

High level reconstruction with DNN for Higgs factories

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- Calorimeter clustering with GravNet/Object condensation

 Slides from S. Tsumura
- b/c tagging with Graph Attention Network
 Slides from T. Once

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3 ILD / SiW ECAL



- Electromagnetic calorimeter (ECAL): Detects positions , and energy of gamma rays
 - \rightarrow Higher accuracy of particle identification: PFA
- SiW ECAL equips a lot of channels (~10⁸) to identify each particle.
- Sandwich structure with 30 alternating layers of Si detection layer and W absorption layer.
- W-absorbing layer: Electromagnetic shower is induced when electrons and gamma rays are incident. $\rightarrow \sim 24 X_0$ in total
- Feature: Moliere radius is small enough to separate each particle

4 Application of Deep Learning to PFA

- Current PFA algorithm : PandoraPFA
 →The pattern recognition based on the human-tuned parameters
- Our targets:
 - Improve performance by reducing confusion term
 - Adding timing information
 - Checking detector effects on
 - Granularity (inc. MAPS?)
 - Timing resolution





5 Calorimeter Clustering

- Input: features of hit in the calorimeter e.g., position, energy, etc.
 → discriminate each cluster
- Deep Learning Architecture
 - Based on Graph Neural Network developed for CMS HGCal









6 Deep Learning

Fully Connected Layer

- One of the most basic structures in deep learning
- Consists of an input layer, a hidden layer, and an output layer
- A more expressive network can be built by increasing the number of layers

Graph Neural Network

- A network is constructed as a graph consisting of nodes (points) and edges (lines)
- Not only can it learn the features of materials with a graph-like structure, but it can also be used in many ways, such as expressing the relationship between features as a graph.





7 GravNet

• Input Data : $V \times F_{IN}$



V: Number of hits for each detector F_{IN} : Number of the features for each hit

- S : Set of coordinates in some learned representation space
- F_{LR} : learned representation of the vertex features
- Input data of initial dimension $V \times F_{IN}$ is converted into a graph.
- The coordinates of the graph is updated by the learning of the network.



8 GravNet

- The contribution of each point is bigger depending on the distance between the points
- The output is calculated for each point based on the contribution
- At last, the outputs $(\widetilde{F_{LR}})$ are concatenated with the initial inputs and previous outputs and pass the FC layer.
- The F_{OUT} output carries collective information from each vertex and its surrounding.





9 Object Condensation

- A loss function technique to recognition for multi-object
- Get the output from GravNet as β and output whether the hit seems to be a representative point of the particle ($0 < \beta < 1$)
- Employs two terms as Loss terms to improve cluster and background identification

$$L = L_V + L_\beta$$

- L_V : The closer the hit is to a particle with high β and belonging to the same particle, the smaller it is, and the more it belongs to a different particle, the larger it is.
 - \rightarrow Equivalent to the attractive and repulsive forces acting on an electric charge
- L_{β} : Converge β to 1 for only one of each particle corresponding to a true cluster The remaining β works its way closer to 0



Output of network

- Beta (condensation)
- 2 x coordinate
 per hit
 Used for clustering

10 Clustering

- Get "condensation point" with hits with beta > threshold
- Cluster other hits to nearest condensation point in the virtual coordinate



II Generation of Input Data

- Two gamma events are generated by ILD detector simulation
- 10000 Events are generated for each of the five data sets from 30 to 150 mrad
- θ : 85/180 π , ϕ : random, momentum: 5.0 GeV



Two gamma event

Gamma-ray

12 Event Display

Large angle (150 mrad): perfect reconstruction



Small angle (30 mrad): a few hits misclustered





Number of hits which is predicted correctly

• Accuracy : Number of hits with true label of each cluster

- The simulation data includes events where photons are converted into other particles.
- As input data, events with only two clusters are selected





Angle[mrad]	30	60	90	120	150
Accuracy[%]	96.08	98.64	99.30	99.68	99.56
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Plans for PFA in ~this year

- Prepare more complicated data (taus, jets, ...)
 - Restructuring data format (npz \rightarrow awkward arrays)
 - Confirm (or tune) MC truth cluster definition
 - How to treat split clusters
- Track-cluster matching
 - Virtual hit representing a track
 - Position at the entry of calorimeter (with "track" flag)
 - To be forced condensation point treated by loss function
 - How to integrate momentum (and direction)
 - Additional input to the hit characteristics or add at later stage
- Comparison with PandoraPFA hoping to be better
 - If better, adapting it to analysis framework (to be used for physics analyses)
- Comparison with timing info included or not included
 - And with different timing resolution

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Jet Flavor Tagging

- Important to identify quarks (b/c/g/uds) of the origin of the jets. e.g., Separation of $h \rightarrow b\overline{b} / c\overline{c} / q\overline{q} / ...$
- Ratio of background can be eliminated determines the limits of analysis cut
- Bottom (b) and charm (c) flavor hadrons have weak interaction
 - \rightarrow b/c hadrons have finite decay lengths
 - \rightarrow Can be identified by finding vertices





Fig. Monte Carlo simulation of the jet near the IP

Graph Data Approach

Concept

Data is represented as a graph

- → Graph structure data can contain interrelationship by connections (Fully-connected neural network has no specific relation between nodes)
- \rightarrow Reduced loss of information when compared to physical phenomena

 \rightarrow High accuracy of identification is expected



Training Data information

- **Data** 240,000 jets of 250 GeV ILD full simulation data $[e^+e^- \rightarrow v\bar{v}h \rightarrow v\bar{v}b\bar{b}/c\bar{c}/q\bar{q} \ (q = u, d, s)]$
 - Build one graph per one jet
 - Define the tracks as nodes in the graph
 - Edges connect between track pairs

Track Input	
d ₀	Longitudinal distance from track to IP
φ	Azimuthal angle of track
ω	the curvature of the track
$\mathbf{z_0}$	Transverse distance from track to IP
tan λ	dz/ds in sz plane
$\sigma(\mathbf{d_0})$	Uncertainty of d ₀
$\sigma(z_0)$	Uncertainty of z ₀





Fig. example of a jet as a graph

Graph Training and GAT

- How to train with graph data (Graph Neural Network; GNN)
 ... Aggregate features from neighboring nodes and update
- We suggest Graph Attention Network (GAT), a GNN with attention mechanism
- <u>Attention mechanism</u> ... Learn the importance score for each weight Take as a coefficient for update parameter.
- \rightarrow Aimed by attention expressing whether tracks has the same vertex.



Training and Network architecture

- Node classification means the origin of tracks as vertices
- Link prediction means whether to form a vertex
- Graph classification means jet flavor tagging
- Loss function

 $L_{total} = L_{Flavor} + \frac{\alpha L_{Vertex}}{\alpha} + \frac{\beta L_{Edge}}{\beta}$ $(\alpha \approx 3, \beta \approx 1)$

Node classification

Label	Description
PV	From primary vertex
SVBB	From secondary vertex of b
SVCC	From secondary vertex of c
TVCC	From tertiary vertex of b
Others	From another particle

Link prediction

Label		Description	
Connected		tracks are connected	
Not-connected		tracks are not connected	
Graph Classification			
Label	Description		
bb	the final state of $b\overline{b}$		
cī	the final state of $c\overline{c}$		
$q\overline{q}$	the final state of $q\overline{q}$ (q = u, d, s)		

Network architecture

Input				
	Fully-connected Layer			
	Graph Attention Layer			
	Batch Normalization			
	LeakyReLU			
	Graph Attention Layer			
	Batch Normalization			
LeakyReLU				
	Graph Attention Layer			
Batch Normalization				
	LeakyReLU			
	Edge Index concat	Poolina		
Fully-connected Layer	Fully-connected Layer	Fully-connected Layer		
Output (Softmax)	Output (Softmax)	Output (Softmax)		
Node classification	Link prediction	Graph classification		
Track classification Vertex Finder Flavor Tagging				

Evaluation of GNN



Tagging		Mis-id fraction		
efficiency = 0.8	background	LCFIPlus	GNN	
<i>b</i> jet	<i>c</i> jet	0.073	0.021	
	<i>uds</i> jet	0.007	0.015	
c jet	<i>b</i> jet	0.22	0.40	
	<i>uds</i> jet	0.24	0.14	



For b jet, the ratio of c jet background is reduced.

- For c jet, the ratio of uds jet background is reduced.
- Integrated of Flavor Tagging with Vertex Finder \rightarrow Implementation with low-level of input than LCFIPlus

Status and plans in flavor tagging

- Tuning of the GAT-based flavor tagging
 - Investigate reasons for degraded performance on node/edge classification
 - Connecting output (or nearly-output) of node/edge to flavor tagging
- Another methods to be considered
 - Importing LHC method (ParticleNet, LorentzNet etc.)
 - Transformer-like method (graph transformer, set transformer etc.)
- Compare among algorithms as well as LCFIPlus
 - Import it to the analysis framework if better than LCFIPlus
- Considering timing information to be included
 - Dependence of timing resolution also to be seen

Backup slides

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Appendix: quark flavor tagging with DNN Flavor tagging with GNN (ongoing effort)

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Modified LSTM with attention NIMA 1047 (2023) 167836



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Performance of vertex finding in this network

Criteria / True label	Primary	Bottom	Charm	Others
All tracks	307 657	187 283	180 143	42 888
In secondary vertex	2.2%	63.3%	68.4%	9.5%
- of same decay chain		62.3%	67.2%	
- of same parent		38.1%	36.2%	6.4%

Performance for vertex finding in LCFIPlus

Criteria / True label	Primary	Bottom	Charm	Others
All tracks	307 657	187 283	180 143	42 888
In secondary vertex	0.2%	57.9%	60.3%	0.5%
- of same decay chain		57.5%	59.9%	
– of same parent		34.0%	37.2%	0.3%

Input Fully-connected Layer Graph Attention Layer **Batch Normalization** LeakyReLU Graph Attention Layer **Batch Normalization** LeakyReLU Graph Attention Layer **Batch Normalization** LeakyReLU Edge Index concat Pooling Fully-connected Laver Fully-connected Laver Fully-connected Layer Output (Softmax) Output (Softmax) Output (Softmax) Link prediction Graph classification Node classification Flavor Tagging Vertex Finder Track classification

	Tagging		Mis-id fraction		
	efficiency = 0.8	background	LCFIPlus	GNN	
	<i>b</i> jet	c jet	0.073	0.021	
		<i>uds</i> jet	0.007	0.015	
	- int	<i>b</i> jet	0.22	0.40	
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Graph Attention Network (GAT)

Partially better than LCFIPlus

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Simultaneous classifications of nodes,

25 GRAVNET - NETWORK -

- Input Data : $B \times V \times F_{IN}$
 - *B* : Number of examples including in a batch
 - V : Number of hits for each detector
 - $F_{\text{IN}}:$ Number of the features for each hit
- S : Set of coordinates in some learned representation space
- F_{LR} : learned representation of the vertex features



26 GRAVNET

- Input example of initial dimension $V \times F_{IN}$ is converted into a graph.
- the f_j^i features of the v_j vertices connected to a given vertex or aggregator v_k are converted into the $\tilde{f_{jk}}^i$ quantities, through a potential (function of euclidean distance d_{ik}).
- The potential function $V(d_{jk})$ is introduced to enhance the contribution of close-by vertices. Example: $V(d_{jk}) = \exp(-d_{jk}^2)$
- The fik i functions computed from all the edges associated to a vertex of aggregator vk are combined, generating a new feature fk i of vk.
 Example : the average of the fik across the j edges / their maximum



27 GRAVNET

- For each choice of gathering function, a new set of featur
- The $\widetilde{F_{LR}}$ vector is concatenated to the initial vector.
- Activation function : tanh
- The F_{OUT} output carries collective information from each vertex and its surrounding.



28 Object Condensation

- Get the output from GravNet as β and output whether the hit seems to be a r point of the particle ($0 < \beta < 1$)
- Employs two terms as Loss terms to improve cluster and background identification

$$L = L_V + L_\beta$$

- L_V : The closer the hit is to a particle with high β and belonging to the same particle, the smaller it is, and the more it belongs to a different particle, the larger it is.
 - \rightarrow Equivalent to the attractive and repulsive forces acting on an electric charge
- L_{β} : Converge β to 1 for only one of each particle corresponding to a true cluster The remaining β works its way closer to 0



29 LOSS FUNCTION - NETWORK LEARNING -

- The value of β_i ($0 < \beta_i < 1$) is used to define a charge q_i per vertex i $q_i = \operatorname{arctanh}^2 \beta_i + q_{\min} \quad (\beta_i \to 1 : q_i \to +\infty)$
- The charge q_i of each vertex belonging to an object k defines a potential $V_{ik}(x) \propto q_i$
- The force affecting vertex j can be described by

 $M_{ik} = \begin{cases} 1 \ (vertex \ i \ belonging \ to \ object \ k) \\ 0 \ (otherwise) \end{cases} \quad q_j \cdot \nabla V_k(x_j) = q_j \nabla \sum_{i=1}^N M_{ik} V_{ik}(x_j, q_i) \end{cases}$



30 LOSS FUNCTION

• The potential of object k can be approximated :

 $V_k(x) \approx V_{\alpha k}(x, q_{\alpha k}), \text{ with } q_{\alpha k} = \max_i q_i M_{ik}.$

• An attractive and repulsive potential are defined as :

$$\vec{V}_k(x) = ||x - x_{\alpha}||^2 q_{\alpha k}, \text{ and}
\hat{V}_k(x) = \max(0, 1 - ||x - x_{\alpha}||) q_{\alpha k}.$$



• The total potential loss L_V :

$$L_{V} = \frac{1}{N} \sum_{j=1}^{N} q_{j} \sum_{k=1}^{K} \left(M_{jk} \check{V}_{k}(x_{j}) + (1 - M_{jk}) \hat{V}_{k}(x_{j}) \right)$$

3I LOSS FUNCTION

- The L_V has the minimum value for $q_i = q_{\min} + \epsilon \ \forall i$
- To enforce one condensation point per object, and none for background or noise vertices, the following additional loss term L_{β} is introduced : s_{B} : hyperparameter describing the

$$L_{\beta} = \frac{1}{K} \sum_{k} (1 - \beta_{\alpha k}) + s_B \frac{1}{N_B} \sum_{i}^{N} n_i \beta_i,$$

background suppression strength K: Maximum value of objects N_B : Number of background n_i : Noise tag (if noise, it equals 1.)

• The loss terms are also weighted by $\operatorname{arctanh}^2\beta_i$:

$$L_p = \frac{1}{\sum_{i=1}^{N} \xi_i} \cdot \sum_{i=1}^{N} L_i(t_i, p_i) \xi_i, \text{ with}$$
$$\xi_i = (1 - n_i) \operatorname{arctanh}^2 \beta_i.$$

 p_i : Featutes $L_i(t_i, p_i)$: Loss term (Difference between true labels and outputs of network)

- Accuracy = Number of hits with predicted label correctly Number of hits with true label
- Opening angle = 0.5 rad (the largest one)
- Event selection : events which include 2 clusters



Opening angle = 0.4 rad



Opening angle = 0.3 rad

Average = 99.30%



Opening angle = 0.2 rad



Opening angle = 0.1 rad (the smallest one)





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COMPARISON BETWEEN PREDICTION AND TRUE LABEL



COMPARISON BETWEEN PREDICTION AND TRUE LABEL



COMPARISON BETWEEN PREDICTION AND TRUE LABEL



NUMBER OF CLUSTER IN EACH EVENT(JUST 100 EVENTS)



Result of GNN



- Not much classification of TVCC and SVCC
- Edge connection is not good
- As a graph, we got better accuracy than nodes and edges