

# Studying hadronization with Machine Learning techniques and event variables

ELTE PARTICLE PHYSICS SEMINAR

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Bence Tankó-Bartalis

**GÁBOR BÍRÓ**

16 11 2021

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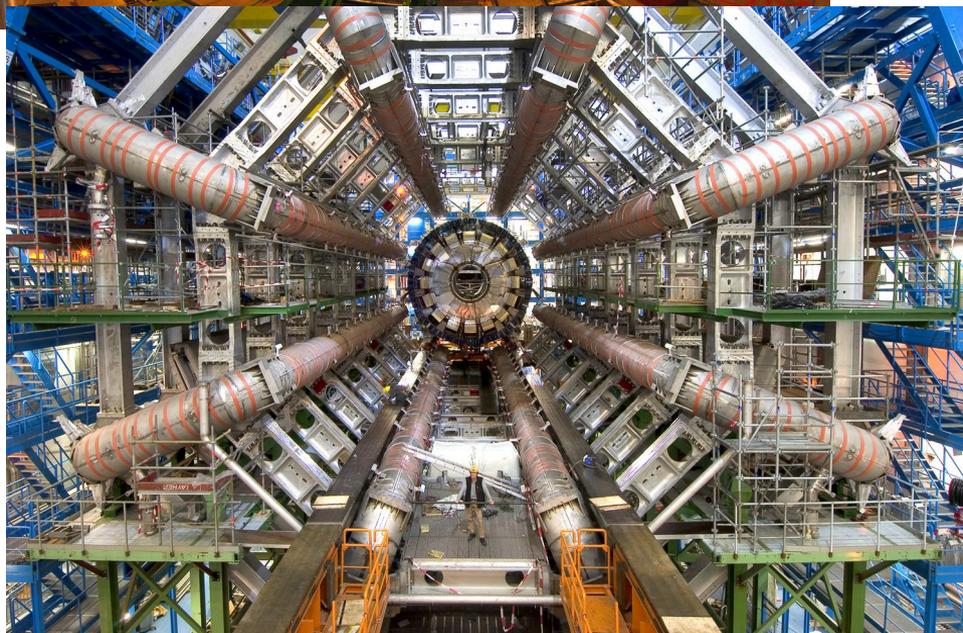
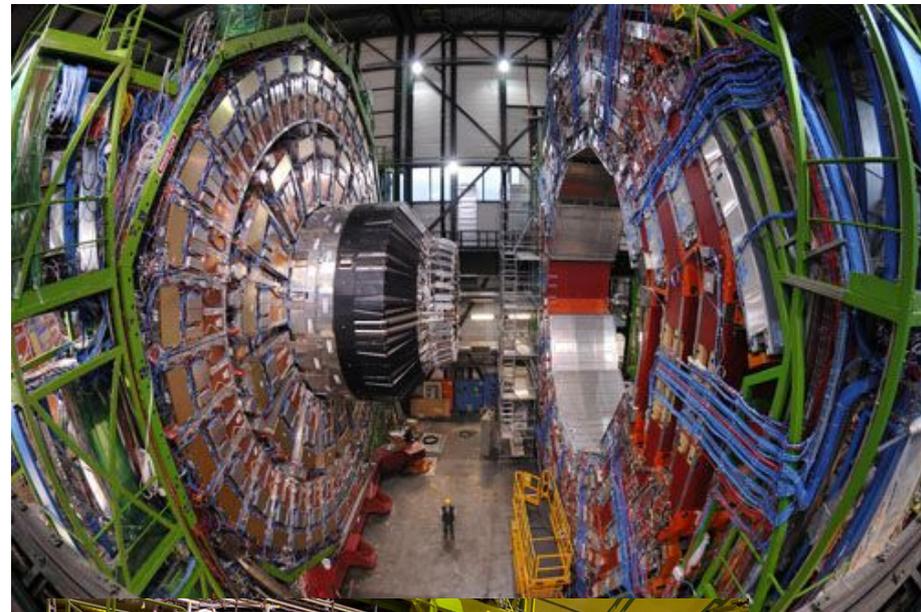


# Outline

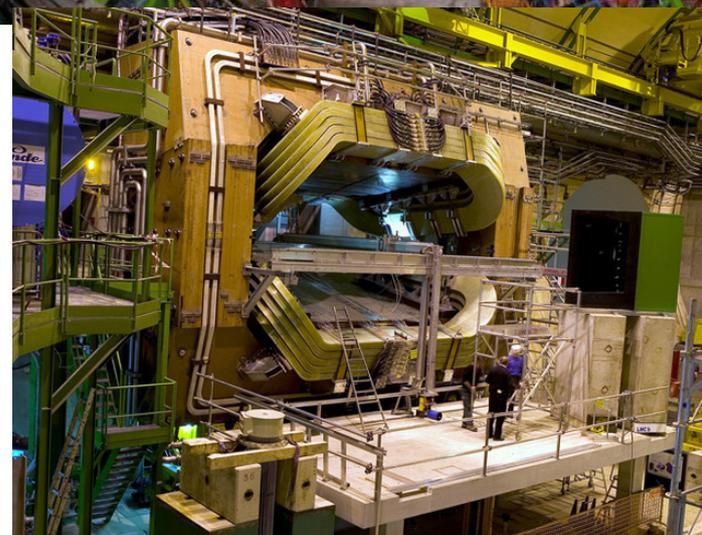
- Machine Learning: motivation
- Applications and examples
- Research goals
- Preliminary results
- Summary



**ALICE  
CMS**



**ATLAS  
LHCb**



# Data, data, and more data



## Large Hadron Collider data:

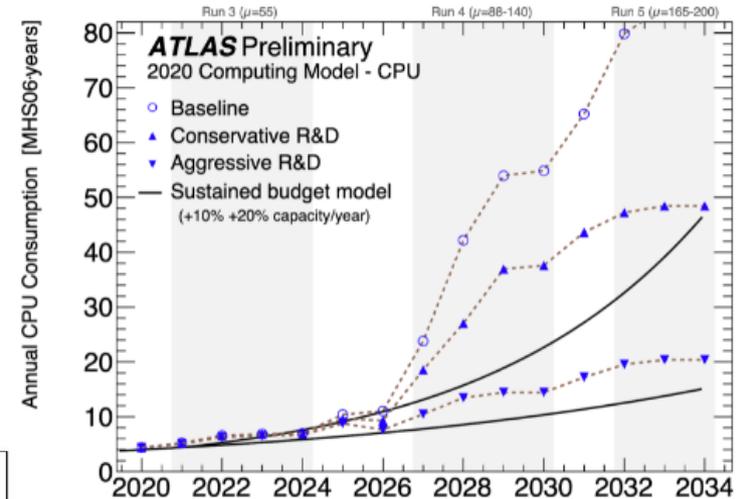
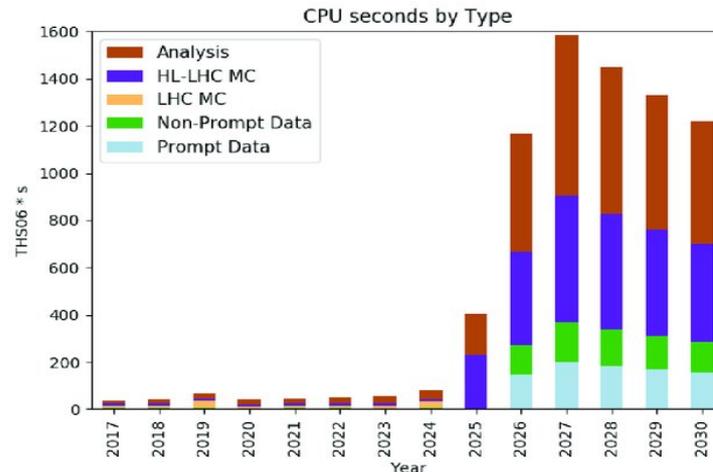
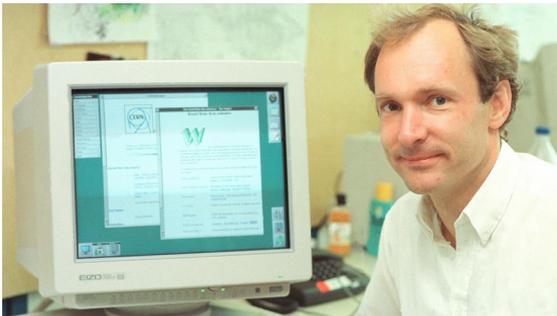
2021: 336 PB

From 2022: 200+ PB/year

## Simulations:

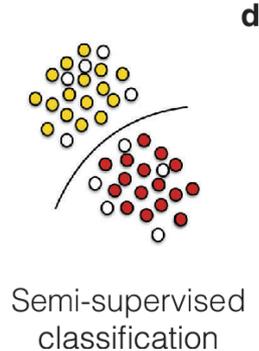
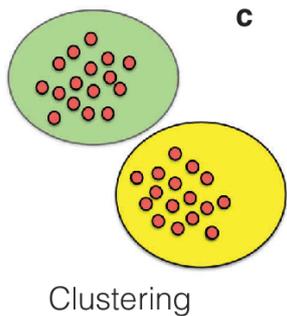
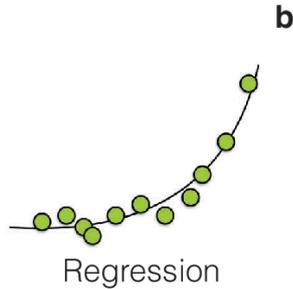
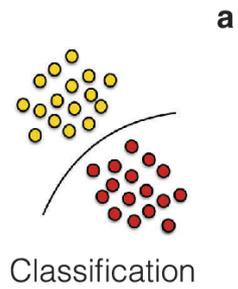
Computationally very expensive

1s LHC data ~ days of CPU time



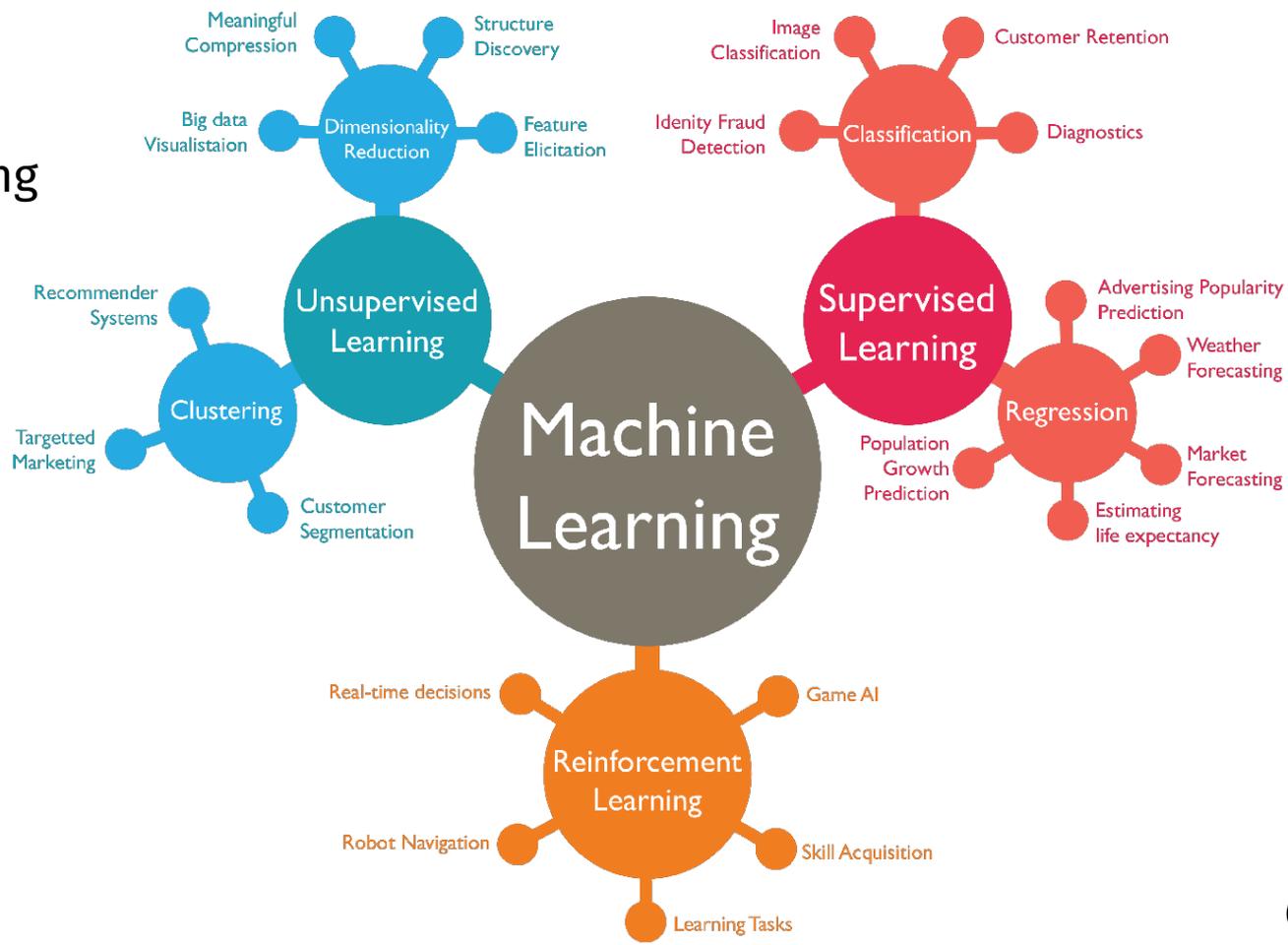
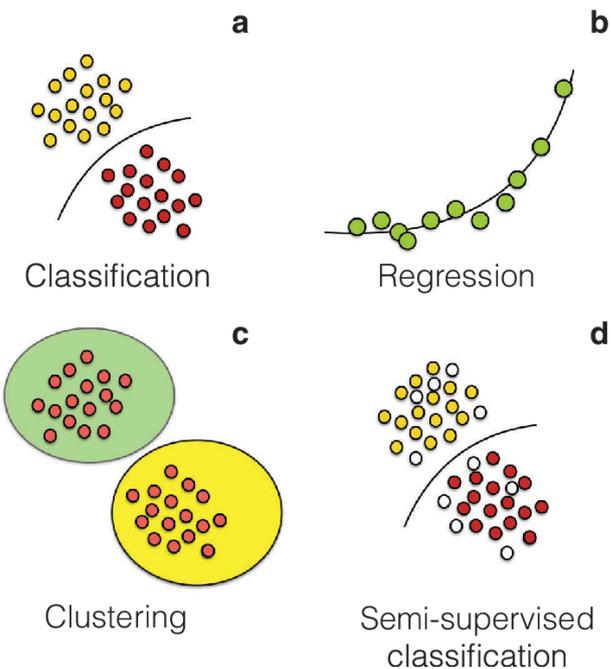
# Machine learning

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



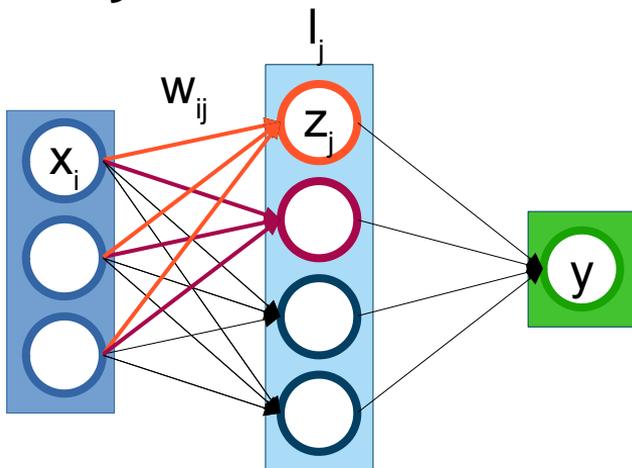
# Machine learning

- Data driven decisions
- Automated analysis
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# Basic building blocks of a neural network

## Fully connected (dense):



## Convolutional:

2	4	9	1	4
2	1	4	4	6
1	1	2	9	2
7	3	5	1	3
2	3	4	8	5

Image

x

1	2	3
-4	7	4
2	-5	1

Filter /  
Kernel

=

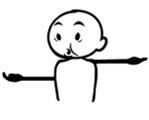
51		

Feature

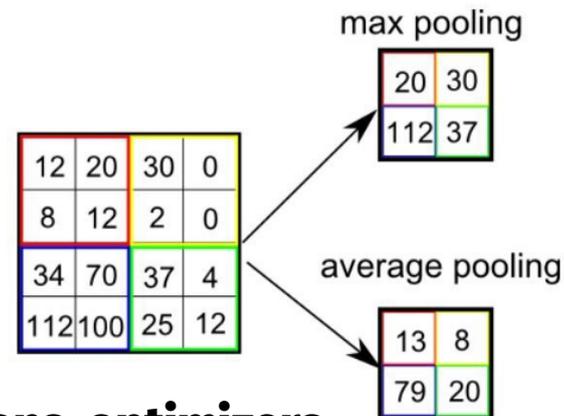
$$z_j = \sum_{i=1}^N x_i w_{ij} + b_j$$

# Basic building blocks of a neural network

## Activation functions:

<p>Sigmoid</p>  $y = \frac{1}{1 + e^{-x}}$	<p>Tanh</p>  $y = \tanh(x)$	<p>Step Function</p>  $y = \begin{cases} 0, & x < n \\ 1, & x \geq n \end{cases}$	<p>Softplus</p>  $y = \ln(1 + e^x)$
<p>ReLU</p>  $y = \begin{cases} 0, & x < 0 \\ x, & x \geq 0 \end{cases}$	<p>Softsign</p>  $y = \frac{x}{1 +  x }$	<p>ELU</p>  $y = \begin{cases} \alpha(e^x - 1), & x < 0 \\ x, & x \geq 0 \end{cases}$	<p>Log of Sigmoid</p>  $y = \ln\left(\frac{1}{1 + e^{-x}}\right)$
<p>Swish</p>  $y = \frac{x}{1 + e^{-x}}$	<p>Sinc</p>  $y = \frac{\sin(x)}{x}$	<p>Leaky ReLU</p>  $y = \max(\alpha x, x)$	<p>Mish</p>  $y = x(\tanh(\text{softplus}(x)))$

## Pooling:



## 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

### Available optimizers

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

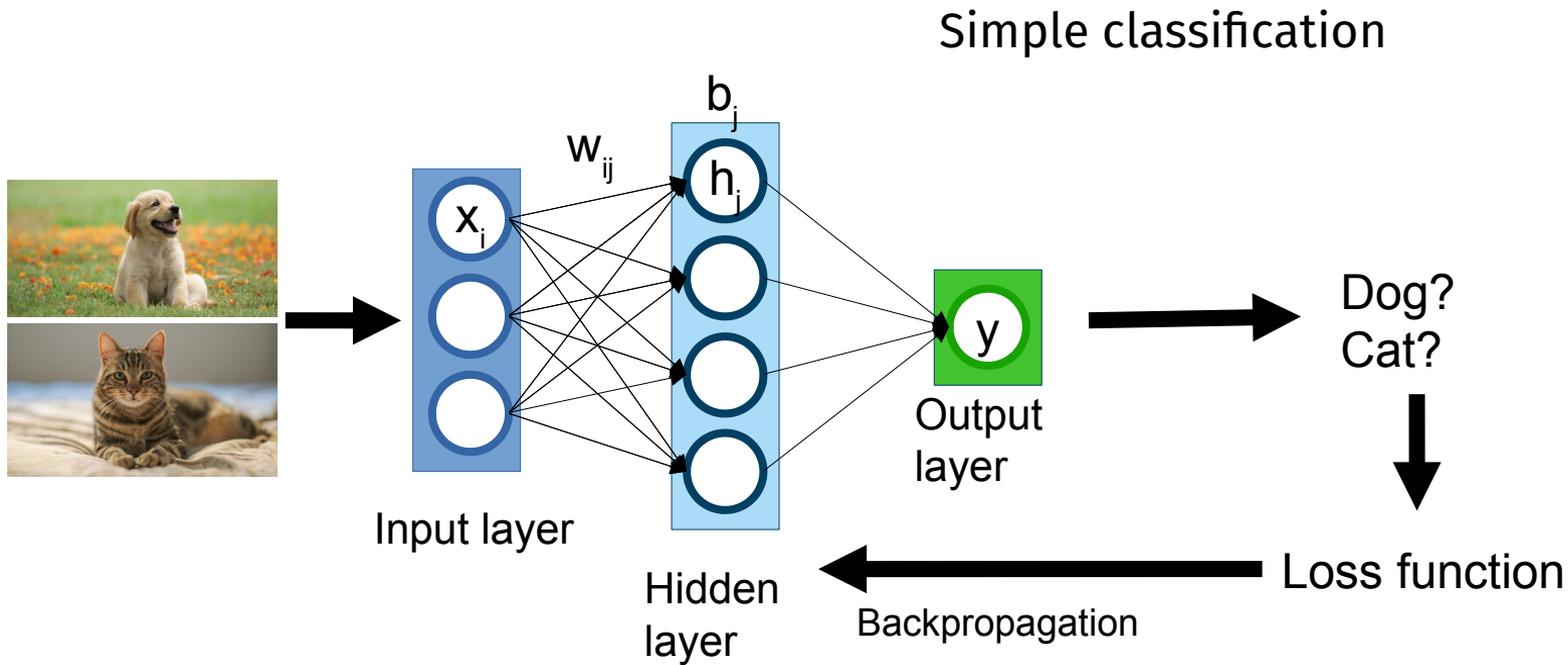
### Probabilistic losses

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

### Hinge losses for "maximum-margin" classification

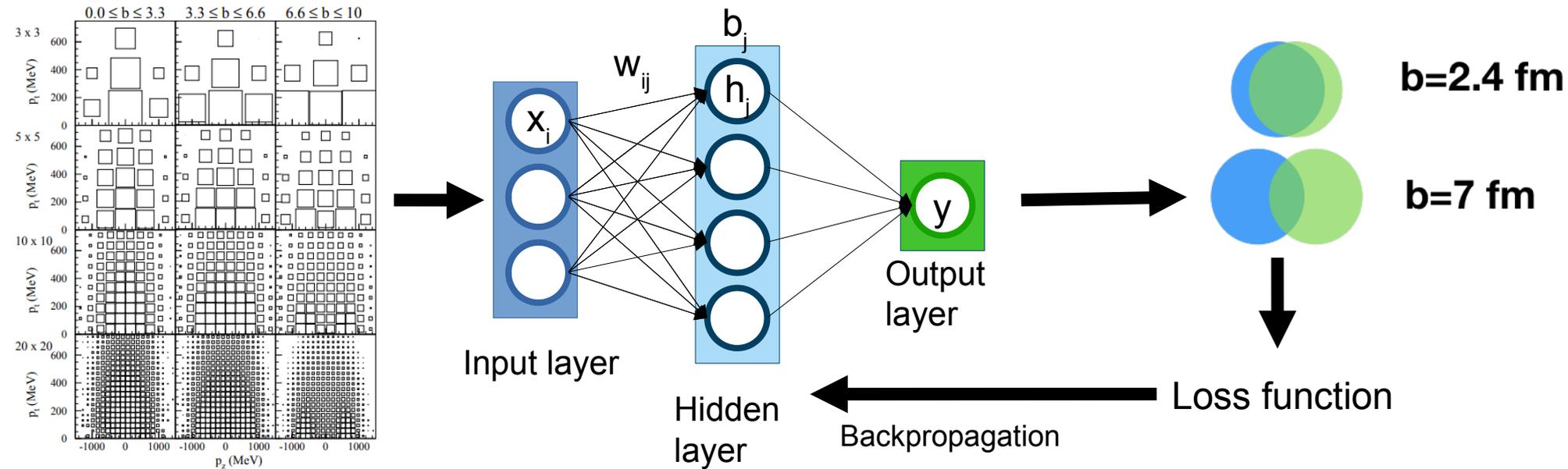
- Hinge class
- SquaredHinge class
- CategoricalHinge class

# Example: FCNN



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

# Example: FCNN



# Popular architectures

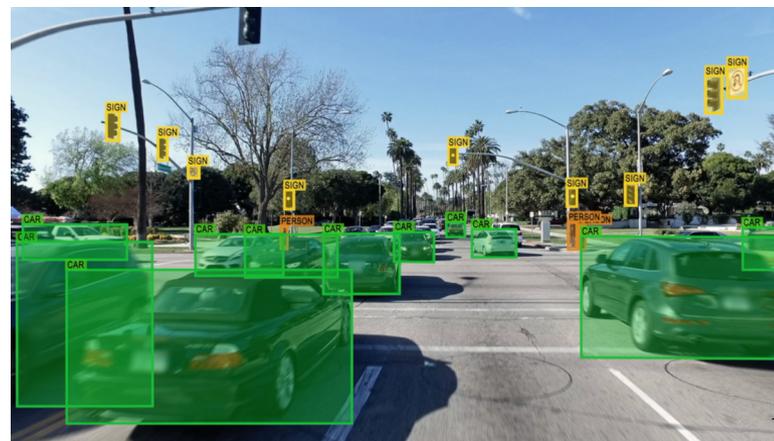
## Classifiers

- 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](https://github.com/facebookresearch/detectron2))



## Autonomous vehicles

## Decision trees

## Transformers

Generative adversarial networks (<https://bit.ly/2YMCfDy>)

(Variational) autoencoders

...

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## 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,spetz,  
atsaris,zurawski}@fnal.gov

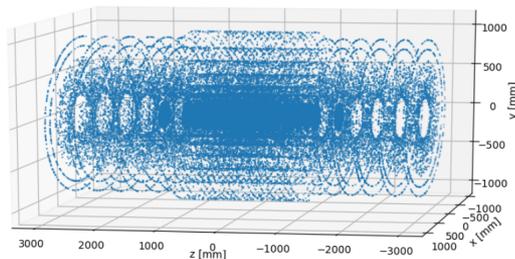
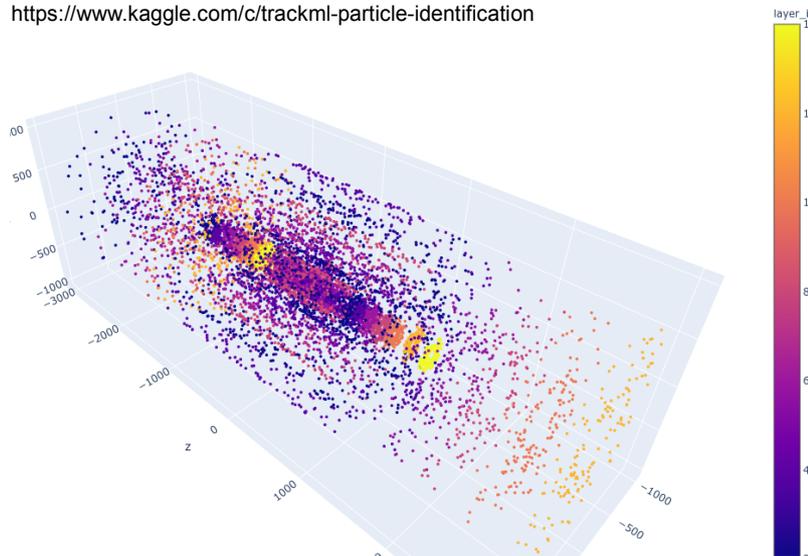


Figure 1: Distribution of particle spacepoints in a particle collision event in a generic simulated HL-LHC tracking detector.

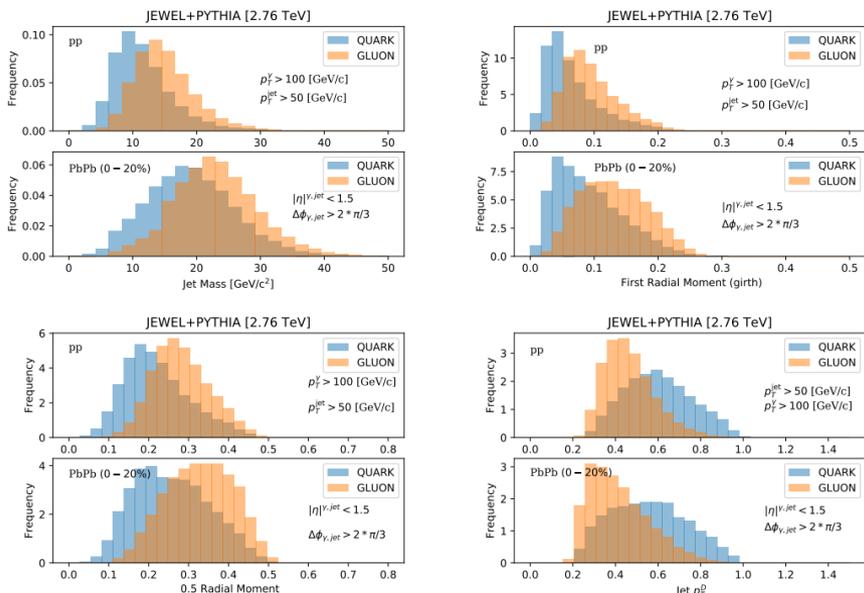


Featured Prediction Competition  
**TrackML Particle Tracking Challenge**  
High Energy Physics particle tracking in CERN detectors  
\$25,000 Prize Money  
CERN · 651 teams · 3 years ago

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



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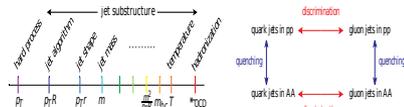
## Probing heavy ion collisions using quark and gluon jet substructure

Yang-Ting Chien<sup>a</sup> and Raghav Kunnawalkam Elayavalli<sup>b,c</sup>

<sup>a</sup> Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139

<sup>b</sup> Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201

<sup>c</sup> Department of Physics and Astronomy, Rutgers, the State University of New Jersey, New Brunswick, NJ 08901



arXiv:1803.03589

## Quark/gluon jet separation

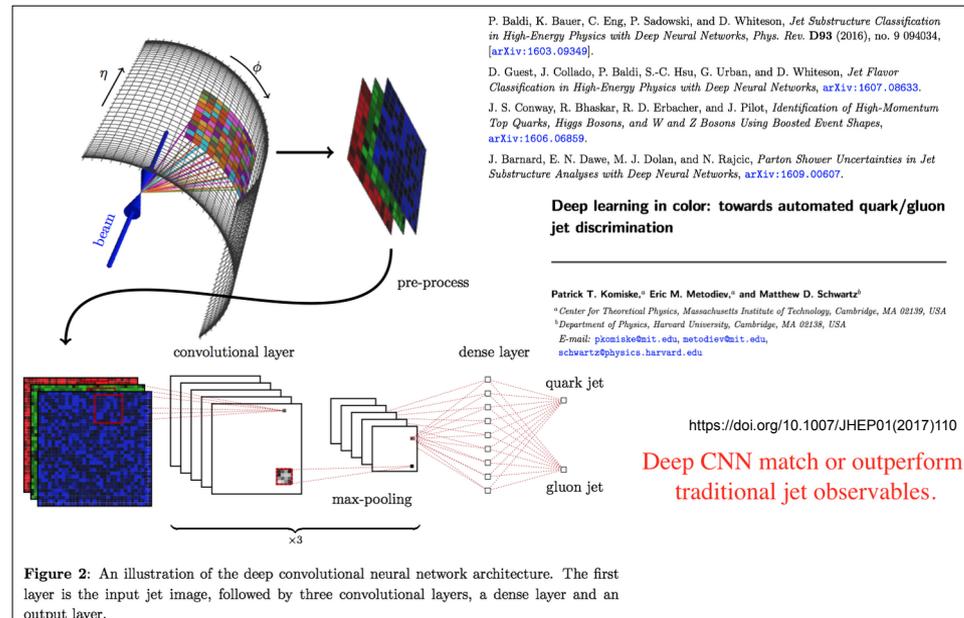


Figure 2: An illustration of the deep convolutional neural network architecture. The first layer is the input jet image, followed by three convolutional layers, a dense layer and an output layer.

# Machine Learning in HEP

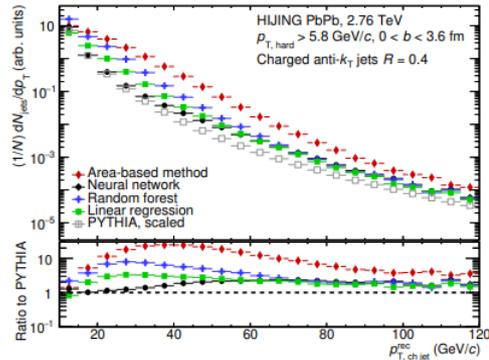
## Machine Learning based jet momentum reconstruction in heavy-ion collisions

Rüdiger Haake<sup>1</sup> and Constantin Loizides<sup>2</sup>

<sup>1</sup>Yale University, Wright Laboratory, New Haven, CT, USA

<sup>2</sup>ORNL, Physics Division, Oak Ridge, TN, USA

(Dated: June 24, 2019)



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

FIG. 9. Reconstructed charged jet spectra in HIJING events and the ratio to ( $N_{\text{coll}}$ -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](mailto:ruediger.haake@cern.ch)

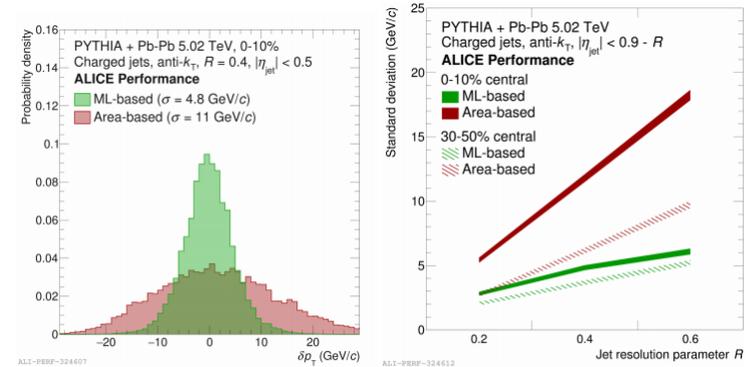
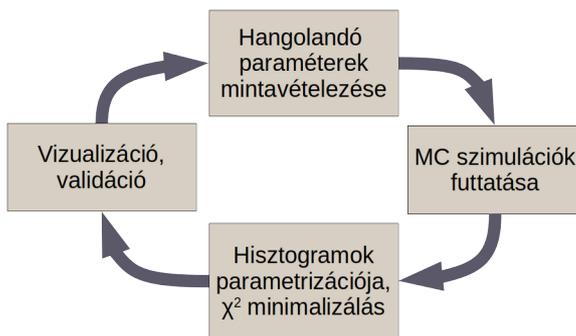


Figure 1: Residual  $p_T$ -distributions of embedded jet probes of known transverse momentum.

<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<sup>1,2,\*</sup> and Benjamin Nachman<sup>2,†</sup>

<sup>1</sup>Department of Physics, University of California, Berkeley, CA 94720, USA

<sup>2</sup>Physics Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

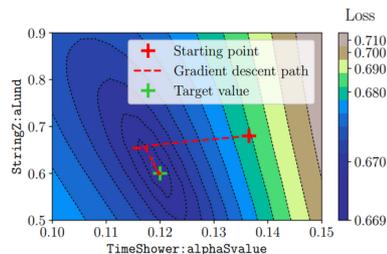


Figure 1: An illustration of the parametrization of the generator response as implemented in the Per Bin Model.

Figure 2: An illustration of the Inverse Model strategy.

MCNNTUNES: tuning Shower Monte Carlo generators with machine learning

Marco Lazzarin<sup>a</sup>, Simone Alioli<sup>b</sup>, Stefano Carrazza<sup>a</sup>

<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>



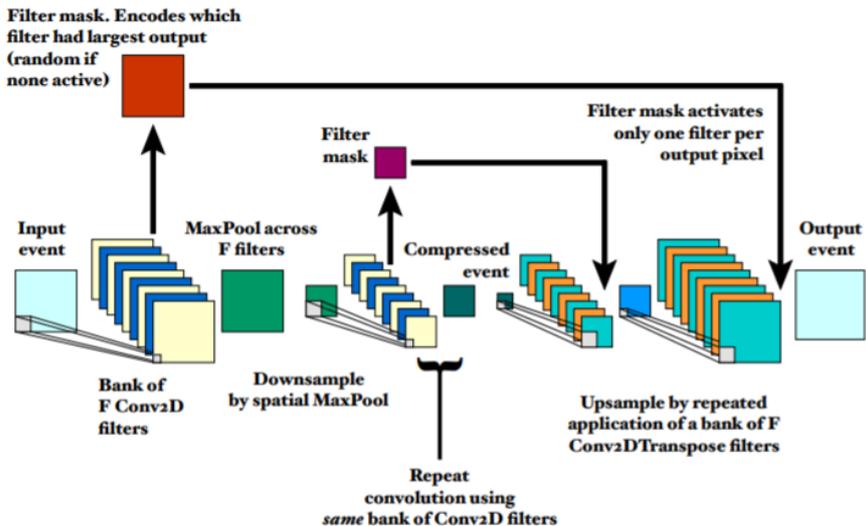
# **Parton shower and hadronization**

# Parton shower

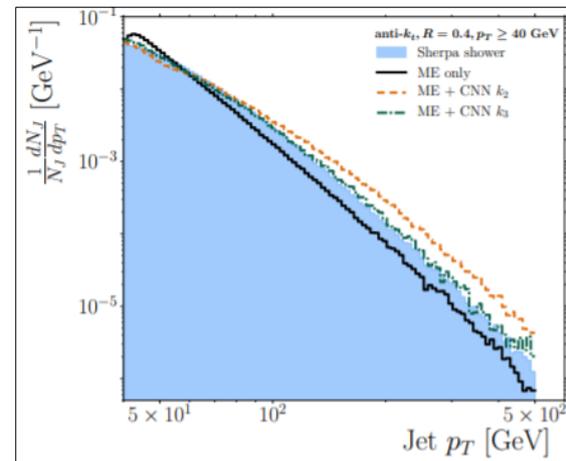
J.W. Monk: Deep Learning as a Parton Shower (arXiv:1807.03685)

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, $\lambda$	500	300
Learning rate	$5 \times 10^{-5}$	$1 \times 10^{-5}$
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



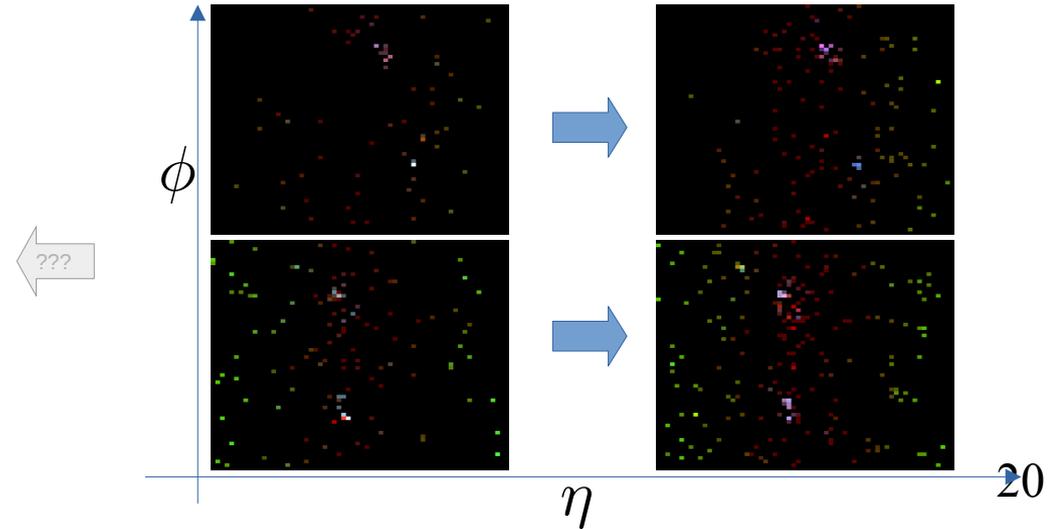
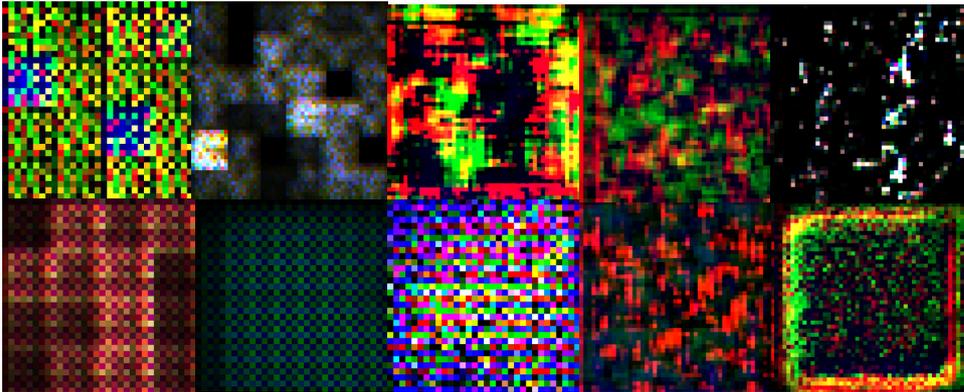
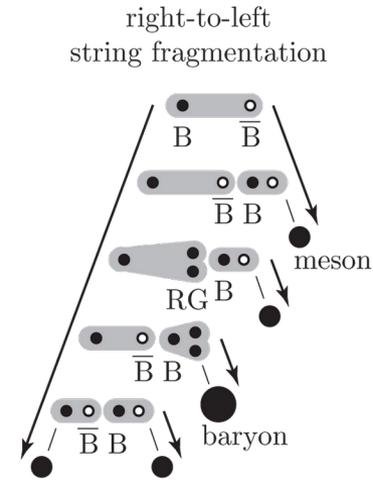
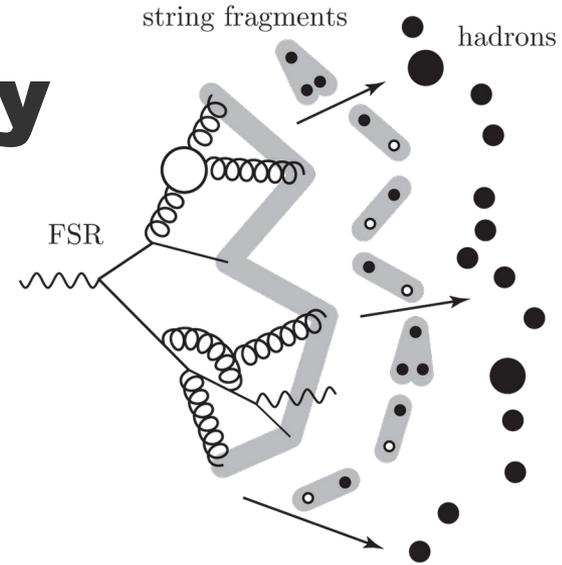
# The goal of this study

## Hadronization

Partons  $\rightarrow$  hadrons

Non-perturbative process

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





“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: 100 000
- Validation: 30 000
- ~17 GB raw data

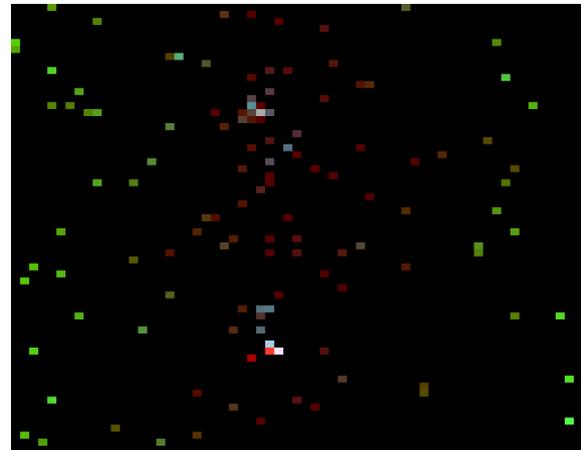
## Input:

Parton level

Discretized in the  $(y, \phi)$  plane:  $p_x, p_y, p_z, E, m$ , multiplicity

$$y \in [-\pi, \pi], \quad 81 \text{ bins}$$

$$\phi \in [0, 2\pi], \quad 54 \text{ bins}$$



# Train and validation sets

## Output:

Hadron level

Event multiplicity, #jets, aplanarity, sphericity, tr-sphericity

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

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

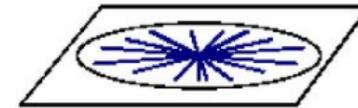
Sphericity:  $S = \frac{3}{2}(\lambda_2 + \lambda_3)$

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

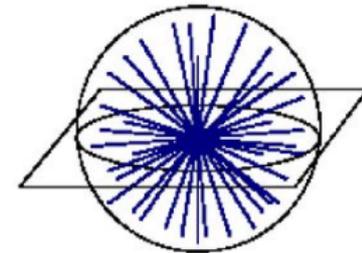
Aplanarity:  $A = \frac{3}{2}\lambda_3$



**S=A=0**



**S=3/4 A=0**



**S=1 A=1/2**

# Models

	<b>Model 1</b>	<b>Model 2</b>	<b>Model 3</b>	<b>Model 4</b>
<b>Base</b>	ResNet-32	ResNet-32	DenseNet-4x4	DenseNet-5x5
<b>Last activation</b>	Sigmoid	Sigmoid	Sigmoid	Sigmoid
<b>Loss</b>	Huber	Binary crossentropy	Binary crossentropy	Binary crossentropy
<b>Trainable parameters</b>	468 373	468 373	422 984	1 137 295

Used hardwares: Nvidia Tesla T4, GeForce GTX 1080, GeForce GTX 980

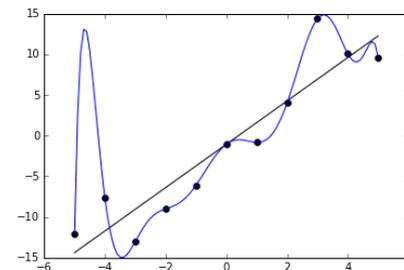
Framework: Tensorflow 2.4.1, Keras 2.4.0

# ResNet and DenseNet variants

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

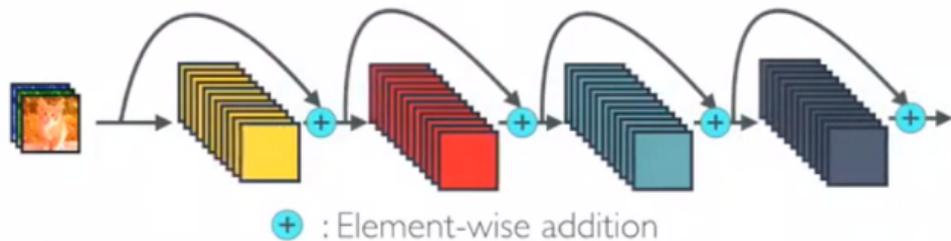
**BUT:**

Vanishing/exploding gradients (not to confuse with overfitting)



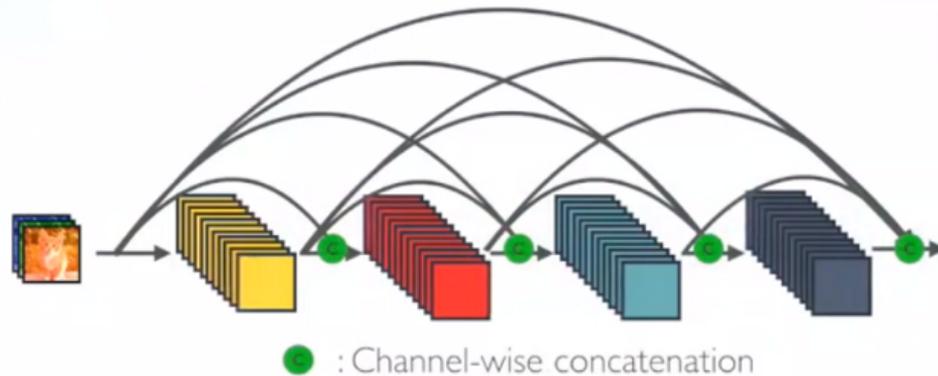
## ResNet

**Residual blocks with “skip connections”**



## DenseNet

**Each layer is receiving a “collective knowledge” from all preceding layers**



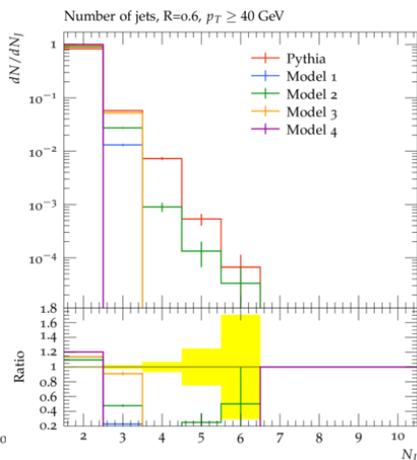
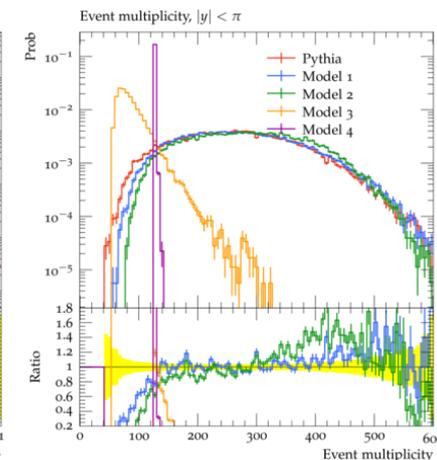
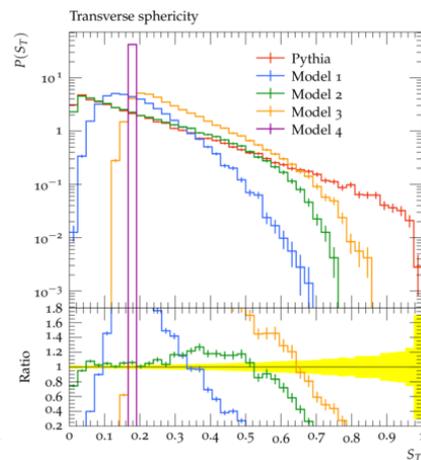
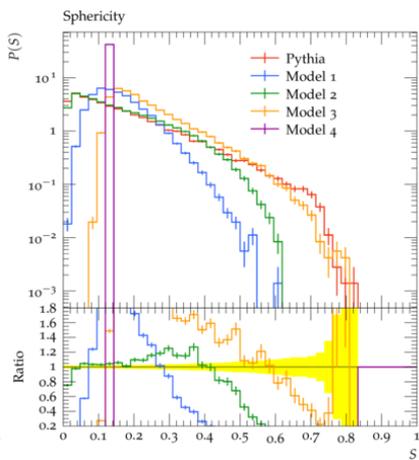
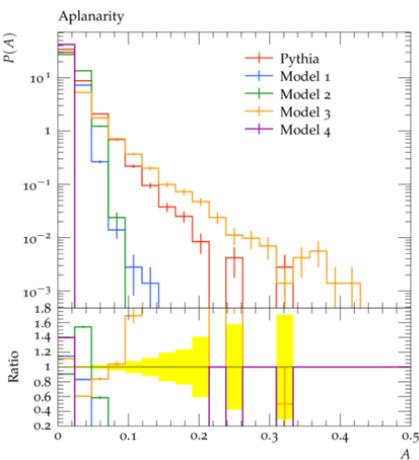
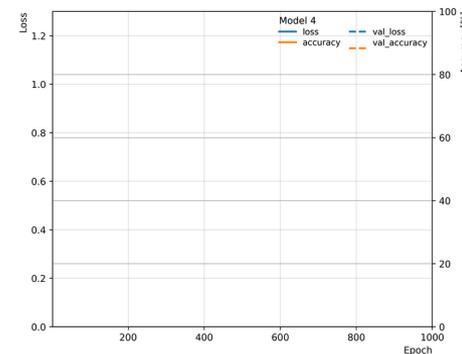
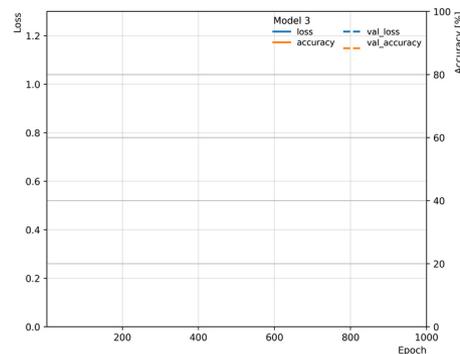
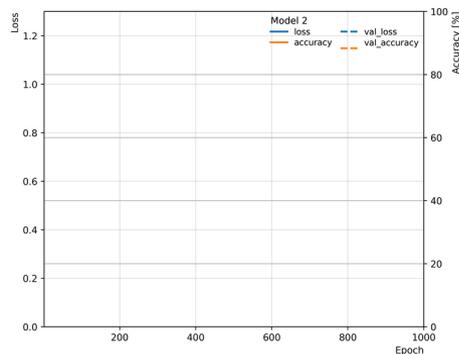
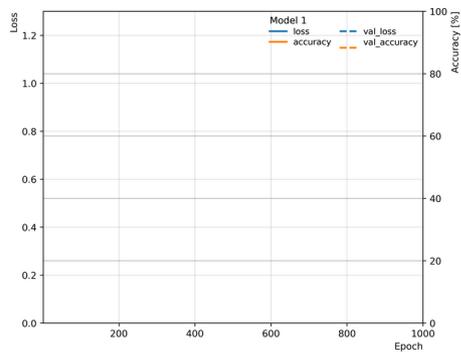


# **Preliminary results**

**(any feedback is very welcome!)**

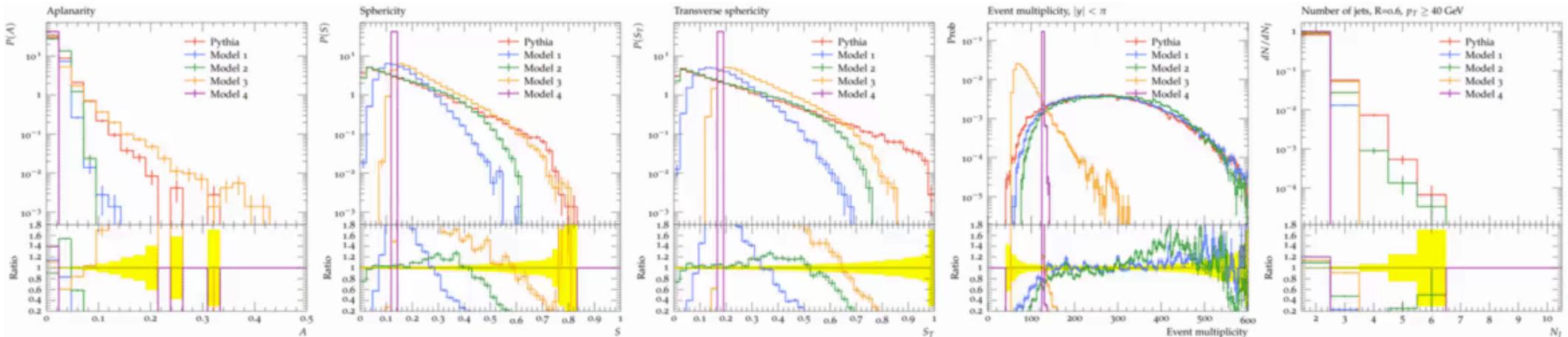
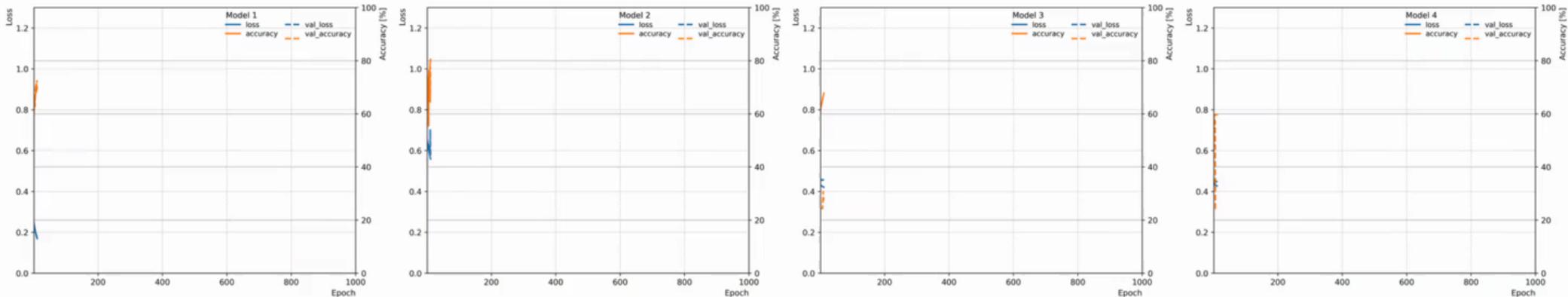
# Proton-proton @ 7 TeV Training + Validation

Model 1	Model 2	Model 3	Model 4
ResNet-Huber	ResNet-BinCrossE	DenseNet small	DenseNet large



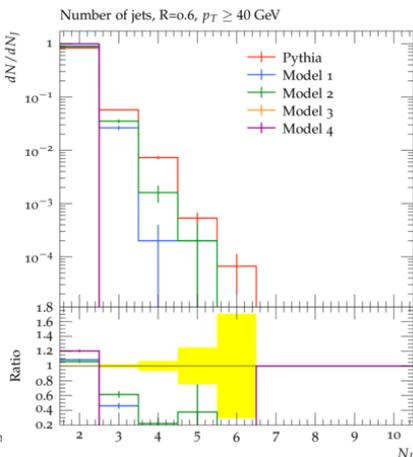
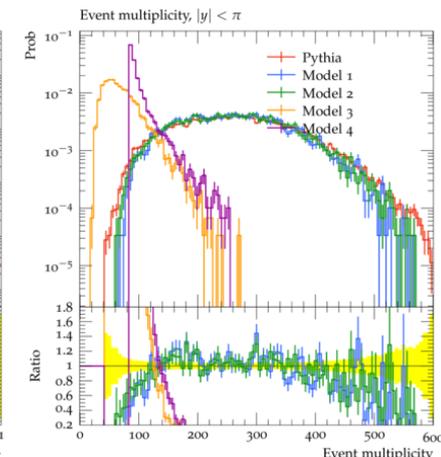
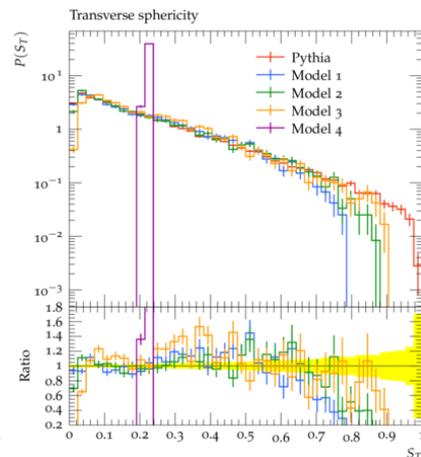
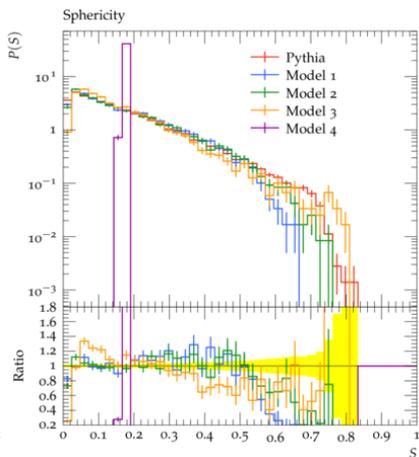
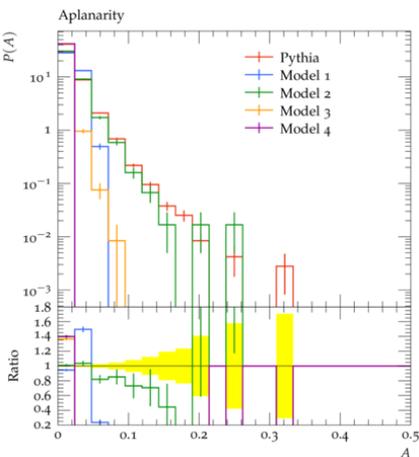
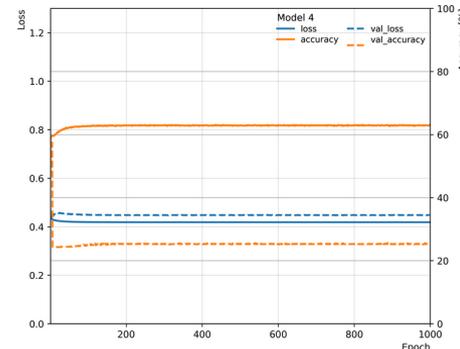
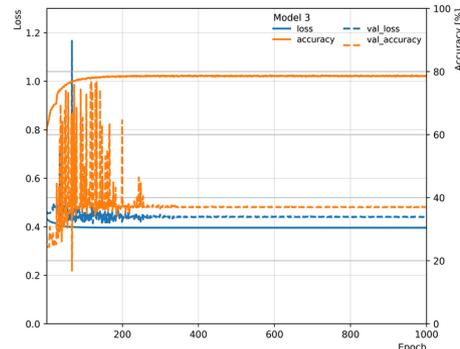
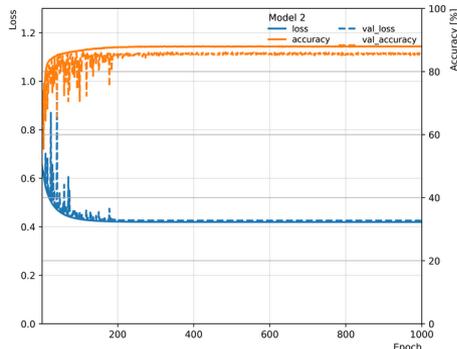
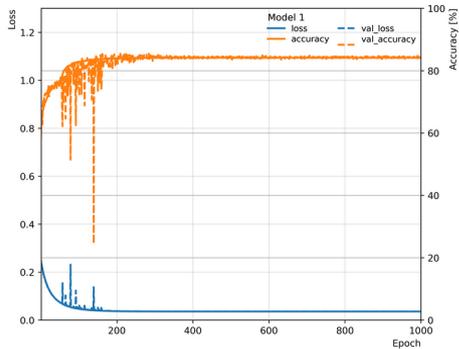
# Proton-proton @ 7 TeV Training + Validation

Model 1	Model 2	Model 3	Model 4
ResNet-Huber	ResNet-BinCrossE	DenseNet small	DenseNet large



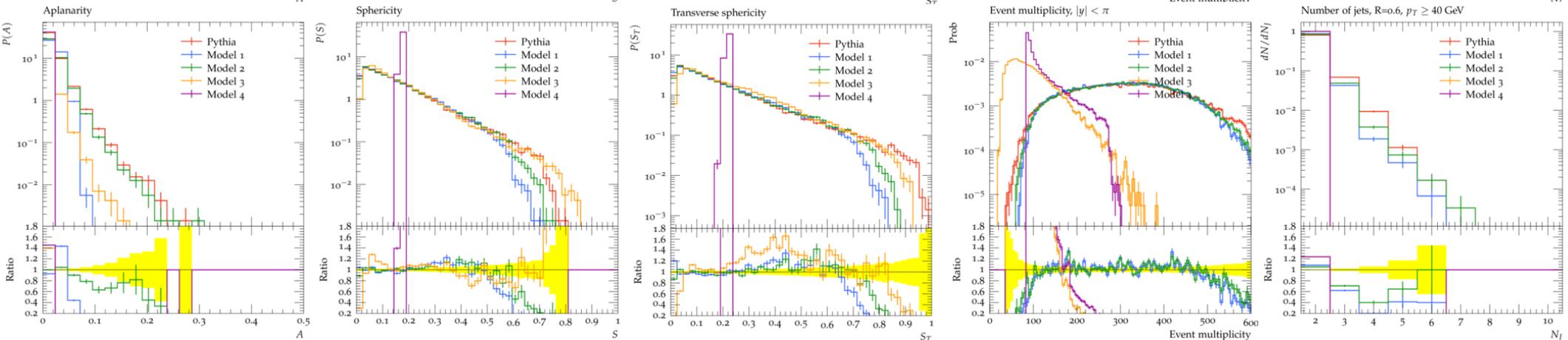
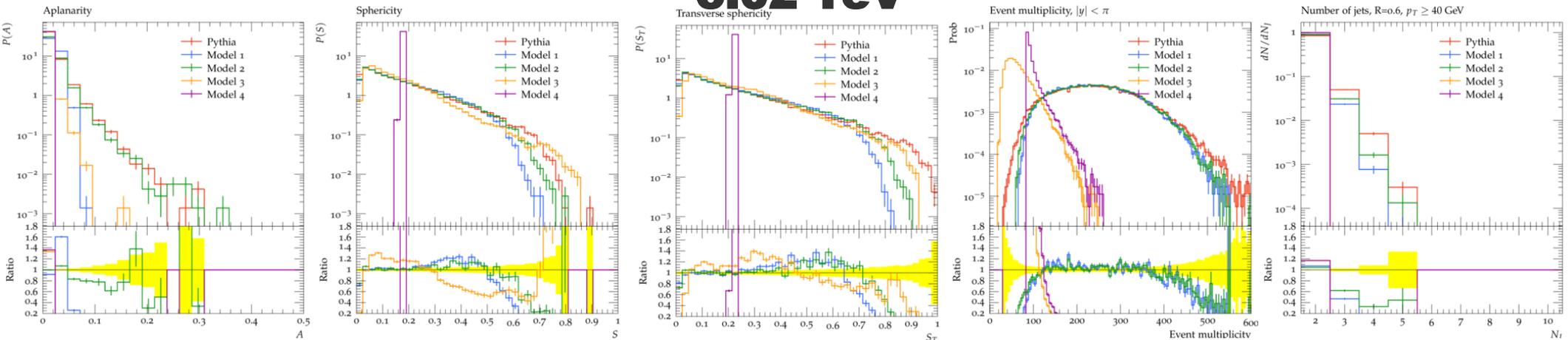
# Proton-proton @ 7 TeV Training + Validation

Model 1	Model 2	Model 3	Model 4
ResNet-Huber	ResNet-BinCrossE	DenseNet small	DenseNet large



# Proton-proton @ 5.02 TeV, 13 TeV Prediction

## 5.02 TeV



## 13 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)

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The research was supported by OTKA grants K135515, K123815, NKFIH 2019-2.1.6-NEMZKI-2019-00011, NKFIH within the framework of the MILAB Artificial Intelligence National Laboratory Program and by the Wigner GPU Laboratory.

**Thank you for your attention!**