# Studying hadronization with Machine Learning techniques and event variables



### 21st ZIMÁNYI SCHOOL WINTER WORKSHOP ON HEAVY ION PHYSICS 6-10 12 2021





biro.gabor@wigner.hu

ELTE EÖTVÖS LORÁND UNIVERSITY

Gergely Gábor Barnaföldi Bence Tankó-Bartalis

arXiv:2111.15655

## Outline

- Machine Learning: motivation
- Applications and examples
- Research goals
- Preliminary results
- Summary

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# Data, data, and more data





### Large Hadron Collider data:

2021: 336 PB From 2022: 200+ PB/year

### Simulations:

Computationally very expensive 1s LHC data ~ days of CPU time









### **Machine learning**

- Data driven decisions
- Automated analysis
- Perform tasks without being explicitly programmed to do so



### **Machine learning**

- Data driven decisions
- Automated analysis
- Perform tasks without being • Meaningful explicitly programmed to do so Structure Image **Customer Retention** Compression Discovery Classification Big data **Idenity Fraud** Feature Diagnostics Classification Visualistaion Detection Reduction Elicitation а b Advertising Popularity Supervised Recommender Unsupervised Prediction Systems Learning Learning Weather Forecasting Clustering Machine Regression Targetted Population Market Marketing Growth Forecasting Prediction Learning Customer Estimating Classification Regression Segmentation life expectancy d С 000 Real-time decisions Game Al 000 000 00000 Reinforcement Learning Robot Navigation Clustering Semi-supervised **Skill Acquisition** classification Learning Tasks

### **Basic building blocks of a neural network**



### **Convolutional:**



Image

Kernel

Х



=

$$z_j = \sum_{i=1}^N x_i w_{ij} + b_j$$

max pooling

### **Basic building blocks of a neural network**

### **Activation functions:**

**Pooling:** 

Nadam

Ftrl



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

## **Example: FCNN**



$$L_{\delta}(y, f(x)) = \begin{cases} \frac{1}{2}(y - f(x))^2, & |y - f(x)| \le \delta \\ \delta(|y - f(x)| - \frac{1}{2}\delta) \end{cases}$$

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## **Example: FCNN**



PRC.53.2358 (1996), Bass, S. A.; Bischoff, A.; Maruhn, J. A.; Stöcker, H.; Greiner, W.

# **Popular architectures**

Classifiers

- AlexNet (Comm. ACM. 60 (6): 84–90, 2012)
- VGG16 (138M parameters, 23 layers, arXiv:1409.1556)
- ResNet (25M+ parameters, arXiv:1512.03385)
- DenseNet (8M parameters, 121 layers, arXiv:1608.06993)

### Object detection

- (Fast(er)) R-CNN (arXiv:1311.2524, arXiv:1504.08083, arXiv:1506.01497)
- YOLO (arXiv:1506.02640)
- Detectron (github.com/facebookresearch/detectron2)

Autonomous vehicles

Decision trees

Transformers

Generative adversarial networks (https://bit.ly/2YMCFdy) (Variational) autoencoders





### 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

Today: **585** references

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- Jet tagging in the Lund plane with graph networks [DOI]
- Vertex and Energy Reconstruction in JUNO with Machine Learning Methods
- MLDE: Efficient machine-learned particle-flow reconstruction using graph neural networks 25th International Conference on Computing in High-Energy and Nuclear Physics

Accelerated Charged Particle Tracking with Graph Neural Networks on EPGAs

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- Graph 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)

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- Zero Dermutation, lat Darton Assignment using a Salf Attention Network
- Learning to Isolate Muons Point Cloud Transformers applied to Collider Physics

### Physics-inspired basis

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- How Much Information is in a Jet? [DOI] Novel Jet Observables from Machine Learning IDOII
- Energy flow polynomials: A complete linear basis for jet substructure [DOI]
- p-learned Top Tagging with a Lorentz Layer [DOI]
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### SW/ZS teoping

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### Classification

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- Parameterized neural networks for high-energy physics [DOI]
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### Trees

- QCD-Aware Recursive Neural Networks for Jet Physics [DOI]
- Recursive Neural Networks in Quark/Gluon Tagging [DOI]

### Graphs

IDOII

Neural Message Passing for Jet Physics

Casting a graph net to catch dark showers [DOI]

Graph neural networks in particle physics [DOI]

Graph Neural Networks for Particle Reconstruction in High Energy Physics detector

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

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### arXiv:1803.03589

Š

Quark/gluon jet separation



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.

in High-Energy Physics with Deep Neural Networks, Phys. Rev. D93 (2016), no. 9 094034, 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.

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 jet discrimination

### Patrick T. Komiske.<sup>a</sup> Eric M. Metodiev.<sup>a</sup> and Matthew D. Schwartz <sup>a</sup> Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA <sup>b</sup>Department of Physics, Harvard University, Cambridge, MA 02138, USA E-mail: pkomiske@mit.edu, metodiev@mit.edu,

schwartz@physics.harvard.edu

https://doi.org/10.1007/JHEP01(2017)110

Deep CNN match or outperform traditional jet observables.



### Jet reconstruction

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



Figure 1: Residual p<sub>T</sub>-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





<sup>a</sup> TIF Lab, Dipartimento di Fisica, Università degli Studi di Milano and INFN Sezione di Milano, Milan, Italy. <sup>b</sup>Dipartimento 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,<sup>1, 2, \*</sup> Luke de Oliveira,<sup>1, †</sup> and Benjamin Nachman<sup>1, ‡</sup> <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA 94720 <sup>2</sup> Yale University, New Haven, CT 06520

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

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# **Parton shower and hadronization**

# The goal of this study



### Hadronization

Partons  $\rightarrow$  hadrons Non-perturbative process Lund-fragmentation (Comput.Phys.Commun. 27 (1982) 243) string fragments hadrons right-to-left string fragmentation  $\overline{\mathbf{B}}$ 0.00 FSR  $\overline{B} B$  $\sim$ ... meson RGB $\overline{B} B$  $\eta$ baryon B B















 $\eta$ 







 $\eta$ 

"The nice thing about artificial intelligence is that at least it's better than artificial stupidity."

Terry Pratchett, Stephen Baxter: The Long War

# **Train and validation sets**

### Monte Carlo data: Pythia 8.303

Monash tune

Selection:

- All final particles with  $|y| < \pi$
- At least 2 jets
  - Anti-k<sub>T</sub>
  - R=0.6
  - p<sub>T</sub>>40 GeV

Event number:

- Train: 150 000
- Validation: 150 000
- ~20 GB raw data



S=1 A=1

S=A=0

**Input:** Parton level Discretized in the  $(y, \phi)$  plane:  $p_{x'}, p_{y'}, p_{z'}$ , E, m, multiplicity  $y \in [\pi, \pi]$ , 62 bins  $\phi \in [0, 2\pi]$  31 bins

### Hadron level output:

(Charged) event multiplicity, (tr-)sphericity, jet p<sub>T</sub>, -mass, -width, -multiplicity

$$M_{xyz} = \sum_{i} \begin{pmatrix} p_{xi}^2 & p_{xi}p_{yi} & p_{xi}p_{zi} \\ p_{yi}p_{xi} & p_{yi}^2 & p_{yi}p_{zi} \\ p_{zi}p_{xi} & p_{zi}p_{yi} & p_{zi}^2 \end{pmatrix}$$
  
Eigenvalues:  $\lambda_1 > \lambda_2 > \lambda_3$   $\sum_i \lambda_i = 1$   
Sphericity:  $S = \frac{3}{2}(\lambda_2 + \lambda_3)$   
Transverse sphericity:  $S_{\perp} = \frac{2\lambda_2}{\lambda_1 + \lambda_2}$  25



S=3/4 A=0

## Models

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

Vanishing/exploding gradients (not to confuse with overfitting)



### **Results**

(any feedback is very welcome!)

### **Proton-proton @ 7 TeV, Training + Validation**



	Model 1	Model 2
Trainable parameters	1.13 M	1.90 M



### **Prediction at other CM energies**

 $\sqrt{s} = 900 \text{ GeV}$ 



### **Prediction at other CM energies**

 $\sqrt{s} = 5.02 \text{ TeV}$ 



### **Prediction at other CM energies**

 $\sqrt{s} = 13 \text{ TeV}$ 



## Summary

Traditional computer vision algorithms capture the main features of high-energy event variables successfully

Generalization to other CM energies: multiplicity scaling

### Plans

Various architectures (hyperparameter fine-tuning)

Other observables ( $p_{T}$ , rapidity, particle species)

Heavy ion (centralities, collective effects)

# Thank you for your attention!

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