Color Singlet clustering and MLPF

GNN based Reconstruction at FCC-ee

Dolores Garcia



ML4Jets2023 - Reconstruction session 06.11.2023

Clustering Color Singlets

- FCC-ee would serve as a Higgs factory, electroweak and top at highest luminosities
 - Measure Higgs particle properties and interactions in challenging decay modes
- Identification of color-neutral resonances relies on clustering final state into jets
- Calorimetry is expected to be much improved at future e+e- colliders, so that the 2-jet invariant mass resolution will be dominated not by detector resolution but rather by mis-clustering [1] (A)
- Jets are not well defined but color connection is physical, this may help improve the mass estimation for color singlets (H,Z,W) and remove more background



A Comparison of clustering performance vs ideal reconstruction





ACKS : Michele Selvaggi

[1]Fujii, K., Grojean, C., Peskin, M. E., Barklow, T., Gao, Y., Kanemura, S., ... & Murayama, H. (2020). ILC study questions for snowmass 2021. arXiv preprint arXiv:2007.03650... [2] Gallicchio, J., & Schwartz, M. D. (2010). Seeing in color: jet superstructure. *Physical review letters*, 105(2), 022001.

Clustering Color Singlets

Loss in performance can be due to:

- Miss matching of jets pairs
- Miss clustering of soft particles leading to degraded resolution

Possible solutions:

- Parameter tuning (BAO)
- Optimize distance metrics?: piecewise continuous function, hard optimization problem
- End-to-end approach



ACKS : Michele Selvaggi

[1]Fujii, K., Grojean, C., Peskin, M. E., Barklow, T., Gao, Y., Kanemura, S., ... & Murayama, H. (2020). ILC study questions for snowmass 2021. arXiv preprint arXiv:2007.03650.. [2] Gallicchio, J., & Schwartz, M. D. (2010). Seeing in color: jet superstructure. Physical review letters, 105(2), 022001.

CSC-Approach

- **GNN** Node classification (instantiation) problem, permutation invariant and equivariant
- Arch: FC Graph Transformer [1]
- Results:
 - Similar performance to classical approach
 - Baselines:
 - Chi-squared
 - $\chi^2 = 1/\sigma_{\rm H} (M_{1/2} M_{\rm H})^2 + 1/\sigma_z (M_{2/1} M_z)^2$
 - Z only $\chi^2 = (M_{1/2} - M_{7})^2$
- Can find events that reduce background by assigning a score per event







CSC-Approach

- Wiring is important
- Using information about **the ordering** (<tree structure) performance can be improved
- Efforts to obtain MLE (A*, beam search...) all for small number of leaves [1,2]





B. Example tree



ACKS : Michele Selvaggi

[1]Brehmer, J., Macaluso, S., Pappadopulo, D., & Cranmer, K. (2020). Hierarchical clustering in particle physics through reinforcement learning. *arXiv preprint arXiv:2011.08191*. [2] Greenberg, C. S., Macaluso, S., Monath, N., Dubey, A., Flaherty, P., Zaheer, M., ... & McCallum, A. (2021, December). Exact and approximate hierarchical clustering using A. In *Uncertainty in Artificial Intelligence* (pp. 2061-2071). PMLR.

5/14

MLPF: Motivation

- The particle flow algorithm aims to identify the produced particles in a collision through the combination of the information from the entire detector and provide best combined energy/momentum resolution
- Hoping to achieve higher reconstruction performance: cluster merging, arbitration of track vs cluster energy
- First step: focus on calorimeter clustering



A Representation of the different layers, hits, tracks and resulting particles (reproduced from [1])



B Example of an event, the shower of secondary particles generated by an individual particle is labelled with one colour [2]



ACKS : Michele Selvaggi, **Gregor Krzmanc**, Jan Kieseler, Philipp Zehetner [1] Pata, J. Machine learning for particle flow reconstruction at CMS, presentation at CDS. [2] Qasim, S. R., Chernyavskaya, N., Kieseler, J., Long, K., Viazlo, O., Pierini, M., & Nawaz, R. (2022). End-to-end multi-particle reconstruction in high occupancy imaging calorimeters with graph neural networks. *The European Physical Journal C*, *82*(8), 753.

Training Data

A Example train event - 15 particles



- Event generation:
 - Use particle gun (10-15 particles)
 - E ∈ [0.5, 50] GeV
 - \circ p, n, K_L, π
- FCC-ee O(100)
- Simulation and reconstruction: Key4HEP turnkey + Geant4



B Number of hits per event (left) and #hits ECAL vs HCAL (right)



ACKS : Michele Selvaggi, Gregor Krzmanc, Jan Kieseler, Philipp Zehetner

Architecture: Object condensation (End-to-End approach)



Input:

- A set of hits from different sensors (coordinates, type of hit, energy, A)
- Each one node in the graph O(600) per particle

$$\begin{aligned} & \bigcup_{i} Q_{\alpha k} = \max_{i} q_{i} M_{i k}. \\ & \widecheck{V}_{k}(x) = \|x - x_{\alpha}\|^{2} q_{\alpha k}, \text{ and} \\ & \widehat{V}_{k}(x) = \max(0, 1 - \|x - x_{\alpha}\|) q_{\alpha k}. \\ & L_{V} = \frac{1}{N} \sum_{j=1}^{N} q_{j} \sum_{k=1}^{K} \left(M_{j k} \widecheck{V}_{k}(x_{j}) + (1 - M_{j k}) \widehat{V}_{k}(x_{j}) \right). \end{aligned}$$

- Each object 1 condensation point (CP)
- Repulsive +Attractive potentials for each CP



Output:

- Coordinate in embedding space (3D>)
- Beta (q)
- Use clustering space to build showers





ACKS : Michele Selvaggi, Gregor Krzmanc, Jan Kieseler, Philipp Zehetner

[1] Kieseler, J. (2020). Object condensation: one-stage grid-free multi-object reconstruction in physics detectors, graph, and image data. *The European Physical Journal C*, 80, 1-12. [2] Qasim, Shah Rukh, et al. "Learning representations of irregular particle-detector geometry with distance-weighted graph networks." *The European Physical Journal C* 79.7 (2019): 1-11

Architecture: Object condensation (End-to-End approach)





Architecture: Gravnet Model

- Input: a set of hits from different sensors (coordinates, type of hit, energy), each one node in the graph O(600) per particle
- Graph representation with **no given graph structure**
- **Dynamically** compute edges in embedding space with knn

- a) Transform input features **F**_{IN} into
 - transformed features \mathbf{F}_{IR}
 - latent coordinates S
- b) Build graph using coordinates S
- d) Aggregate weighted features
 - Weights depending on distance
 - Aggregation typically is mean or max
- e) Concatenate the new features





ACKS : Michele Selvaggi, Gregor Krzmanc, Jan Kieseler, Philipp Zehetner

[1] Kieseler, J. (2020). Object condensation: one-stage grid-free multi-object reconstruction in physics detectors, graph, and image data. *The European Physical Journal C*, 80, 1-12. [2] Qasim, Shah Rukh, et al. "Learning representations of irregular particle-detector geometry with distance-weighted graph networks." *The European Physical Journal C* 79.7 (2019): 1-11.

10/14

Efficiency and fake rate



- Efficiency approaches 100% with high p_T
- Adding tracks will improve efficiency



- Most fakes with E< 1 GeV
- Other clustering methods in the embedding space can improve fakes
- Resulting from bad beta distributions



Response and Resolution (clustering metrics)



• Evaluated on reco values (for clustering evaluation)



- Resolution performance must be improved for low energies
- Can be improved with better clustering in embedding space



Calorimeter clustering - Results

- Containing: percentage of reco energy that belong to the reconstructed particle (G+R)/(G+B)
- Purity: Percentage of reco energy contained in reconstructed cluster (G)/(G+R)





Summary and next steps MLPF

Summary:

- Color singlet clustering seems promising with ML but more research is necessary
- MLPF
 - Promising performance, we will soon compare to PFA (baseline for CLD)
 - Demonstrated generalization over different types of events (for now kept particle number low)
 - Fast execution time, linear scaling with number of hits

Ongoing work and next steps:

- Add tracks as inputs to the graph
- Regress particle properties
- Try heterogeneous graph architectures
- Compare to the performance of PFA



Thank you!