# Machine learning for data reconstruction at the LHC

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#### Overview

A high-level summary of various aspects of machine learning in LHC data reconstruction, mostly based on CMS examples.

A short summary of a particular use case: ML for combining signals across detector subsystems with particle flow.

This talk is in personal capacity (not representing CMS or CERN), representing my biased views.

You can find a great and fairly complete overview of ML papers in HEP at <u>https://iml-wg.github.io/HEPML-LivingReview/</u>.



*"The primary goal of the experiments at the CERN Large Hadron Collider (LHC) is to answer fundamental questions in particle physics."* 

#### LHC schedule



2028	2029	2030	2031	2032	2033	2034	2035	2036
J F MAMJJASOND	Run 4	J F MAMJ JASOND		J F MAM J J A SOND	Run 5	J F MAMJ JASOND		JIFIMAMJJASOND

-	

Shutdown/Technical stop Protons physics Ions Commissioning with beam Hardware commissioning/magnet training

Last updated: June 2021

#### How do particles acquire mass?

Higgsdependence (2012) **CMS** Preliminary 35.9 fb<sup>-1</sup> (13 TeV) GeV VKV V  $\kappa_F \frac{m_F}{\sqrt{}}$  or  $10^{-1}$ Higgs self-interaction (~2030) Higgs potential  $10^{-2}$ /(φ) SM Higgs boson ..... Our Stable - Data vacuum [M, ε] fit - S+B Fit  $10^{-3}$ Metastable ----- Bkg Fit Component  $\pm 1\sigma$ Higgs field ±10 m (ø) +20 Re (\$\$  $\pm 2\sigma$ 150 120 130 140 110 10-4 m<sub>yy</sub> (GeV) SM 1.5 Ratio to 0.5 The first and so far only observed 0 spinless elementary particle!  $10^{2}$  $10^{-1}$ 10 Particle mass [GeV]

Higgs couplings (2019)



#### General purpose detectors



## The cylindrical onion



#### Particles in detector layers



## Reconstruction, simplified

Charged particle tracking



#### Energy clustering



#### 19.7 fb<sup>-1</sup> (8 TeV) + 5.1 fb<sup>-1</sup> (7 TeV) events / GeV CMS S/(S+B) weighted sum 3.5 $H \rightarrow \gamma\gamma$ Data S+B fits (weighted sum) Combining detector subsystems B component +10 weighted ( +20 1000 <u>credit</u> $\hat{\mu} = 1.14^{+0.26}_{-0.23}$ S/(S+B) 0.5 m., = 124.70 ± 0.34 GeV B component subtracte 500 115 120 125 130 135 140 145 110 m<sub>yy</sub> (GeV) y/mm Jets 0 137 fb<sup>-1</sup> (13 TeV Events/bin CMS Data SR PYTHIA SR △ Data CR<sub>middle</sub> - PYTHIA CR -500 Data CR 10 . .. - PYTHIA CR 10 102 $|\eta| < 2.5$ 10 -1000 $CR_{high}$ : 1.5 < $|\Delta \eta|$ < 2.6 500 1000 1500 2000 2500 $CR_{middle}$ : 1.1 < $|\Delta \eta|$ < 1.5 x/mm SR: |An| < 1.1 10 5 6 7 8

Photons

Dijet mass [TeV]

## Jet formation

Jets are an emergent phenomenon!

Evolution from femtoscale to meter-scale, 15 orders of magnitude!

The jet structure encodes information about the underlying physics: particle origins, energies, coupling strengths.

00000

credit

Fragmentation

partons  $gud \dots$ 

Hadronization

hadrons  $\pi^{\pm} K^{\pm} \dots$ 

Detection



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## Jet origins



#### Observing jets



What is the originating particle of the jet?

#### Simulated datasets



We can use the full Standard Model predictive machinery to simulate millions of examples with full detector interactions!



#### Discriminating with observables



Construct observables based on theory or prior physics knowledge.

Things get complicated in the real world: systematics, irreducible backgrounds.

Always need to validate and calibrate on real data!

#### Supervised ML ~ fitting nonlinear models on large datasets



Table 1: Input variables used for the Run 1 version of the CSV algorithm and for the CSVv2 algorithm. The symbol "x" ("—") means that the variable is (not) used in the algorithm

# B-jet identification: multivariate classification



Combine individual observables nonlinearly, classify examples using a decision boundary.

Input variable	Run 1 CSV	CSVv2
SV 2D flight distance significance	x	x
Number of SV		x
Track nrel	x	x
Corrected SV mass	x	x
Number of tracks from SV	x	x
SV energy ratio	x	x
$\Delta R(SV, jet)$		x
3D IP significance of the first four tracks	x	x
Track p <sub>T.rel</sub>		x
$\Delta R(\text{track}, \text{jet})$		x
Track p <sub>T.rel</sub> ratio		x
Track distance		x
Track decay length		x
Summed tracks ET ratio		x
$\Delta R(\text{summed tracks, jet})$		x
First track 2D IP significance above c threshold		x
Number of selected tracks		x
Jet p <sub>T</sub>	_	x
Jet n		x



#### Observation of Higgs to b quarks: energy regression



- jet kinematics: jet  $p_{\rm T}$ ,  $\eta$ , mass, and transverse mass, defined as  $\sqrt{E^2 p_{\star}^2}$ ;
- information about pileup interactions: the median energy density in the event, p, corresponding to the amount of transverse momentum per unit area that is due to overlapping collisions[35];
- information about semileptonic decays of b hadrons when an electron or muon candidate is clustered within a jet: the transverse component of lepton mom<u>entum perpen</u>dicular to the jet axis, the distance  $AR = \sqrt{(A\eta)^2 + (A\phi)^2}$ , and a categorical variable that encodes information about the lepton candidate's flavor:
- information about the secondary vertex, selected as the highest p<sub>T</sub> displaced vertex linked to the jet: number of tracks associated to the vertex, transverse momentum, and mass (computed assigning the pion mass to all reconstructed tracks forming the secondary vertex); the

distance between the collision vertex and the secondary vertex computed in three-dimensional space with its associated uncertainty[36, 37];

- jet composition: largest  $p_T$  value of any charged hadron candidates, fractions of energy carried by jet constituents; namely charged hadrons, neutral hadrons, muons, and an electromagnetic component coming from electrons and photons. These fractions are computed for the whole jet, and separately in five rings of *AR* around the jet axis (AR = 0-0.5, 0.05-0.1, 0.1-0.2, 0.2-0.3, 0.3-0.4);
- multiplicity of PF candidates clustered to form the jet; information about jet energy sharing among the jet constituents computed as

(1)



 $\sqrt{\sum_i p_{T,i}^2}$ 

#### Neural networks



Multivariate, nonlinear, highly over-parameterized functions.

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#### Neural network models for various data types

Feedforward networks ~ simple feature vectors

Convolutional neural networks ~ 2D/3D images

Recurrent neural networks / LSTM ~ ordered sequences

Graph neural networks ~ sets, graphs

Transformers ~ ordered sequences, sets

#### Jets as images





## **Encoding symmetries**

Process the image with learnable translation-invariant filters: Convolutional Neural Networks



block1conv2			
block2conv2			
block3conv3			
block4conv3			
block5conv1			
block5conv2			
block5conv3			

#### Tau identification with CNNs



 $\tau^{\pm} \to \pi^{\pm} \nu_{\tau} \qquad \tau^{\pm} \to \rho^{\pm} \nu_{\tau} \to \pi^{\pm} \pi^{0} \nu_{\tau} \qquad \tau^{\pm} \to a_{1}^{\pm} \nu_{\tau} \to \pi^{\pm} \pi^{\mp} \pi^{\pm} \nu_{\tau} \qquad \tau^{\pm} \to \rho^{\prime \pm} \nu_{\tau} \to \pi^{\pm} \pi^{\mp} \pi^{\pm} \pi^{0} \nu_{\tau}$ 



#### The computing challenge



LHC is compute-limited, we fight for every CPU cycle and kilobyte.

#### Sets of feature vectors



#### set of inputs with N constituents, M features

{..., (pT, η, φ, particle ID), ...}

feature matrix (N, M)



jet constituents

#### Set to graph



#### Neural nets on graphs



## Constructing graphs



Physics data as graphs

Particle tracking (neighborhood)



(b)

Jet

MET

Lepton

(c)

Jet

2007.13681

Calorimeter clustering (learned)



Event identification (all-to-all)



(d)

Jet constituents (all-to-all)

#### Graph nets in a nutshell



J. Leskovec et al [2021]

# A concrete case: machine learned particle flow reconstruction

- 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]
  - The Boosted Higgs Jet Reconstruction via Graph Neural Network
  - 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
  - Towards a realistic track reconstruction algorithm based on graph neural networks for the HL-LHC
  - Deep Learning strategies for ProtoDUNE raw data denoising
  - 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
- Anomaly detection with Convolutional Graph Neural Networks
- Energy-weighted Message Passing: an infra-red and collinear safe graph neural network algorithm
- Improved Constraints on Effective Top Quark Interactions using Edge Convolution Networks
- Particle Graph Autoencoders and Differentiable, Learned Energy Mover's Distance
- 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
  - SPANet: Generalized Permutationless Set Assignment for Particle Physics using Symmetry Preserving Attention
  - Particle Convolution for High Energy Physics
  - Deep Sets based Neural Networks for Impact Parameter Flavour Tagging in ATLAS

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

#### Particle reconstruction



The particle flow algorithm aims to identify and reconstruct individually all of the particles produced in a collision, through an optimal combination of the information from the entire detector.

#### Particle Flow algorithm



Figure 2. Schematic of particle flow algorithm for CMS Level-1 trigger correlator.

Particle-flow reconstruction and global event description with the CMS detector					
CMS Collaboration • A.M. Sirunyan et al. (Jun 15, 2017)					
Published in: JINST 12 (2017) 10, P10003 • e-Print: 1706.04965 [physics.ins-det]					
▶ pdf & links & DOI					



#### Machine learned particle flow reconstruction



"Efficient machine-learned particle-flow reconstruction using graph neural networks"; **JP**, J. Duarte, J-R Vlimant, M. Pierini, M. Spiropulu; Eur. Phys. J. C (2021) 81: 381
### Open benchmark dataset for particle flow reconstruction

February 24, 2021

Dataset Open Access

Simulated particle-level events of ttbar and QCD with PU200 using Pythia8+Delphes3 for machine learned particle flow (MLPF)

Pata, Joosep; Duarte, Javier Mauricio; Vlimant, Jean-Roch; Pierini, Maurizio; Spiropulu, Maria

<b>Publication date:</b> February 24, 202	21			
DOI:				
DOI 10.5281/zenodo.4559324				
Keyword(s):				
particle physics	high-energy physics	machine learning		
Communities:				
Machine Learning for Particle Physics				
License (for files):				





**Fig. 3** Functional overview of the end-to-end trainable MLPF setup with GNNs. The event is represented as a set of detector elements  $x_i$ . The set is transformed into a graph by the graph building step, which is implemented here using an locality sensitive hashing (LSH) approximation of kNN. The graph nodes are then encoded using a message passing step, implemented using graph convolutional nets. The encoded elements are decoded to the output feature vectors  $y_i$  using elementwise feedforward networks.

### Model implementation

As an example (batches, elements, features) = (2, 6400, 25)



# Scalable graph building

# Avoid a quadratic bottleneck with locality-sensitive hashing.





Requires batch-mode graphs. No N<sup>2</sup> allocation or computation needed.

One scalable combined graph layer. The input elements are projected into a learnable embedding space. Nearby elements in the embedding space are binned to fixed-size bins. A fully-connected graph is built in each bin, which is used for one or multiple graph convolutions that are used to transform the input elements. Finally, the transformed elements are unbinned.

<u>credit</u>

#### Learned binning



The learned binning structure in the first two layers of the model. We show one simulated ttbar event, with each point corresponding to a PFElement in the event. The colors correspond to the assignment of the PFElements into the bins in each layer.

# Learned graph structure



# Application in the CMS experiment

#### Reconstructed with standard particle flow.

#### Machine-learned particle flow



"Machine Learning for Particle Flow Reconstruction at CMS", CMS Collaboration, 2021 [JP on behalf of CMS, ACAT2021, Daejeon, South Korea; CERN CDS]

# Training on simulation

- Trained on 40k events with pileup + 2.4M single-particle events
- ~5 days on 5 GPUs in the KBFI cluster
- Hyperparameter optimization at the Julich supercomputing center [E. Wulff]

sample fragment	PU configuration	MC events
top-antitop pairs	flat 55-75	20k
$Z \rightarrow  au  au$ all-hadronic	flat 55-75	20k
single electron flat $p_T \in [1, 100]$ GeV	no PU	400k
single muon flat $p_T \in [0.7, 10]$ GeV	no PU	400k
single $\pi^0$ flat $p_T \in [0, 10]$ GeV	no PU	400k
single $\pi$ flat $p_T \in [0.7, 10]$ GeV	no PU	400k
single $\tau$ flat $p_T \in [2, 150]$ GeV	no PU	400k
single $\gamma$ flat $p_T \in [10, 100]$ GeV	no PU	400k

Table 1: MC simulation samples used for optimizing the MLPF model.



#### Particle distributions



### Jets in full reconstruction





#### Missing transverse energy



Validate performance under different physics conditions (=datasets). We found that we need to augment the training dataset with more high-energy neutral hadrons for better generalization to e.g. QCD events.

# Interpreting ML models

- What inputs are relevant for a particular model output?
- Compute layerwise relevance scores
- Aggregate along the graph structure

$$\mathbf{R}_{j}^{(l)} = \sum_{k} \frac{x_{j} A_{jk}}{\sum_{m} x_{m} A_{mk}} \mathbf{R}_{k}^{(l+1)}$$





"Explaining machine-learned particle-flow reconstruction"; Farouk Mokhtar, Raghav Kansal, Daniel C Diaz Javier Duarte, **JP**, Maurizio Pierini, Jean-Roch Vlimant <u>NeurIPS 2021, Machine Learning and the Physical Sciences</u>, 2111.12840 [physics.data-an]

# Speeding up reconstruction

- Besides good physics performance, reconstruction needs to be fast and computationally efficient
- Neural nets are well-suited for GPUs & other parallel processors
- Important to avoid a quadratic scaleup with occupancy
- Next steps are to test the MLPF algorithm on real data in CMS in Run3
- Also looking into extending this for FCC reconstruction



# Next steps on MLPF

- Improve the training statistics, additional validation in the tails of distributions
- Improve GPU inference integration in CMS reconstruction software
- LHC Run 3 is an opportunity to test machine-learned particle flow reconstruction on real data!
- The algorithm is generic possible feasibility studies for future detectors
- This dataset for further studies on interpretability
- Integrate with machine-learned tracking and clustering from upstream reconstruction

# Summary

- **Fundamental physics + ML**: a unique combination of large datasets, accurate underlying quantitative models and hard physics problems
- The LHC is a rich area for applied ML methods, hundreds of models running in production at any given time
- Machine learning is about **fitting distributions on data** with numerical optimization, can **augment imperative algorithms**
- Data reconstruction at the LHC is a challenging problem, well-suited to differentiable, machine-learned algorithms:
  - "Efficient machine-learned particle-flow reconstruction using graph neural networks"; JP, J. Duarte, J-R Vlimant, M. Pierini, M. Spiropulu; Eur. Phys. J. C (2021) 81: 381
  - "Machine Learning for Particle Flow Reconstruction at CMS", CMS Collaboration, 2021 [JP on behalf of CMS, ACAT2021, Daejeon, South Korea; CERN CDS]
  - "Explaining machine-learned particle-flow reconstruction"; Farouk Mokhtar, Raghav Kansal, Daniel C Diaz Javier Duarte, JP, Maurizio Pierini, Jean-Roch Vlimant; <u>NeurIPS 2021, Machine</u> <u>Learning and the Physical Sciences</u>
- Encoding physics priors (=symmetries) can improve the representation power of neural networks

# Backup

### Optimization over large datasets



<u>credit</u>

#### Loss surface of ANN-s



# Overfitting



#### Train, test and validate





# Lessons learned

- It's all about the dataset!
- Set up a simple baseline method and simple performance metrics!
- Decouple the model and how you measure the performance of a model.
- Change one thing at a time.
- Visualize a few predictions, understand where and why they fail.
- Visualize the learning dynamics. What is learnt quickly, what takes time?
- Don't try fancy methods before you get a simple method to work.
- Try to reuse existing models before inventing your own.
- ML can only attempt to answer to questions that you can pose quantitatively.
- All models are wrong, some models are useful.

# Top quark / Higgs jets



One top jet, one W jet. Credit: CMS.

<u>credit</u>

### Jet substructure to jet identification



Which is which?

- q/g
- H->bb
- t->bW->bqq
- b
- W->qq

# A full event



#### This event has: A. ~5 jets B. ~10 jets C. ~20 jets D. ~50 jets

We need X numbers to represent this event at the level of momentum vectors of the jets and leptons:

- A. X~10
- B. X~50
- C. X~500
- D. X~5000

# Identifying collision events





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Statistical discriminator

Machine learning: mathematical models optimized on data.



<u>credit</u>

#### Classification



# Regression



x	У
0.0	0.1
0.0	0.15
0.2	0.02

### Supervised learning



# Optimization

Our model: y = mx + c



Which model has a lower overall error?

- A. Left
- B. Right

How many parameters does the linear model (blue line) have?

- A. One
- B. Two
- C. Three
- D. Undefined

What are the units of the mean squared error E?

- C. The units of y
- D. The units of  $y^2$
- E. Unitless

# **Optimization game**

Compute total error

$$E = rac{1}{n} \sum_{i=0}^n (y_i - (m x_i + c))^2$$

Compute derivatives of dE/dm, dE/dc

$$egin{aligned} D_m &= rac{1}{n} \sum_{i=0}^n 2(y_i - (mx_i + c))(-x_i) \ D_m &= rac{-2}{n} \sum_{i=0}^n x_i(y_i - ar{y}_i) \ D_c &= rac{-2}{n} \sum_{i=0}^n (y_i - ar{y}_i) \end{aligned}$$

Update m, c

$$m=m-L imes D_m$$

 $c = c - L \times D_c$ 



#### Batched gradient descent



# Choosing the right learning rate



#### Artificial/deep neural network



How many tunable parameters does this model have?

A. 
$$k_m + 1$$
  
B.  $k_m (k_m + 1)$   
C.  $2 k_m$ 

In this image,  $u_k$ ,  $v_k$ ,  $y_k$  are

- Scalars (single numbers) Α.
- Β. Vectors (1D lists of numbers)
- C. Tensors (nD matrices)

Output



Leaky ReLU  $\max(0.1x, x)$ 

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 $\begin{array}{l} \textbf{Maxout} \\ \max(w_1^T x + b_1, w_2^T x + b_2) \end{array}$ 



What would be a suitable activation function for binary classification, with output values from 0...1

- A. Sigmoid
- B. ReLU
- C. Linear

What would be a suitable output activation function for regression, where the output domain is 0...500 (e.g. reconstructed mass)

- A. Sigmoid
- B. ReLU
- C. Linear


The number of nodes in the hidden layer *p* should be

- A. Larger than the number of inputs *n*
- B. Smaller than the number of inputs *n*
- C. Exactly the same as the number of inputs *n*
- D. Is not fixed and can be chosen as needed

## Representing data



Collider events contain a variable number of particles of various types.



Typical DNNs require a fixed size *n* input.

## **Categorical variables**



One-hot encoding.

<u>credit</u>

Your MC simulation can contain jets, electrons, muons and photons. How many bits are required to represent objects of all classes?

- A. One
- B. Two
- C. Three
- D. Four
- E. Five

### Bias vs. variance



<u>credit</u>

Low Variance **High Variance** Low Bias High Bias <u>credit</u>

## Training and validation datasets



# Regularization

Building robust models with respect to fluctuations in the input dataset.

Dropout: randomly disable neural network nodes at training time.



What would happen if the dropout was applied not only in training, but also during inference?

- A. The network output would always be zero
- B. The network output would be even more regularized
- C. The network output would be more noisy from one prediction to the next.

## Regularization with more data



## Example of overfitting and regularization







## Recap

#### Training on MC simulation forward "Higgs event" labels "ttbar event" backward Large N еггог Inference on MC simulation + real data forward "ttbar event" Smaller, varied N

<u>credit</u>

# Tensorflow playground

#### https://playground.tensorflow.org



How many hidden neurons required to fit the "two blobs" dataset?

- A. One
- B. Two
- C. Three

How many hidden neurons required to fit the circle dataset?

- D. One
- E. Two
- F. Three

# Clustering



## **Reconstructing particle showers**

Hits  $\rightarrow$  clusters  $\rightarrow$  particle candidates.

How many clusters do we expect?

What's the "cost" of incorrectly merging/splitting a cluster?

How do you determine the particle properties from the cluster?



## Particle tracking





<u>link</u>

### Reconstruction across different detector systems





## Generative modelling



MC generation

**Detector simulation** 

Comparison with data

# Generative modeling with ML



https://openai.com/blog/generative-models/

### Overparameterization



credit

## Semi-supervised methods





FIG. 2. The jet topics method applied to constituent multiplicity, starting with Z+jet (pink) and dijet (purple) distributions from Pythia 8.226. There is good agreement between the two extracted jet topics (orange and green) and pure Z+quark and Z+gluon distributions (red and blue).