Studying hadronization with Machine Learning techniques

GPU Day 2022

by the

Wigner Scientific Computing Laboratory

20-21 06 2022

GÁBOR BÍRÓ

biro.gabor@wigner.hu

Gergely Gábor Barnaföldi
Bence Tankó-Bartalis

arXiv:2111.15655

Outline

- Machine Learning: the motivation
- Research goals
- Results
- Future directions
- Summary

Data, data, and more data

Large Hadron Collider data:

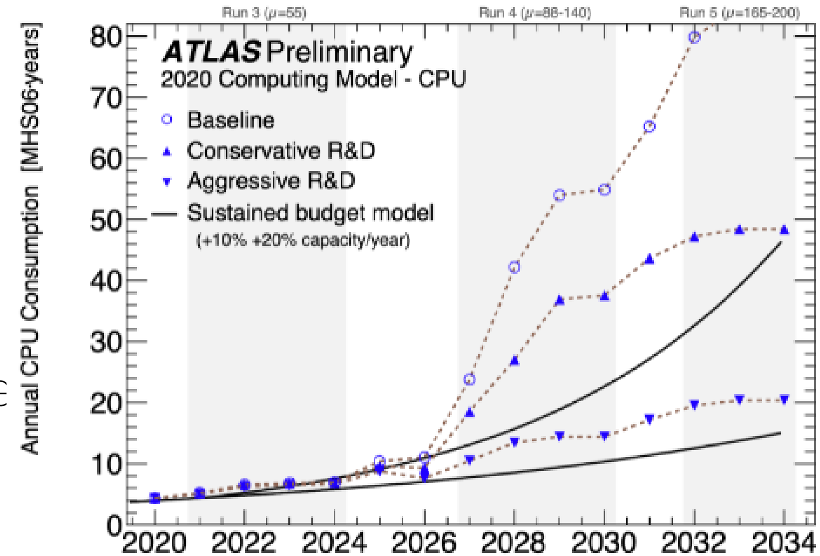
2021: 336 PB

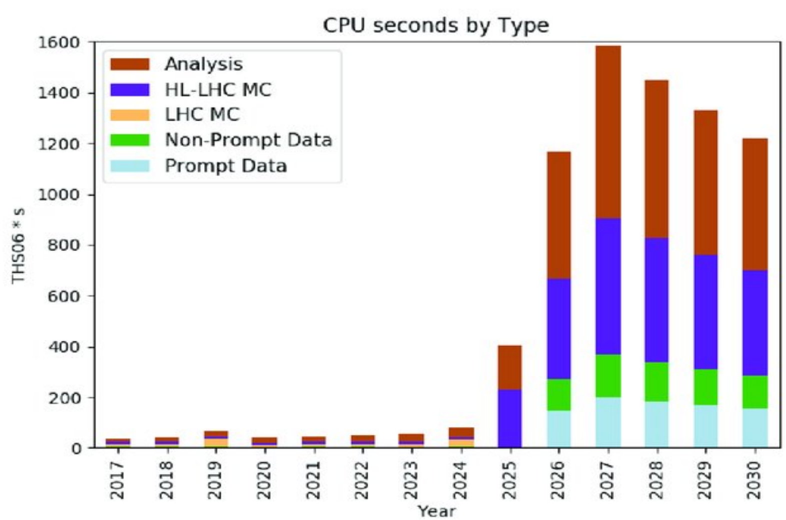
From 2022: 200+ PB/year

Simulations:

Computationally very expensive

1s LHC data ~ days of CPU time

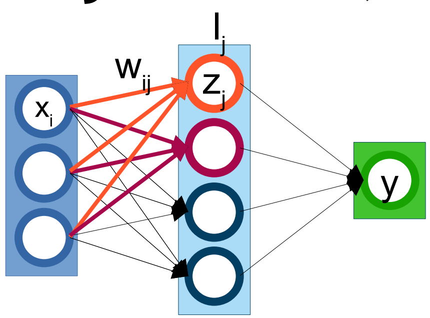




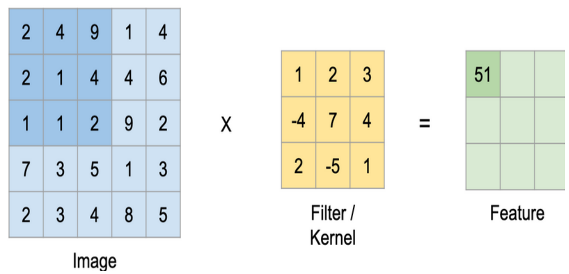
Basic building blocks of a neural network

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

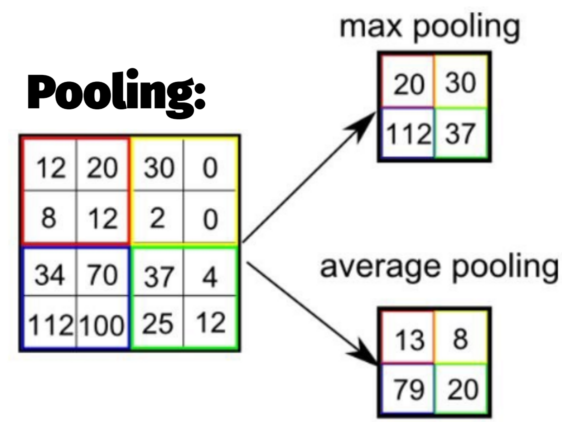
Fully connected (dense):



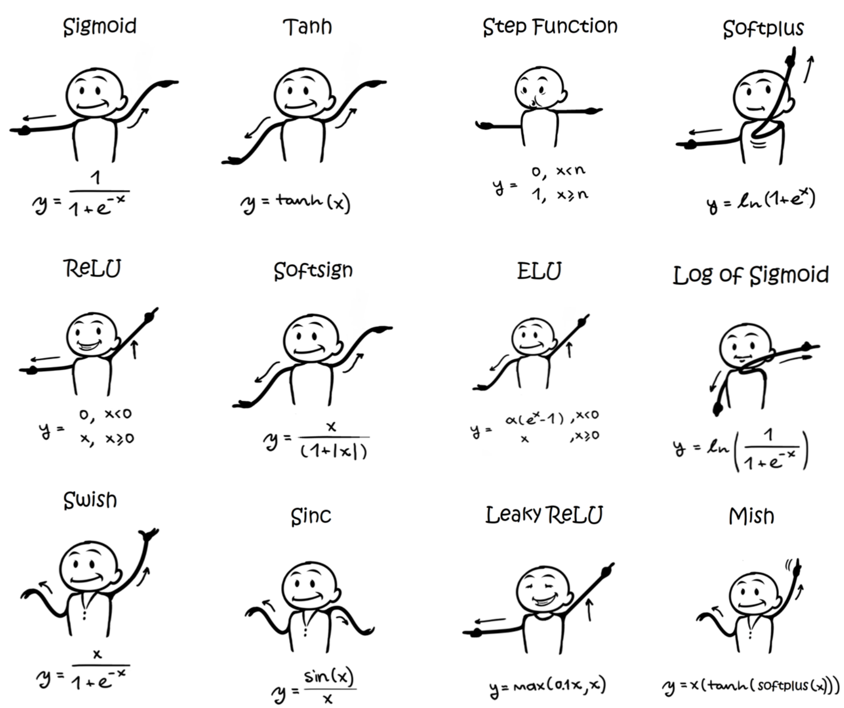
Convolutional:



Pooling:



Activation functions:



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

Loss functions, optimizers...

Regression losses

- MeanSquaredError class
- MeanAbsoluteError class
- MeanAbsolutePercentageError class
- MeanSquaredLogarithmicError class
- CosineSimilarity class
- mean_squared_error function
- mean_absolute_error function
- mean_absolute_percentage_error function
- mean_squared_logarithmic_error function
- cosine_similarity function
- Huber class
- huber function
- LogCosh class
- log_cosh function

Probabilistic losses

- BinaryCrossentropy class
- CategoricalCrossentropy class
- SparseCategoricalCrossentropy class
- Poisson class

Hinge losses for "maximum-margin" classification

- Hinge class
- SquaredHinge class
- CategoricalHinge class

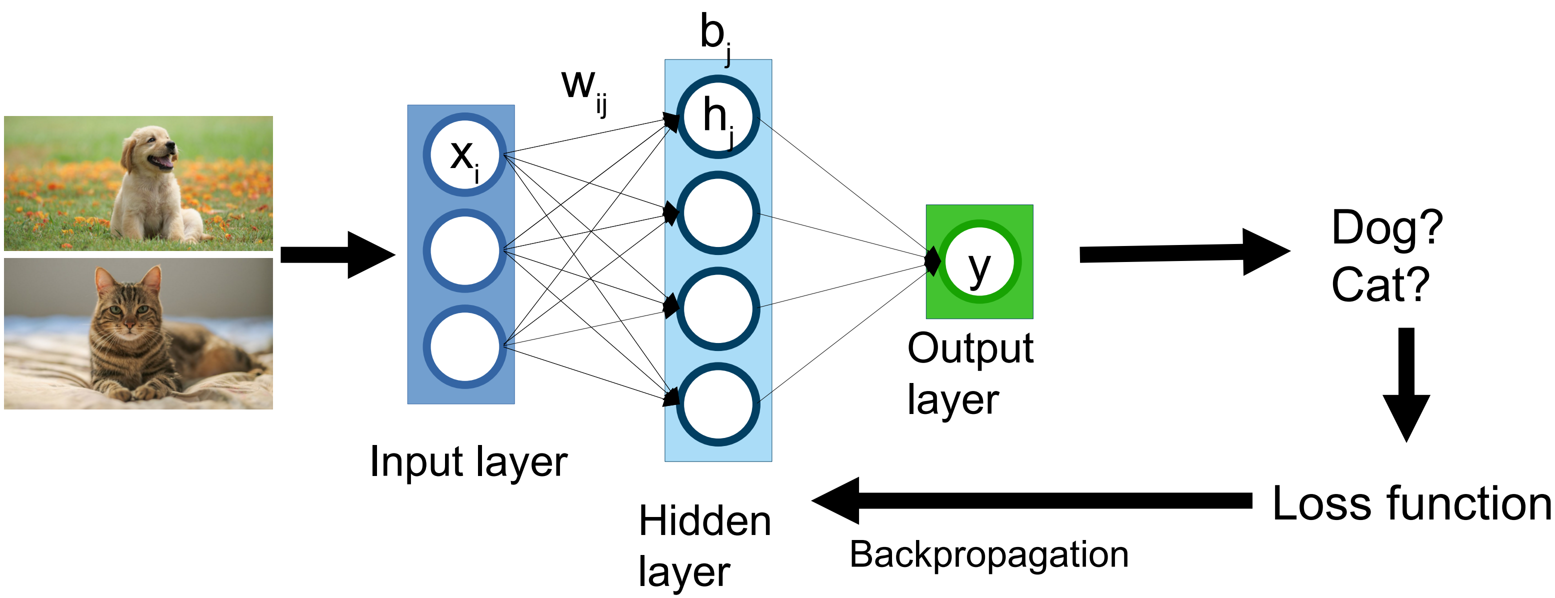
Available optimizers

- SGD
- RMSprop
- Adam
- Adadelta
- Adagrad
- Adamax
- Nadam
- Ftrl

https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

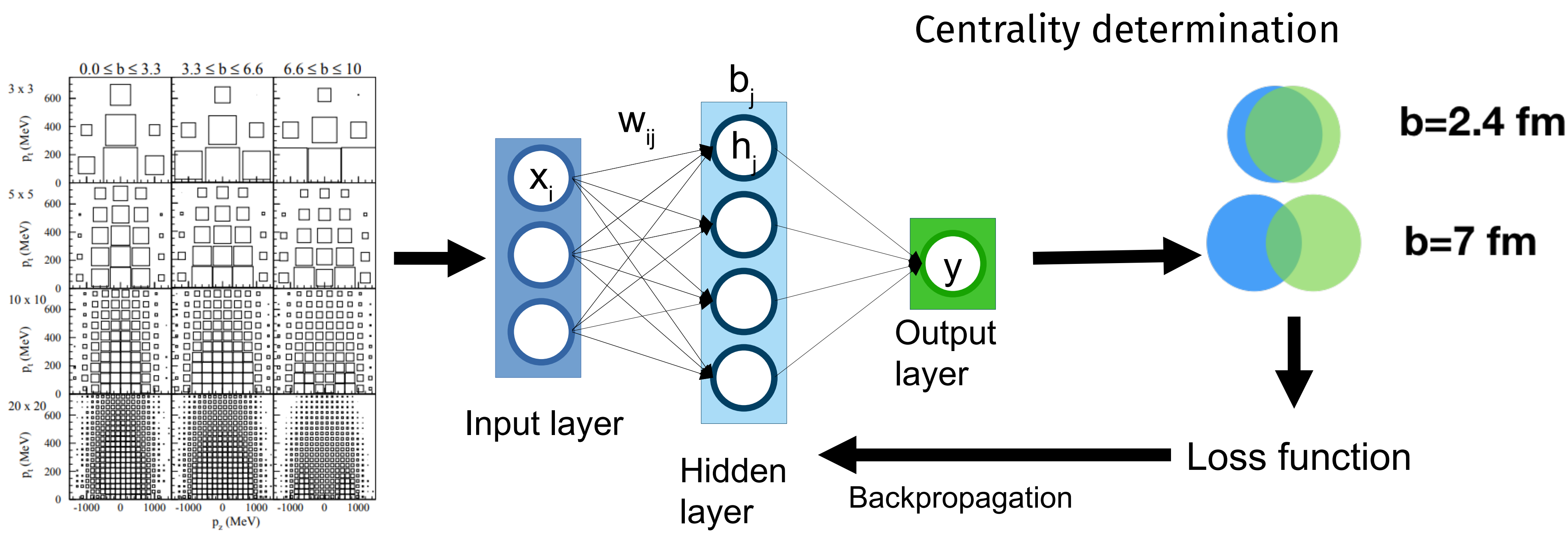
Example: FCNN

Simple classification



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

Example: FCNN



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

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)

Regression
Autonomous vehicles
Decision trees
Transformers
Generative adversarial networks (https://bit.ly/2YMCFdy)
(Variational) autoencoders
...

Machine Learning in HEP

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

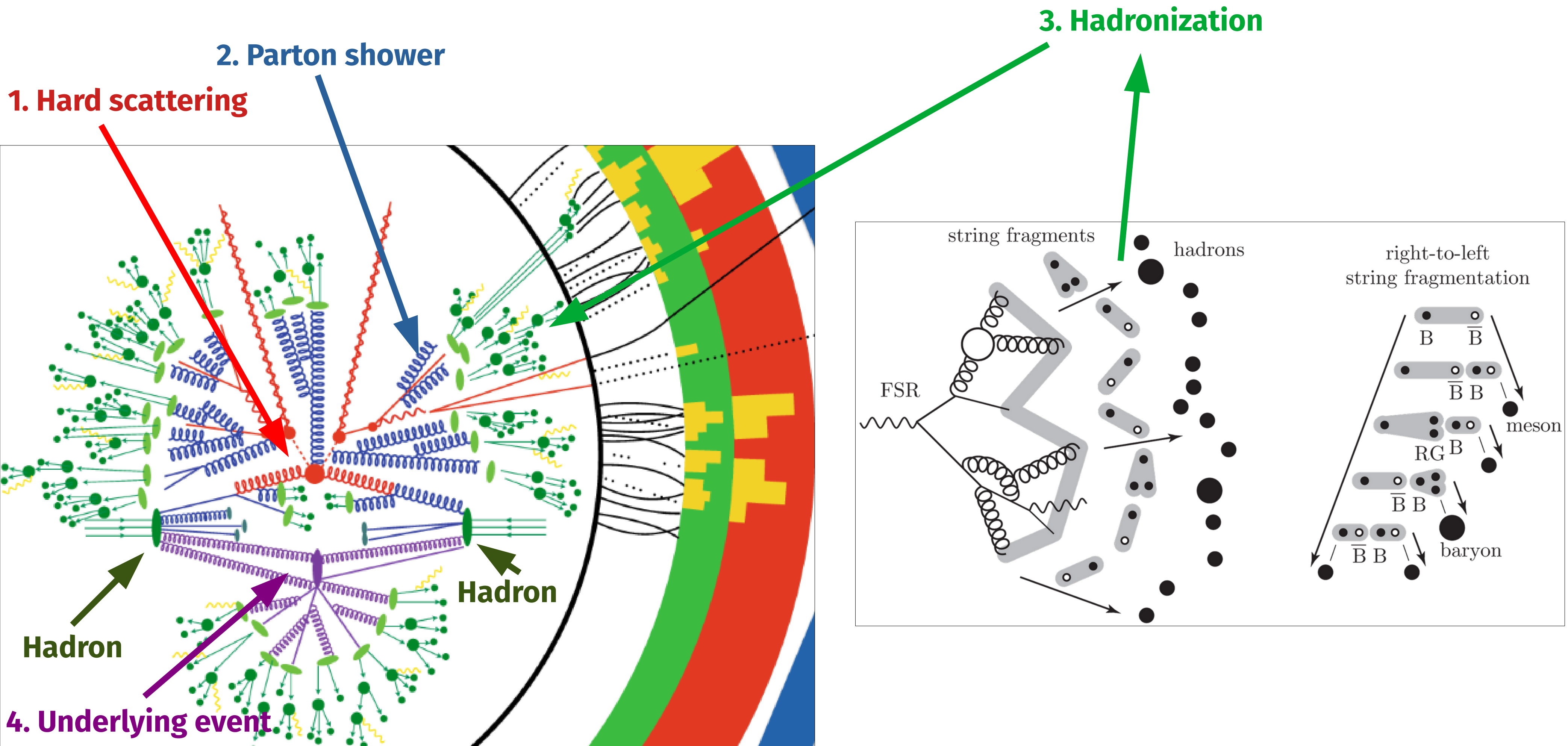
Today: **631** references

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

  - Accelerated Charged Particle Tracking with Graph Neural Networks on FPGAs
  - Particle Track Reconstruction using Geometric Deep Learning
  - Jet tagging in the Lund plane with graph networks [DOI]
  - Vertex and Energy Reconstruction in JUNO with Machine Learning Methods
  - MLPF: Efficient machine-learned particle-flow reconstruction using graph neural networks
  - 25th International Conference on Computing in High-Energy and Nuclear Physics
  - 25th International Conference on Computing in High-Energy and Nuclear Physics
  - Graph Neural Network for Object Reconstruction in Liquid Argon Time Projection Chambers
  - Instance Segmentation GNNs for One-Shot Conformal Tracking at the LHC
  - Charged particle tracking via edge-classifying interaction networks
  - Jet characterization in Heavy Ion Collisions by QCD-Aware Graph Neural Networks
  - 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)
  - Energy Flow Networks: Deep Sets for Particle Jets [DOI]
  - ParticleNet: Jet Tagging via Particle Clouds [DOI]
  - ABCNet: An attention-based method for particle tagging [DOI]
  - Secondary Vertex Finding in Jets with Neural Networks
  - Equivariant Energy Flow Networks for Jet Tagging
  - Permutationless Many-Jet Event Reconstruction with Symmetry Preserving Attention Networks
  - Zero-Permutation Jet-Parton Assignment using a Self-Attention Network
  - Learning to Isolate Muons
  - Point Cloud Transformers applied to Collider Physics
- 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 Layer [DOI]
  - Resurrecting $b\bar{b}h$ with kinematic shapes
- W/Z tagging
  - Jet-images — deep learning edition [DOI]
  - Parton Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks [DOI]
  - QCD-Aware Recursive Neural Networks for Jet Physics [DOI]
  - Identification of heavy, energetic, hadronically decaying particles using machine-learning techniques [DOI]
  - Boosted W and Z tagging with jet 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 $W^\pm$ polarization analyzer from Deep Neural Networks
- $H\rightarrow b\bar{b}$
  - Automating the Construction of Jet Observables with Machine Learning [DOI]
  - Boosting $H\to b\bar b$ with Machine Learning [DOI]
  - Interaction networks for the identification of boosted $H \rightarrow b\overline{b}$ decays [DOI]
  - Interpretable deep learning for two-prong jet classification with jet spectra [DOI]
  - Identification of heavy, energetic, hadronically decaying particles using machine-learning techniques [DOI]
  - Disentangling Boosted Higgs Boson Production Modes with Machine Learning
  - Benchmarking Machine Learning Techniques with Di-Higgs Production at the LHC
  - 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 $\text{t}\bar{\text{t}}\text{b}\bar{\text{b}}$ process
- quarks and gluons
  - Quark versus Gluon Jet Tagging Using Jet Images with the ATLAS Detector
  - Deep learning in color: towards automated quark/gluon [DOI]
  - Recursive Neural Networks in Quark/Gluon Tagging [DOI]
  - DeepJet: Generic physics object based jet multiclass classification for LHC experiments
  - Probing heavy ion collisions using quark and gluon jet substructure
  - JEDI-net: a jet identification algorithm based on interaction networks [DOI]
  - Quark-Gluon Tagging: Machine Learning vs Detector [DOI]
  - Towards Machine Learning Analytics for Jet Substructure [DOI]
  - Quark Gluon Jet Discrimination with Weakly Supervised Learning [DOI]

- Classification
  - Parameterized classifiers
    - Parameterized neural networks for high-energy physics [DOI]
    - Approximating Likelihood Ratios with Calibrated Discriminative Classifiers
    - 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 $H\to b\bar b$ 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/gluon [DOI]
    - Deep-learning Top Taggers or The End of QCD? [DOI]
    - Pulling Out All the Tops with Computer Vision and Deep Learning [DOI]
    - Reconstructing boosted Higgs jets 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 collisions
  - 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 $H\to b\bar b$ with Machine Learning [DOI]
    - End-to-End Physics Event Classification with the CMS Open Data: Applying Image-based Deep Learning on Detector Data to Directly Classify Collision Events at the LHC [DOI]
    - 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]
  - Sequences
    - 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
    - QCD-Aware Recursive Neural Networks for Jet Physics [DOI]
    - Recursive Neural Networks in Quark/Gluon Tagging [DOI]
  - Graphs
    - Neural Message Passing for Jet Physics
    - Graph Neural Networks for Particle Reconstruction in High Energy Physics detectors
    - Probing stop pair production at the LHC with graph neural networks [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]
    - Learning representations of irregular particle-detector geometry with distance-weighted graph networks [DOI]
    - Interpretable deep learning for two-prong jet classification with jet spectra [DOI]
    - Neural Network-based Top Tagger with Two-Point Energy Correlations and Geometry of Soft Emissions [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]
    - Distance-Weighted Graph Neural Networks on FPGAs for Real-Time Particle Reconstruction in High Energy Physics [DOI]
    - Supervised Jet Clustering with Graph Neural Networks for Lorentz Boosted Bosons [DOI]
    - Track Seeding and Labelling with Embedded-space Graph Neural Networks
    - Graph neural network for 3D classification of ambiguities and optical crosstalk in scintillator-based neutrino detectors [DOI]

Parton shower and hadronization

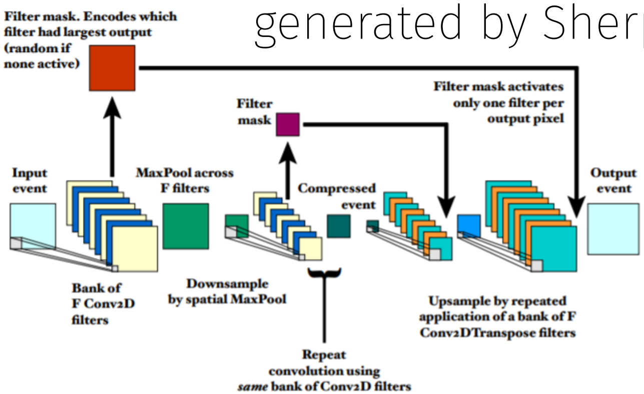


Nature Reviews Physics 3, 73 (2021)

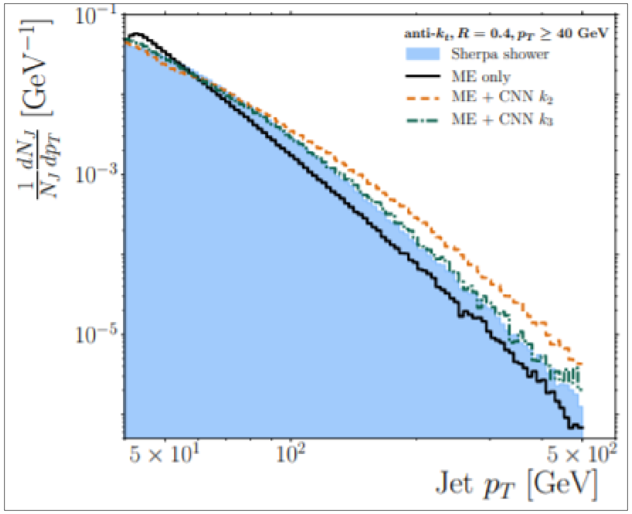
The goal of this study

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	5×10^{-5}	1×10^{-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

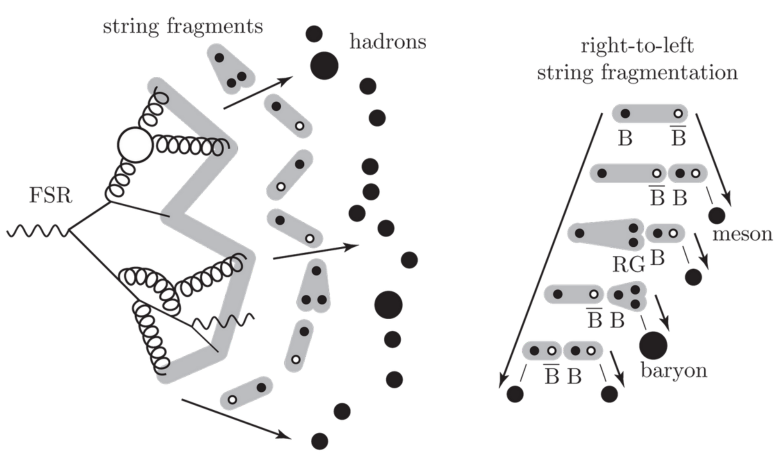


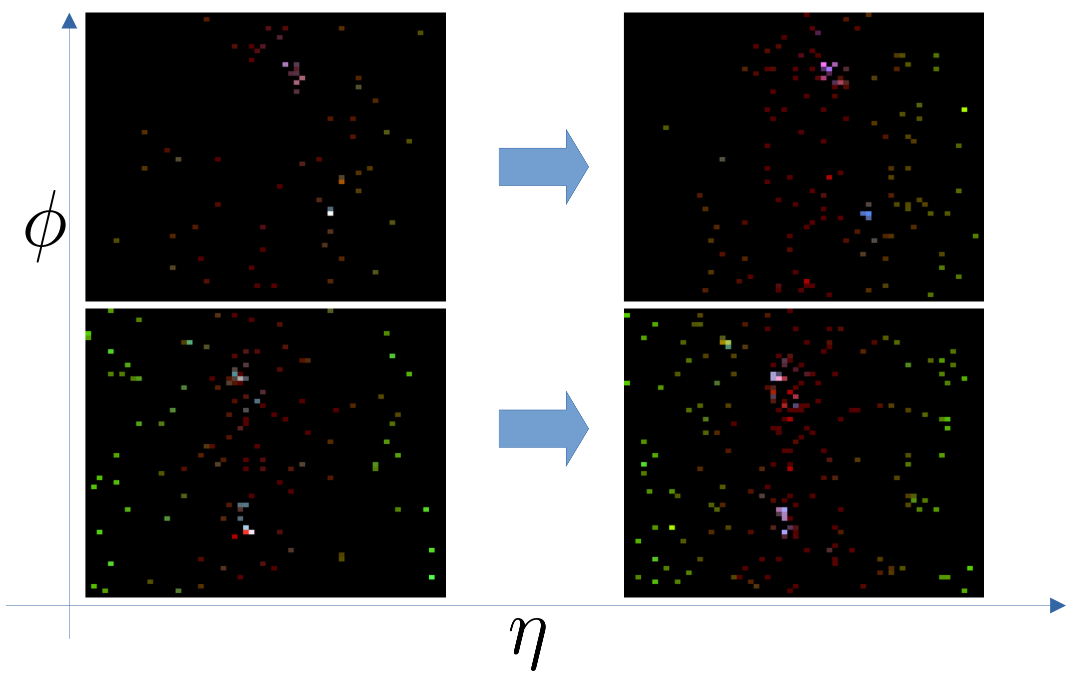
Hadronization

Partons → hadrons

Non-perturbative process

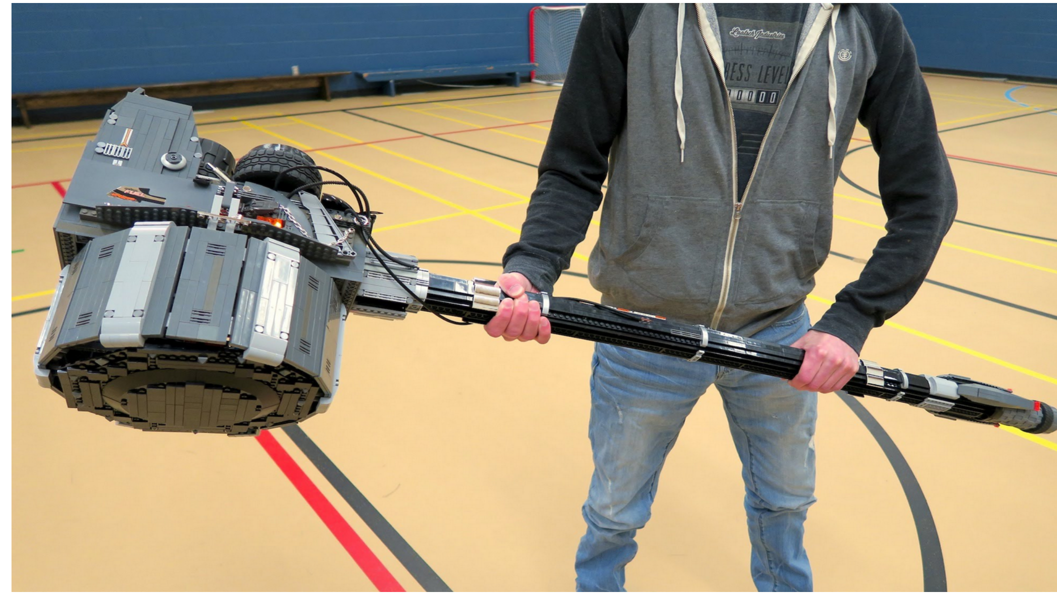
Lund-fragmentation (Comput.Phys.Commun. 27 (1982) 243)



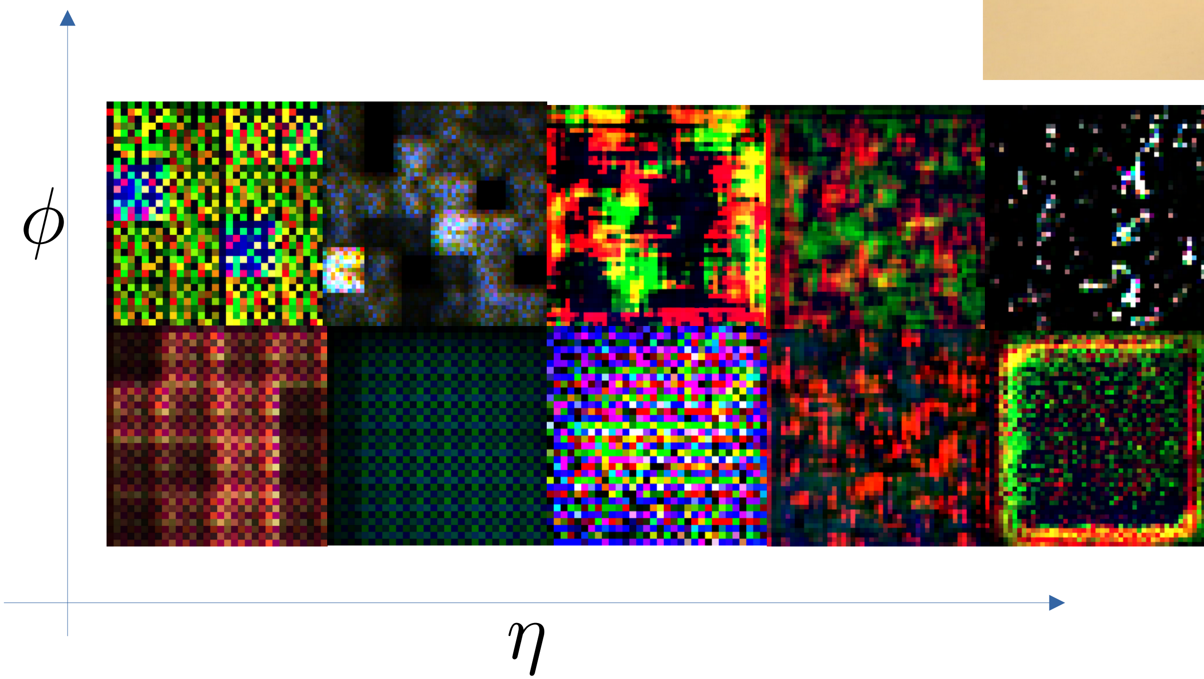


ML: a great tool...

ML: a great tool...



https://www.youtube.com/watch?v=WhvMvbqWNYo



“The nice thing about artificial intelligence is that at least it’s better than artificial stupidity.”

Terry Pratchett, Stephen Baxter: The Long War

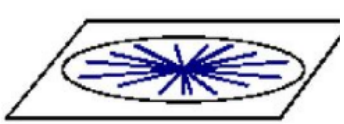
Train and validation sets

Monte Carlo data: Pythia 8.303

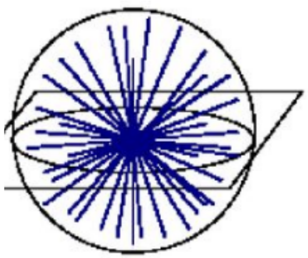
Monash tune

Selection:
- All final particles with $|y| < \pi$
- At least 2 jets
  - Anti-k_T
  - R=0.6
  - p_T>40 GeV

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



S=3/4 A=0



S=1 A=1/2

Input:

Parton level

Discretized in the (y, ϕ) plane: p_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_T, -mass, -width, -multiplicity

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

Eigenvalues: $\lambda_1 > \lambda_2 > \lambda_3$ $\sum_i \lambda_i = 1$

Sphericity: $S = \frac{3}{2}(\lambda_2 + \lambda_3)$

Transverse sphericity: $S_\perp = \frac{2\lambda_2}{\lambda_1+\lambda_2}$

Models

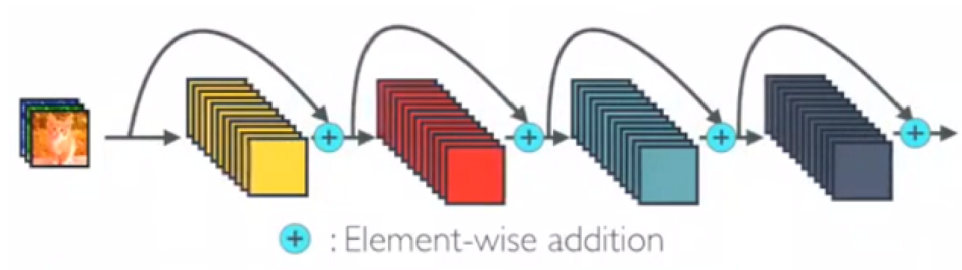
Stacking more layers: solve complex problems more efficiently, get highly accurate results

BUT:

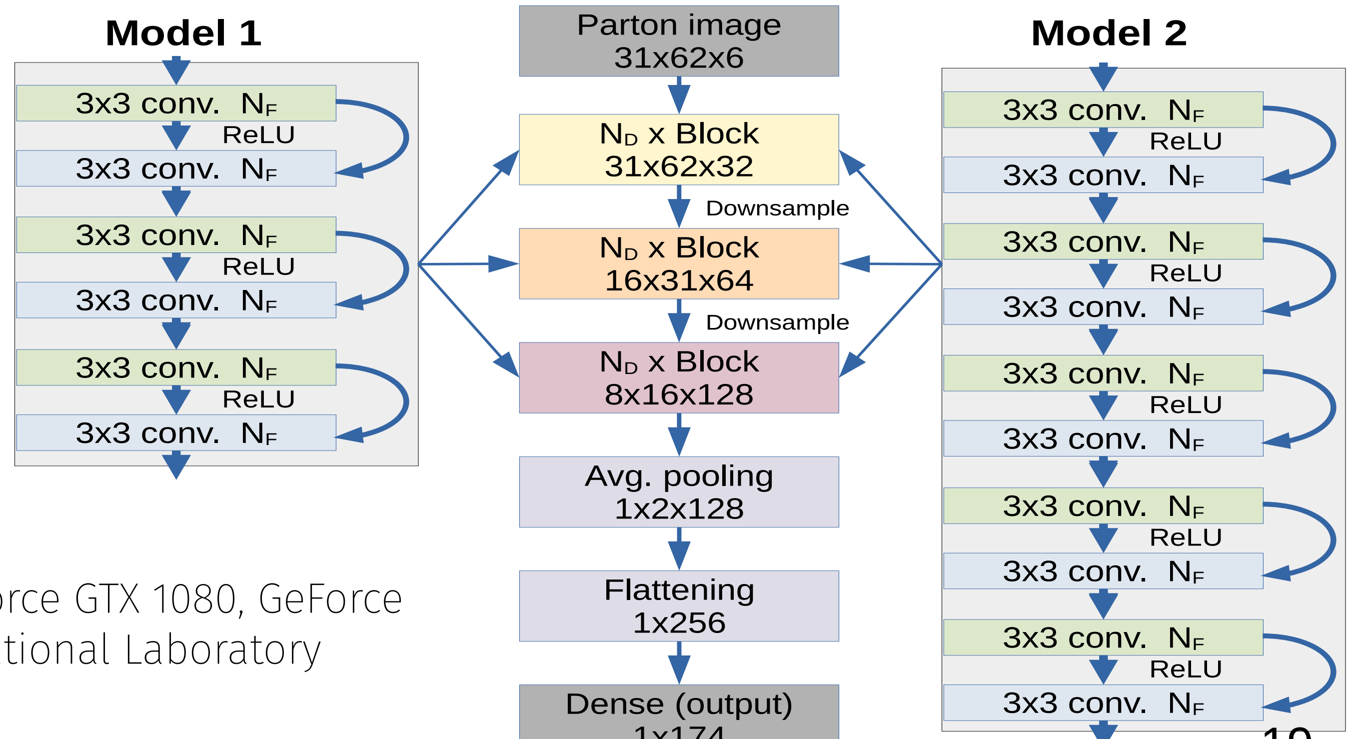
Vanishing/exploding gradients (not to confuse with overfitting)

ResNet

Residual blocks with "skip connections"



	Model 1	Model 2
Trainable parameters	1.13 M	1.90 M



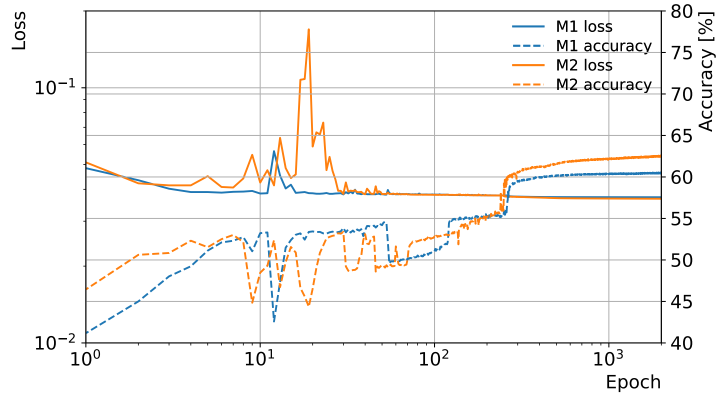
Used hardwares: Nvidia Tesla T4, GeForce GTX 1080, GeForce GTX 980 @ Wigner Scientific Computational Laboratory

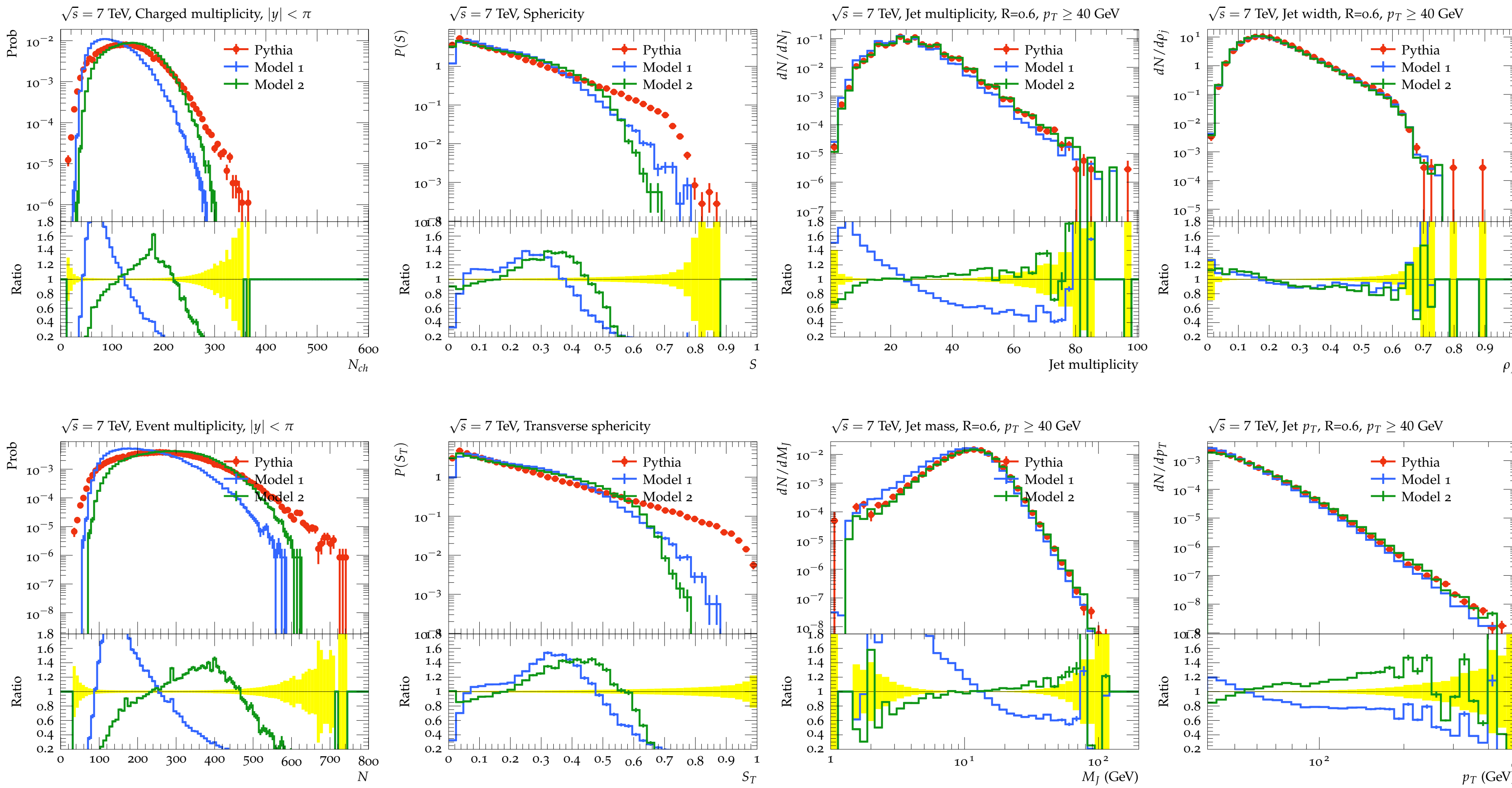
Framework: Tensorflow 2.4.1, Keras 2.4.0

Results

Proton-proton @ 7 TeV, Training + Validation

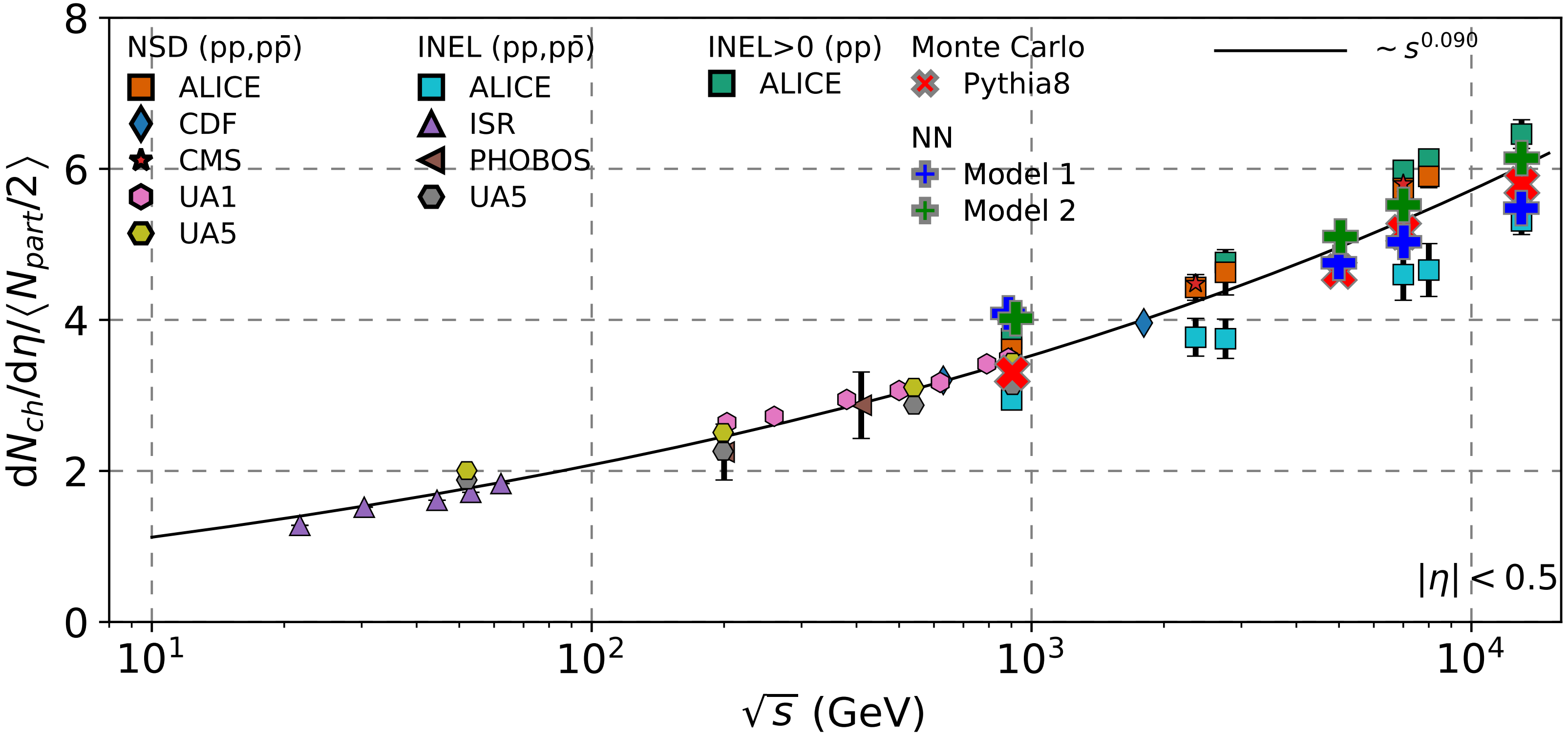
	Model 1	Model 2
Trainable parameters	1.13 M	1.90 M





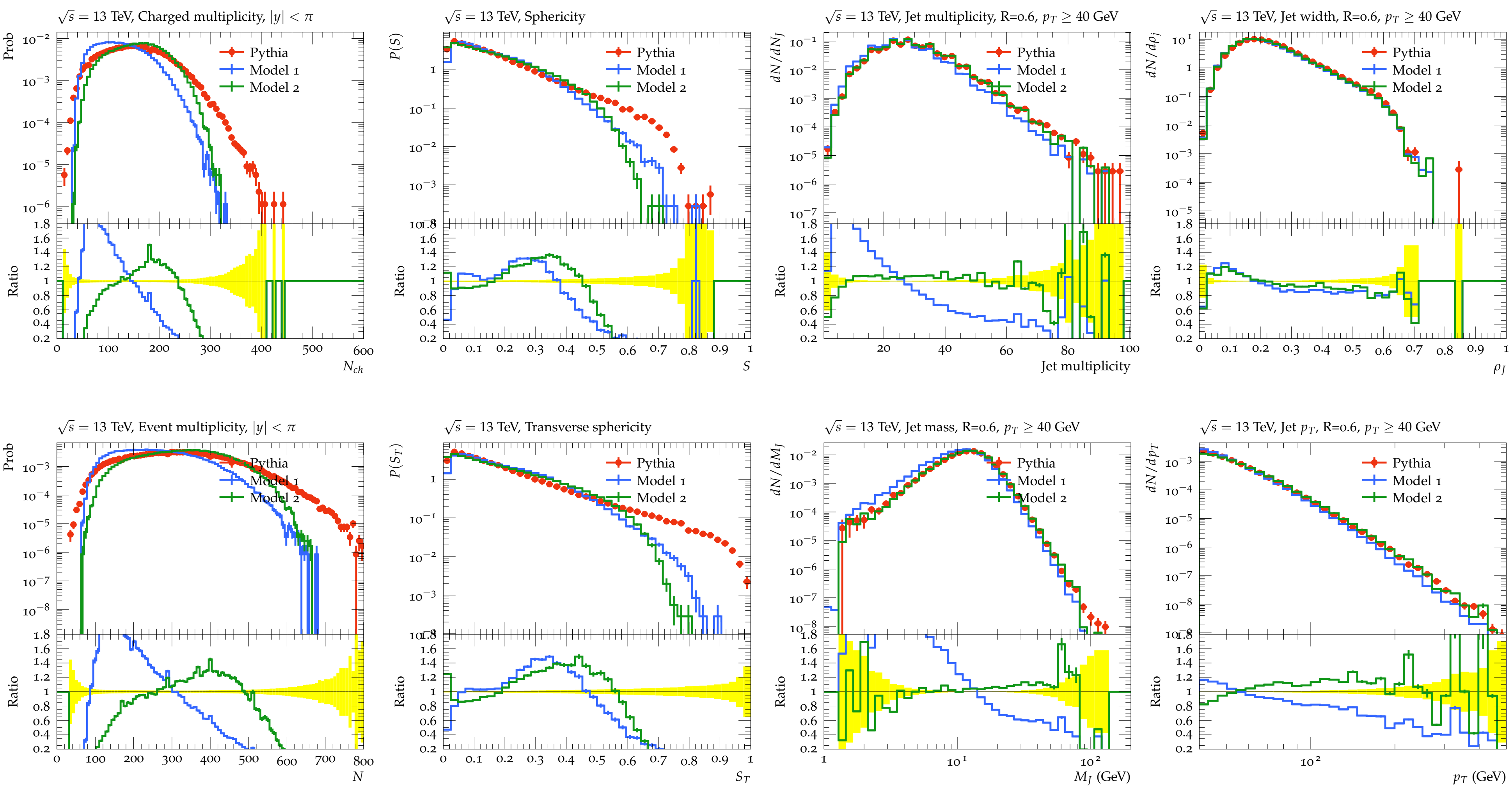
Center-of-mass energy scaling

	Model 1	Model 2
Trainable parameters	1.13 M	1.90 M



Prediction at other CM energies

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



How to do it more effectively?

(WIP)

Dimensionality

Input:

Parton level

Discretized in the (y, ϕ) plane: p_x, p_y, p_z, E, m, multiplicity

$$\left.\begin{array}{ll} y \in [\pi, \pi], & \text{62 bins} \\ \phi \in [0, 2\pi] & \text{31 bins} \end{array}\right\} := M$$

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

vs

$\mathcal{O}(10^2)$ Pixels with information

Reduction with Singular Value Decomposition:

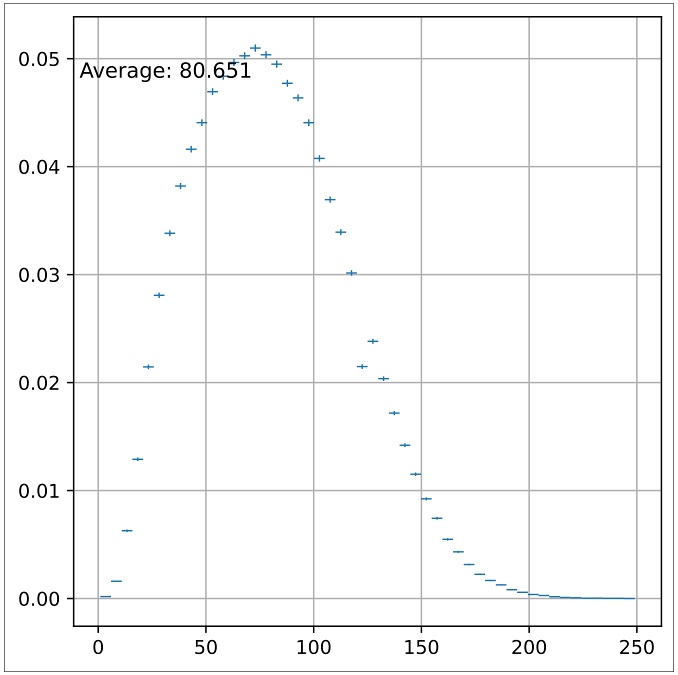
$$M_{n\times m} = U_{n\times n}\Sigma_{n\times m}V^T_{m\times m}$$

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

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

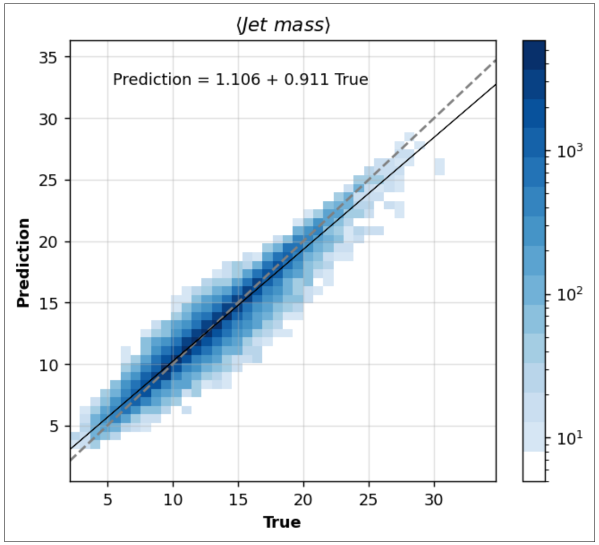
Reduce the input to $\mathcal{O}(10^2)$

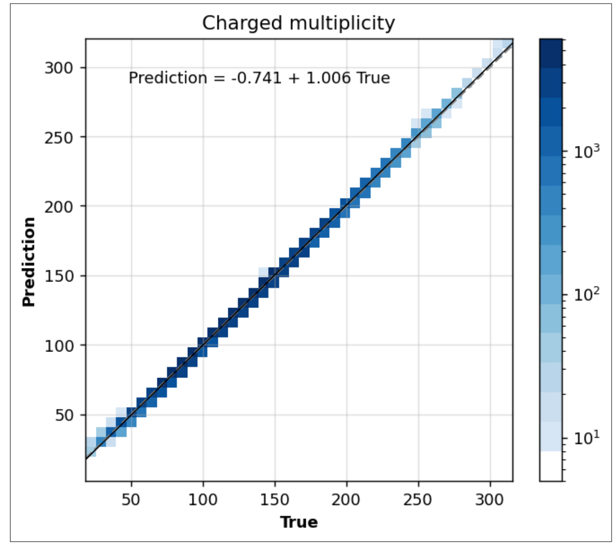
doi:10.1007/BF02288367

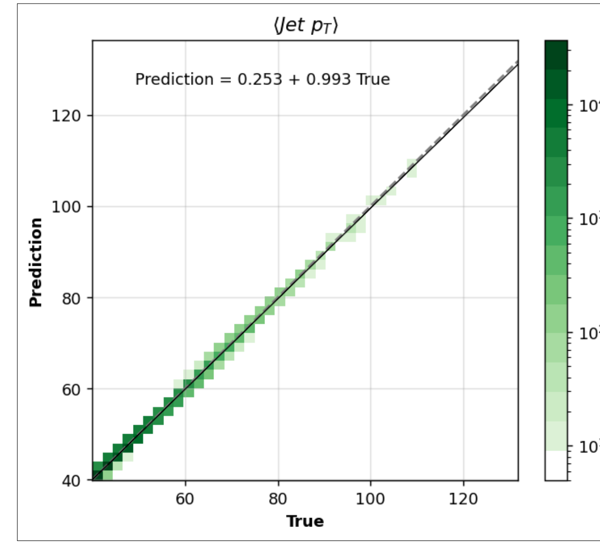


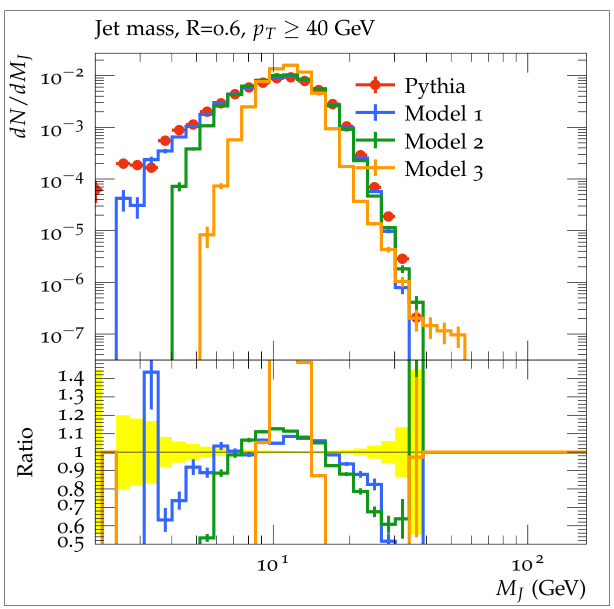
Data-Driven Science and Engineering (S. L. Brunton, J. N. Kutz)

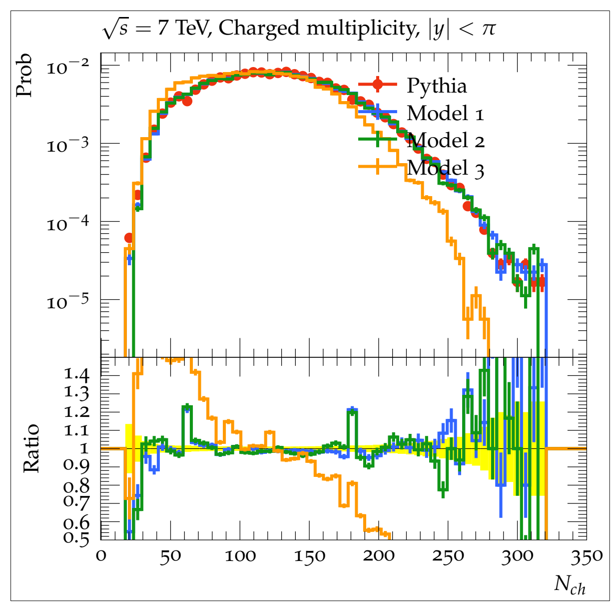
Dimensionality (work in progress)

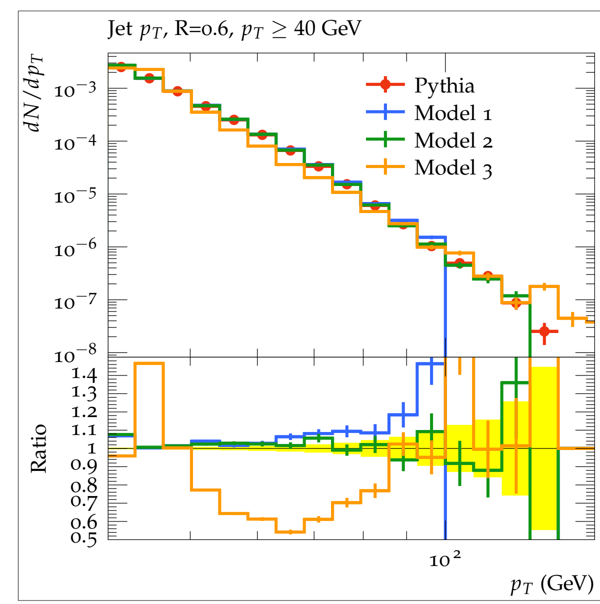












Summary

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

Generalization to other CM energies: multiplicity scaling

Prospects

Dimensional reduction

Various architectures (hyperparameter fine-tuning)

Other observables (p_T, rapidity, particle species)

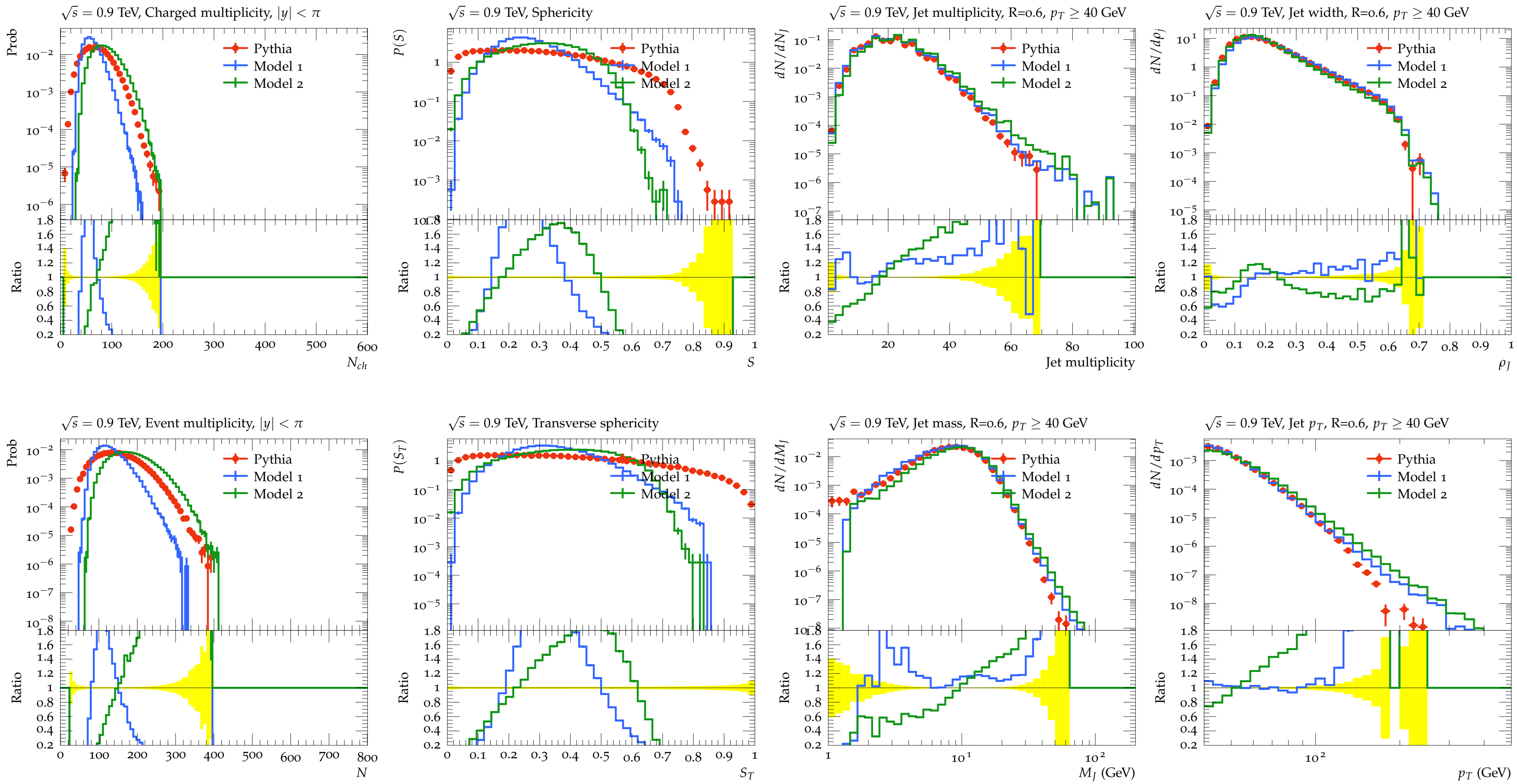
Heavy ion (centralities, collective effects)

Thank you for your attention!

The research was supported by OTKA grants K135515, K123815, NKFIH 2019-2.1.6-NEMZKI-2019-00011, 2020-2.1.1-ED-2021-00179, the **Wigner Scientific Computational Laboratory** (former Wigner GPU Laboratory) and NKFIH within the framework of the MILAB Artificial Intelligence National Laboratory Program.

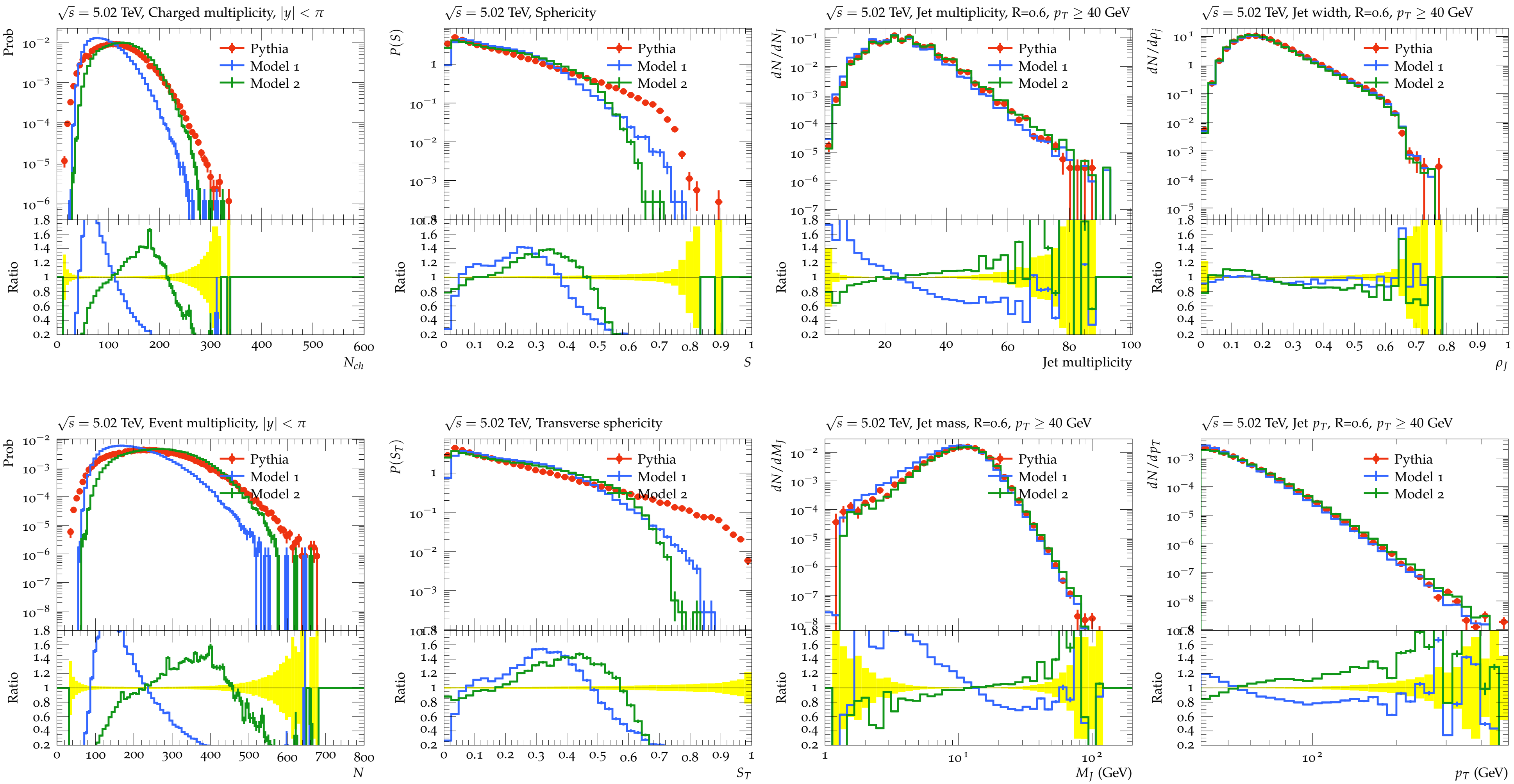
Prediction at other CM energies

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



Prediction at other CM energies

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



Machine Learning in HEP

Track reconstruction

Particle Track Reconstruction with Deep Learning

Steven Farrell, Paolo Calafiura, Mayur Mudigonda, Prabhat
Lawrence Berkeley National Laboratory
{SFarrell,PCalafiura,Mudigonda,Prabhat}@lbl.gov

Dustin Anderson, Josh Bendavid, Maria Spiropoulou, Jean-Roch Vlimant, Stephan Zheng
California Institute of Technology
{dustinanderson111,joshbendavid,maria.spiropulu, jeanroch.vlimant,st.t.zheng}@gmail.com

Giuseppe Cerati, Lindsey Gray, Keshav Kapoor, Jim Kowalkowski, Panagiotis Spentzouris, Aristeidis Tsaris, Daniel Zurawski
Fermi National Accelerator Laboratory
{cerati,lagray,kkapoor,jbk,spentz, atsaris,zurawski}@fnal.gov

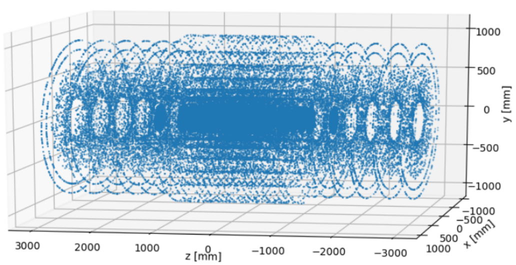
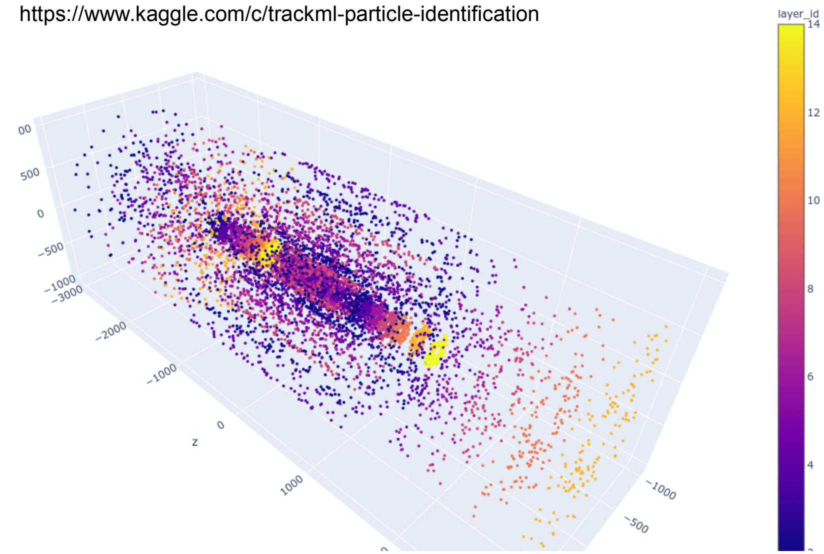
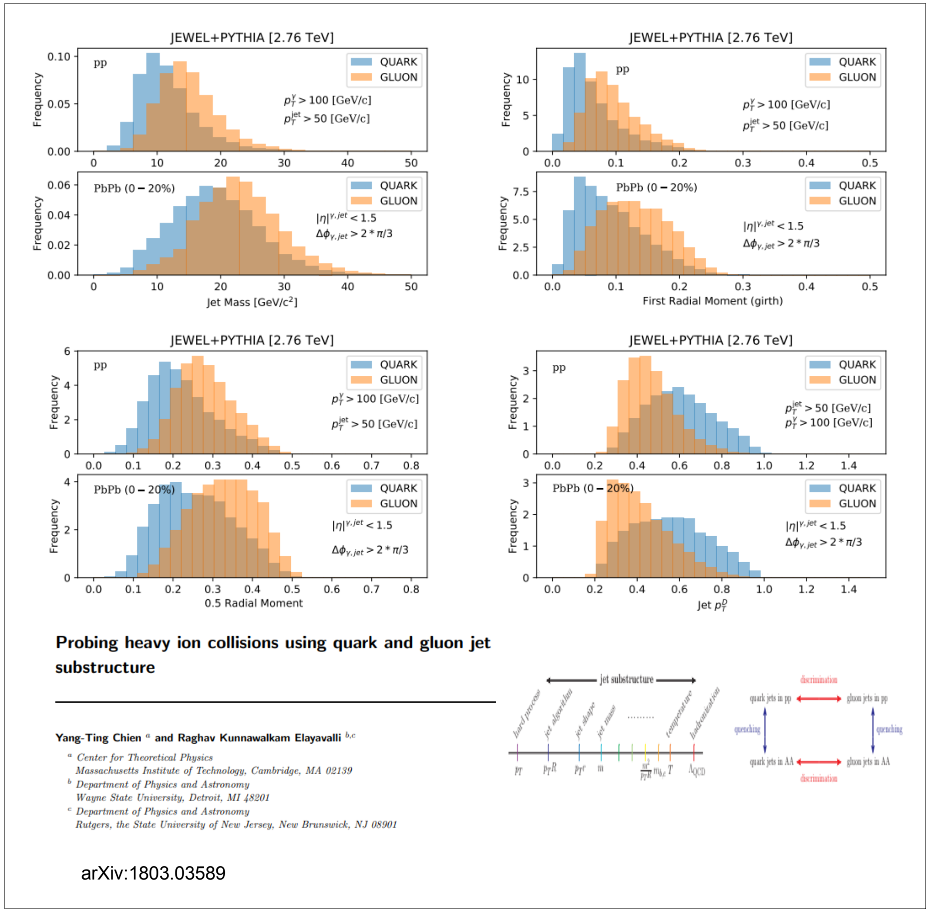


Figure 1: Distribution of particle spacepoints in a particle collision event in a generic simulated HL-LHC tracking detector.

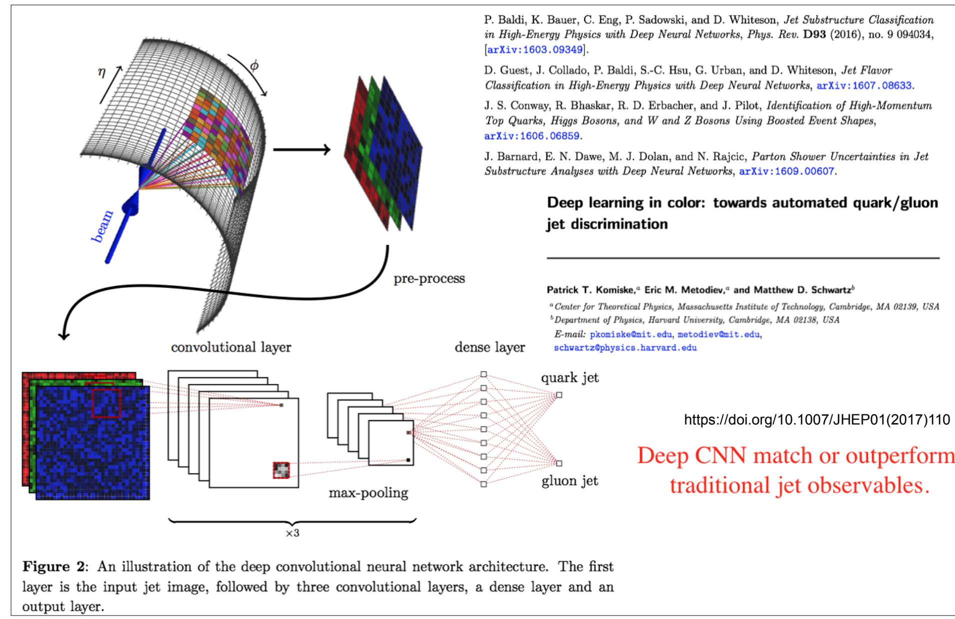
https://www.kaggle.com/c/trackml-particle-identification



Machine Learning in HEP



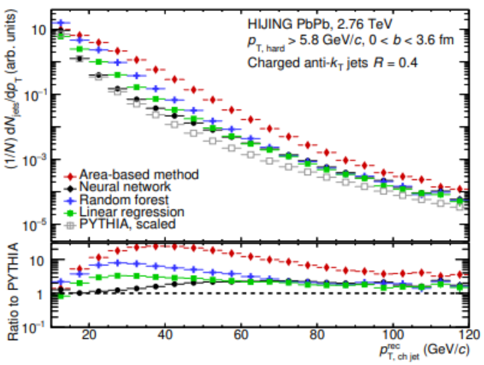
Quark/gluon jet separation



Machine Learning in HEP

Machine Learning based jet momentum reconstruction in heavy-ion collisions

Rüdiger Haake[1] and Constantin Loizides[2]
[1]*Yale University, Wright Laboratory, New Haven, CT, USA*
[2]*ORNL, Physics Division, Oak Ridge, TN, USA*
(Dated: June 24, 2019)



Feature	Score	Feature	Score
Jet p_T (no corr.)	**0.1355**	$p^1_{\mathrm{T,const}}$	0.0012
Jet mass	0.0007	$p^2_{\mathrm{T,const}}$	**0.0039**
Jet area	0.0005	$p^3_{\mathrm{T,const}}$	0.0015
Jet p_T (area-based corr.)	**0.7876**	$p^4_{\mathrm{T,const}}$	0.0011
LeSub	0.0004	$p^5_{\mathrm{T,const}}$	0.0009
Radial moment	0.0005	$p^6_{\mathrm{T,const}}$	0.0009
Momentum dispersion	0.0007	$p^7_{\mathrm{T,const}}$	0.0008
Number of constituents	0.0008	$p^8_{\mathrm{T,const}}$	0.0007
Mean of const. p_T	**0.0585**	$p^9_{\mathrm{T,const}}$	0.0006
Median of const. p_T	0.0023	$p^{10}_{\mathrm{T,const}}$	0.0007

FIG. 9. Reconstructed charged jet spectra in HIJING events and the ratio to (N_{coll}-scaled) PYTHIA jet spectra.

https://doi.org/10.1103/PhysRevC.99.064904

Jet reconstruction

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

Rüdiger Haake* **for the ALICE Collaboration**
Yale University, Wright Laboratory, New Haven, CT, USA
E-mail: ruediger.haake@cern.ch

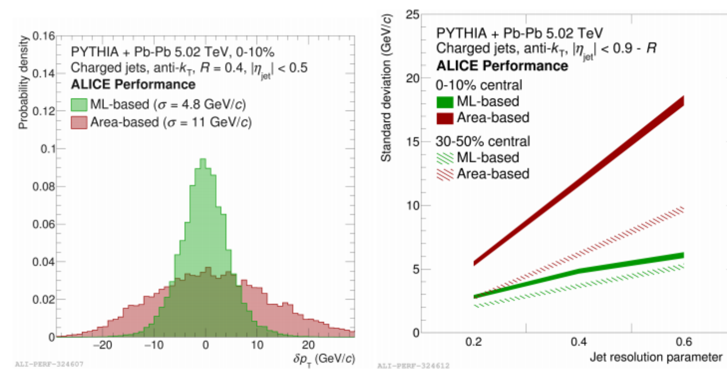
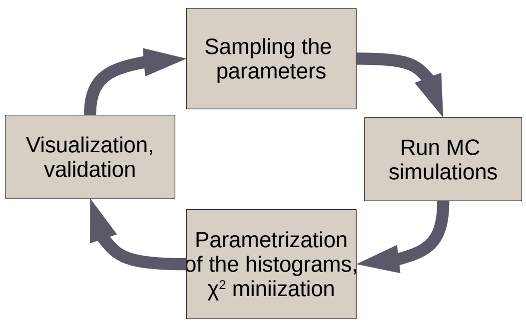


Figure 1: Residual p_T-distributions of embedded jet probes of known transverse momentum.

https://doi.org/10.22323/1.364.0312

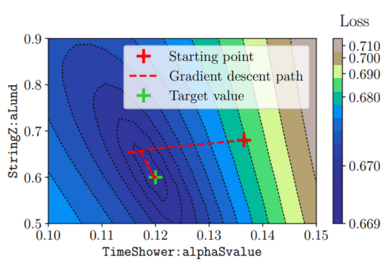
Machine Learning in HEP

Tuning Monte Carlo event generators



Neural Networks for Full Phase-space Reweighting and Parameter Tuning

Anders Andreassen[1,2,*] and Benjamin Nachman[2,†]
[1] *Department of Physics, University of California, Berkeley, CA 94720, USA*
[2] *Physics Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*



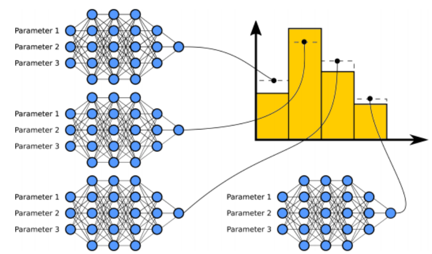


Figure 1: An illustration of the parametrisation of the generator response as implemented in the Per Bin Model.

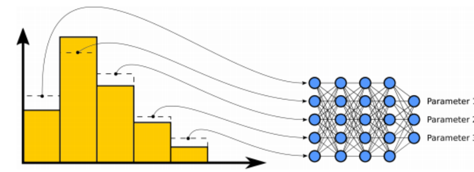


Figure 2: An illustration of the Inverse Model strategy.

MCNNTUNES: tuning Shower Monte Carlo generators with machine learning

Marco Lazzarin[a], Simone Alioli[b], Stefano Carrazza[a]
[a] *TIF Lab, Dipartimento di Fisica, Università degli Studi di Milano and INFN Sezione di Milano, Milan, Italy.*
[b] *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,[1,2,*] Luke de Oliveira,[1,†] and Benjamin Nachman[1,‡]
[1] *Lawrence Berkeley National Laboratory, Berkeley, CA 94720*
[2] *Yale University, New Haven, CT 06520*

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