# Jet as a Particle Cloud

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### INTRODUCTION

- How to represent a jet is one of the key aspects of machine learning algorithms for jet physics
  - better representation can improve the performance/efficiency of the ML algorithms, therefore extend the reach of physics analyses
  - new representations (and ML algorithms) may lead to fresh insights into jets themselves, thus deepen our understanding of jet physics
  - Lots of the approaches and techniques has been proposed in the past few years...



 $250 < p_T/GeV < 260 GeV, 65 < mass/GeV < 95$ Pythia 8, W' $\rightarrow$  WZ,  $\sqrt{s} = 13 \text{ TeV}$ 10<sup>3</sup> [Translated] Azimuthal Angle ( $\phi$ ) Pixel  $p_{_{T}}$  [GeV] 10<sup>2</sup> 10 10<sup>-1</sup> 10<sup>-2</sup> 10<sup>-3</sup> 10-4 10<sup>-5</sup> -0.5 10<sup>-6</sup> 10<sup>-7</sup> 10<sup>-8</sup> 10<sup>-9</sup> 0.5 -0.5 0 [Translated] Pseudorapidity (η) 1511.05190



1603.09349



609.00607



ATL-PHYS-PUB-2017-017



red = transverse momenta of charged particles
green = the transverse momenta of neutral particles
blue = charged particle multiplicity

1612.01551





# AS SEQUENCES...



### AS... POINT CLOUDS?



arXiv:1801.07829

### AS... POINT CLOUDS?



### Point cloud

From Wikipedia, the free encyclopedia

A point cloud is a set of data points in space.

### AS... POINT CLOUDS?



### Point cloud

From Wikipedia, the free encyclopedia

A **point cloud** is a set of data points in space. Point clouds are generally produced by **3D** scanners, which measure a large number of points on the external surfaces of objects around them.

## JET AS A PARTICLE CLOUD

simulated top quark jet anti- $k_T$ , R = 0.8,  $p_T = 600$  GeV



### Jet (Particle cloud)

From Wikipedia, the free encyclopedia

A jet (particle cloud) is a set of particles in space. Particle clouds are generally created by clustering a large number of particles measured by particle detectors, e.g.,  $\mathcal{F}_{\text{EXPERIMENT}}$  and  $\mathcal{F}_{\text{EXPERIMENT}}$ .

# POINT CLOUDS VS PARTICLE CLOUDS



### Point cloud

- points are intrinsically unordered
- primary information:
  - 3D coordinates in the xyz space



- Particle cloud
  - particles are intrinsically unordered
  - primary information:
    - = 2D coordinates in the  $\eta$ - $\phi$  space
  - but also additional "features":
    - energy/momenta
    - charge/particle type
    - track quality/impact parameters/etc.

Much richer content than typical point clouds!

# WHY PARTICLE CLOUD?

- Image
  - can benefit directly from powerful and sophisticated algorithms (CNNs) from the computer vision community
  - images are uniform grids of pixels:
    - projecting particles into pixels leads to high sparsity and loss of granularity
    - also nontrivial to include features other than particle energy/momenta (e.g., track impact parameters)
  - Sequence
    - preserves full granularity, no loss of information from pixelation
    - straightforward to include any features for each particle
    - all sequence-based algorithm (RNN/RecNN/1D CNN) assumes an explicit ordering
      - but jet constituents are intrinsically unordered
  - Point cloud
  - shares all the benefits of sequence
  - and points are unordered

# LEARNING FROM POINT CLOUDS

- Efficient representation already half of success
  - but only half...
  - the other half: a powerful network that fully exploits all the information in the representation
- Learning from point clouds
  - active research area in the ML community mainly due to the prosperity of autonomous driving technology
  - many custom algorithms proposed recently
  - One of the key aspects is to respect/exploit the permutation invariance of the inputs
    - one approach: use a "global" symmetric function over inputs (e.g., <u>Deep Sets</u>)
      - adapted to particle clouds -> <u>Energy Flow Network</u> see <u>Patrick's talk</u>!
    - another approach: hierarchical learning from "local" to "global"
      - an example: convolution operation
        - key contributor to the overwhelming success of CNNs in image recognition
      - can we adapt convolution to work on point clouds?

## CONVOLUTION ON REGULAR GRIDS

Regular grid



- Conventional convolution only operates on regular grids and cannot be applied on point clouds
- point clouds are irregular
  - how to define a "local" patch to convolve?
- point clouds are unordered
  - conventional convolution operation (Σ<sub>i</sub> K<sub>i</sub> x<sub>i</sub>)
     is not invariant under permutation of the points (x<sub>i</sub>)



?

# CONVOLUTION ON POINT CLOUDS



- Convolution on point clouds: EdgeConv [arXiv:1801.07829]
  - treating a point cloud as a graph:
    - each point is a vertex
- for each point, a local patch is defined by getting the K-nearest neighbors to it
  - distance defined based on the point "coordinates"
- designing a symmetric "convolution" function
  - define "edge feature" for each center-neighbor pair:  $e_{ij} = h_{\Theta}(x_i, x_j)$ 
    - same  $h_{\Theta}$  for all neighbor points, and all center points, for symmetry
  - aggregate the edge features in a symmetric way:  $x_i' = \sum_j e_{ij}$

# DYNAMIC GRAPH CNN

- EdgeConv shares many nice properties of regular CNNs
  - incorporates local neighborhood information (correlations)
  - can be stacked to perform a hierarchical learning from local to global features
- Dynamic Graph CNN (DGCNN)
  - when stacking the EdgeConv layers, it is possible to recompute the graph using nearest neighbors in the features space produces by each layer
    - i.e., the output features of each EdgeConv layer can be treated as a new "coordinate" for each point
    - point distances can be updated using these learned coordinates (in a latent space)
  - found to be beneficial in the ML paper

#### Customization for particle clouds

- the original DGCNN is actually not directly applicable to jets, as the particle inputs have not only "coordinates" (i.e.,  $\eta$ ,  $\varphi$ ), but also additional features ( $p_T$ , charge, particle ID, etc.)
- to apply DGCNN on particle clouds, some customizations are made to the first EdgeConv layer:
  - the nearest neighbor finding is purely based on the  $(\eta, \varphi)$  coordinates
  - then, the other features are added to the (η, φ) coordinates of each particle for producing the edge features

## NETWORK ARCHITECTURE



- 3 stages: k-nearest neighbors updated at the beginning of each stage
- batch normalization (BN) used after each EdgeConv operation
- residual connection (RC) [1512.03385, 1603.05027] added between EdgeConv layers
- BN and RC helped greatly for stabilizing the training and also improving the performance

### PERFORMANCE COMPARISON

- The performance of DGCNN is benchmarked on two jet tagging tasks using public datasets:
  - top tagging dataset: A. Butter, G. Kasieczka, T. Plehn and M. Russell [arXiv:1707.08966, Link]
  - quark/gluon tagging dataset: P. T. Komiske, E. M. Metodiev and J. Thaler [arXiv:1810.05165, link]
  - very nice public datasets
    - ML-friendly format, convenient for developing/testing new algorithms
    - allow for consistent comparison between algorithms
    - the community needs more public datasets
      - especially ones closer to real experiments (pileup, tracking, detector resolution, etc.)
      - open data/simulation in ML-friendly format from CMS and ATLAS would be of great help!
  - Results compared with a few alternative algorithms
    - 1D CNN over particle sequence (P-CNN)
      - CMS "DeepAK8" architecture [CMS-DP-2017-049]
      - but using only information available in the datasets (e.g., no tracking)
    - 2D CNN over 64x64 jet image
      - state-of-the-art model from image recognition: ResNeXt50 [arXiv:1611.05431]
      - #filters reduced by a factor or 4 to avoid overfitting and also to speed up training
    - Particle Flow Network (PFN) [arXiv:1810.05165]

## PERFORMANCE: TOP TAGGING

#### Top tagging:

- only particle 4-momentum is available
- train/val/test 1.2M/400k/400k
- results of more algorithms available at <u>link</u>

#### We managed to push the boundary a bit further

- >20% lower background at signal efficiency of 30%
- Is the gain real? Or is it just learning more details of the parton shower model?
- but personally I would not really consider the jet tagging problem as "solved"
  - especially facing realistic experimental challenges like pileup, detector effects, and additional information (e.g., tracking, timing, etc.)



#### Performance on top-tagging dataset

Algorithm	Accuracy	ROC AUC	$I/\epsilon_{bkg} @ \epsilon_{sig}=30\%$
1D P-CNN	0.930	0.9804	780
2D CNN [ResNeXt50]	0.936	0.9838	1086
DGCNN	0.937	0.9842	1160
PFN-r.r. [arXiv:1810.05165]	0.932	0.9819 ± 0.0001	888±17

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### PERFORMANCE: QUARK/GLUON TAGGING

### Quark/gluon tagging

- dataset from P. T. Komiske, E. M. Metodiev and J. Thaler [arXiv:1810.05165, link]
- train/val/test 1.6M/200k/200k
- two versions with different information:
  - momentum-only
  - momentum + realistic particle ID (e/μ/γ/ charged hadron/neutral hadron) + charge



#### Performance on quark/gluon-tagging dataset

	Algorithm	Accuracy	ROC AUC	$I/\epsilon_g @ \epsilon_q = 50\%$
Momentum	PFN [ <u>arXiv:1810.05165]</u>	-	0.8911 ± 0.0008	$30.8 \pm 0.4$
	2D CNN [ResNeXt50]	0.821	0.8960	30.9
	DGCNN	0.826	0.8988	32.8
Momentum + realistic particle ID	PFN-Ex [arXiv:1810.05165]	-	0.9005 ± 0.0003	34.7 ± 0.4
	1D P-CNN	0.826	0.8996	34.9
	DGCNN	0.835	0.9073	36.8

# TRAINING AND INFERENCE SPEED

- Another important factor of a ML algorithm is the training and inference speed
  - benchmarked on a GTX 1080Ti
  - current ML package not well optimized for graph network
    - future implementation/hardware(e.g., FPGA) may greatly improve the speed



## OUTLOOK

We present another point cloud inspired approach for jet tagging

- a jet can be viewed as a cloud of unordered particles
- dynamic graph CNN, based on permutation-invariant EdgeConv operation, is applied on particle clouds for jet tagging
- better performance for jet tagging compared to existing approaches based on jet images and sequences
- Point cloud: a natural and flexible representation for jets as well as collision events, with a rich connection yet to be fully explored
  - point cloud classification (labelling the whole cloud) <-> jet tagging
  - point cloud segmentation (labelling each point)
    - pileup identification?
    - particle tracking?
- so far we are importing expertise from ML community
  - can we propose better ML algorithms based on physics?
  - can we export better ideas to the ML community?

# OUTLOOK (CONT.)

- Point cloud: a natural and flexible representation for jets as well as collision events, with a rich connection yet to be fully explored
  - can we peek in the ML model to see what/how it learned?
  - can we learn jet physics from ML?



label: top, score: 0.9969, pt: 598.9



### TOP TAGGING COMPARISON

Approach	AUC	Acc.	1/eB (@ eS=0.3)	Contact	Comments
LoLa	0.979	0.928		GK / SImon Leiss	Preliminary number, based on LoLa
LBN	0.981	0.931	863	Marcel Rieger	Preliminary number
CNN	0.981	0.93	780	David Shih	Model from Pulling Out All the Tops with Computer Vision and Deep Learning (1803.00107)
P-CNN (1D CNN)	0.980	0.930	782	Huilin Qu, Loukas Gouskos	Preliminary, use kinematic info only (https://indico.physics.lbl.gov/i ndico/event/546/contributions/ 270/)
6-body N-subjettiness (+mass and pT) NN	0.979	0.922	856	Karl Nordstrom	Based on 1807.04769 (Reports of My Demise Are Greatly Exaggerated: N-subjettiness Taggers Take On Jet Images)
8-body N-subjettiness (+mass and pT) NN	0.980	0.928	795	Karl Nordstrom	Based on 1807.04769 (Reports of My Demise Are Greatly Exaggerated: N-subjettiness Taggers Take On Jet Images)
Linear EFPs	0.980	0.932	380	Patrick Komiske, Eric Metodiev	d<= 7, chi <= 3 EFPs with FLD. Based on 1712.07124: Energy Flow Polynomials: A complete linear basis for jet substructure.
Particle Flow Network (PFN)	0.982	0.932	888	Patrick Komiske, Eric Metodiev	Median over ten trainings. Based on Table 5 in 1810.05165: Energy Flow Networks: Deep Sets for Particle Jets.
Energy Flow Network (EFN)	0.979	0.927	619	Patrick Komiske, Eric Metodiev	Median over ten trainings. Based on Table 5 in 1810.05165: Energy Flow Networks: Deep Sets for Particle Jets.