, maintainability, intuitive usage







Test of KNO-scaling for the predictions - Hijing++



Summary

Developed hadronization models with different complexities

- Traditional computer vision algorithms capture the main features of high-energy event variables successfully → training only at a single c.m. energy, predictions at other energies
- Generalization to other CM energies: KNO scaling in jetty events
- Valuable input for MC developments

Prospects

Architecture variations (hyperparameter fine-tuning)

Heavy ion (centralities, collective effects)

Thank you for your attention!

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U-Net: biomedical image segmentation





(Conditional (Variational)) autoencoders

Dimension reduction Denoising data Latent space conditioning





Fig. 4. Generating new concrete formulas and evaluating their properties

https://arxiv.org/pdf/2204.05397.pdf



Diffusion models: https://huggingface.co/spaces/stabilityai/stable-diffusion

Gradually perturbate he input data over several steps by adding Gaussian noise



GAN: data generation via competing generator-discriminator





GAN: data generation via competing generator-discriminator



Attention and Transformers :

A revolution in natural language processing



https://arxiv.org/abs/1706.03762

Graph Neural Networks





Track reconstruction

Particle Track Reconstruction with Deep Learning



Figure 1: Distribution of particle spacepoints in a particle collision event in a generic simulated HL-LHC tracking detector.







arXiv:1803.03589

Quark/gluon jet separation



P. Baldi, K. Bauer, C. Eng, P. Sadowski, and D. Whiteson, Jet Substructure Classification in High-Energy Physics with Deep Neural Networks, Phys. Rev. D93 (2016), no. 9 094034, [arXiv:1603.09349].

D. Guest, J. Collado, P. Baldi, S.-C. Hsu, G. Urban, and D. Whiteson, Jet Flavor Classification in High-Energy Physics with Deep Neural Networks, arXiv: 1607.08633. J. S. Conway, R. Bhaskar, R. D. Erbacher, and J. Pilot, Identification of High-Momentum Top Quarks, Higgs Bosons, and W and Z Bosons Using Boosted Event Shapes. arXiv:1606.0685

J. Barnard, E. N. Dawe, M. J. Dolan, and N. Rajcic, Parton Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks, arXiv: 1609.00607.

> Deep learning in color: towards automated quark/gluon iet discrimination

> Patrick T. Komiske," Eric M. Metodiev," and Matthew D. Schwartz "Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA Department of Physics, Harvard University, Cambridge, MA 02138, USA E-mail: pkomiske@mit.edu, metodiev@mit.edu. schwartz@physics.harvard.edu

quark jet

gluon jet

https://doi.org/10.1007/JHEP01(2017)110 Deep CNN match or outperform traditional jet observables.

Figure 2: An illustration of the deep convolutional neural network architecture. The first layer is the input jet image, followed by three convolutional layers, a dense layer and an output layer.



Jet reconstruction

Machine Learning based jet momentum reconstruction in Pb–Pb collisions measured with the ALICE detector



Figure 1: Residual p_T-distributions of embedded jet probes of known transverse momentum.

https://doi.org/10.22323/1.364.0312

Tuning Monte Carlo event generators



Neural Networks for Full Phase-space Reweighting and Parameter Tuning







Figure 1: An illustration of the parametrisation of the generator response as implemented in the Per Bin Model. Figure 2: An illustration of the Inverse Model strategy.

MCNNTUNES: tuning Shower Monte Carlo generators with machine learning

Marco Lazzarin^a, Simone Alioli^b, Stefano Carrazza^a

^aTIF Lab, Dipartimento di Fisica, Università degli Studi di Milano and INFN Sezione di Milano, Milan, Italy. ^bDipartimento di Fisica, Università degli Studi di Milano Bicocca and INFN Sezione di Milano Bicocca, Milan, Italy.

https://doi.org/10.1016/j.cpc.2021.107908

Accelerating Science with Generative Adversarial Networks: An Application to 3D Particle Showers in Multi-Layer Calorimeters

Michela Paganini,^{1,2,*} Luke de Oliveira,^{1,†} and Benjamin Nachman^{1,‡} ¹Lawrence Berkeley National Laboratory, Berkeley, CA 94720 ²Yale University, New Haven, CT 06520

https://doi.org/10.1103/PhysRevLett.120.042003

Dimensionality

Input:

Parton level

Discretized in the (y,ϕ) plane: p_,m, multiplicity

 $\left.\begin{array}{l} y\in [\pi,\pi], \quad 32 \text{ bins} \\ \phi\in [0,2\pi], \quad 32 \text{ bins} \end{array}\right\} := M$

Reduction with Singular Value Decomposition:

Reduce the input to $\mathcal{O}(10^2)$

 $M_{n \times m} = U_{n \times n} \Sigma_{n \times m} V_{m \times m}^T$

- Unitarity
- Ordered by importance
- Guaranteed to exist, unique

$$M \approx \sum_{i=1}^{r} \sigma_i u_i v_i^T + \mathcal{O}(\epsilon), \quad r \le \min\{n, m\}$$

Data-Driven Science and Engineering (S. L. Brunton, J. N. Kutz)

 $\mathcal{O}(10^3-10^4)$ Total pixels vs $\mathcal{O}(10^2)$

50

100

doi:10.1007/BF02288367



150

200

250

Dimensionality (work in progress)











