Day 4: Introduction to Graph Neural Networks

François Drielsma
(with Kazu and Aashwin)

drielsma@slac.stanford.edu

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U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

Day 4 Lecture | Outline

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1. **Graph Neural Networks (GNNs): what are they good for?**
   - Motivation behind the creation of GNNs
   - Introduction to graphs, graph-structured data
   - Presentation of typical tasks on graphs
2. **GNN feature learning: how does information flow in graphs ?**
   - Graph convolutions
   - Message passing
   - Graph pooling operations
3. **GNN examples: what are common GNN architectures ?**
   A. Classifying people in a social network with a GCN + *Tutorial*
   B. Particle clustering with MetaLayers + *Tutorial*
   C. Protein graph classification with with DiffPool + *Tutorial*
4. **Conclusions**

Machine Learning: learning a transformation from data (classification, regression, etc.)

Inductive bias: assumptions about the model in a learning process (very good read)

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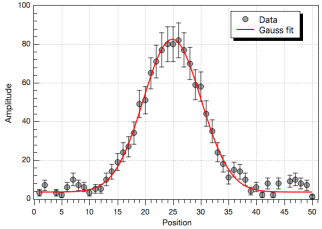
Hand-engineered function

- Strong inductive bias
- Extremely limited freedom
- Strong potential for underfitting
- Computationally cheap



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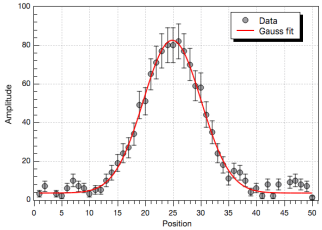

Fully-connected Neural Network

- Virtually no inductive bias
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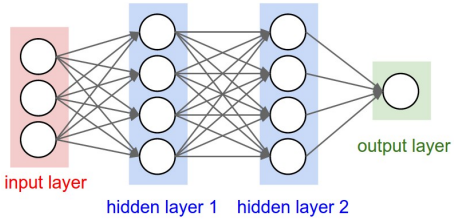
- No by-design overfitting prevention
- Computationally expensive for deep nets



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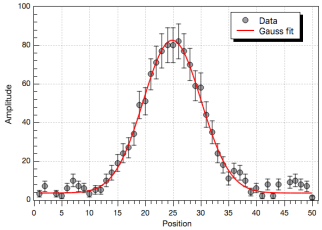

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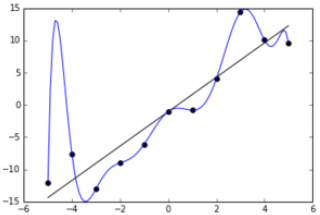

Convolutional Neural Networks: freedom of MLPs but **locality** and **translation invariance**

- Inductive biases:
  - Strong correlation between adjacent input pixels (receptive field small compared to full input)
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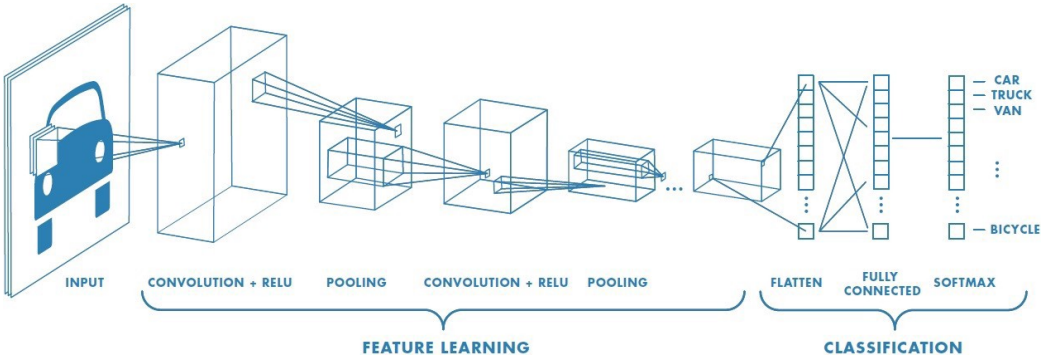

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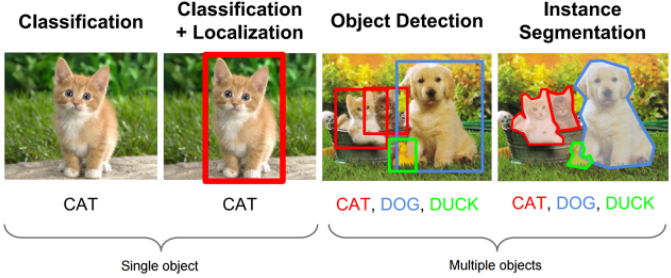
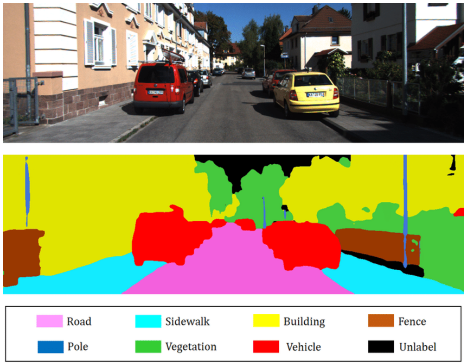
- **State-of-the-art** in Computer Vision, exclusively for **data on a grid**





Recurrent Neural Network: freedom of MLPs but with **locality** and **temporal invariance**

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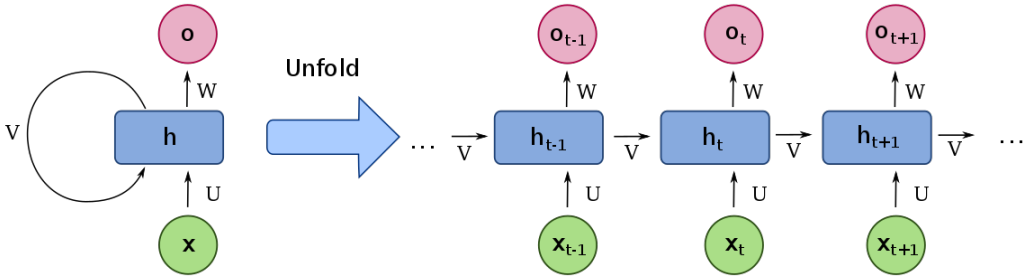

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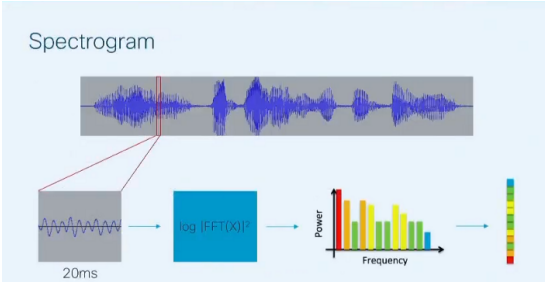
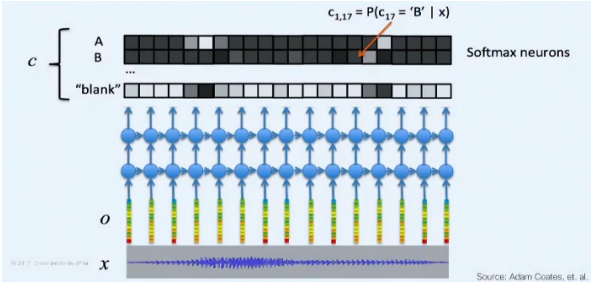
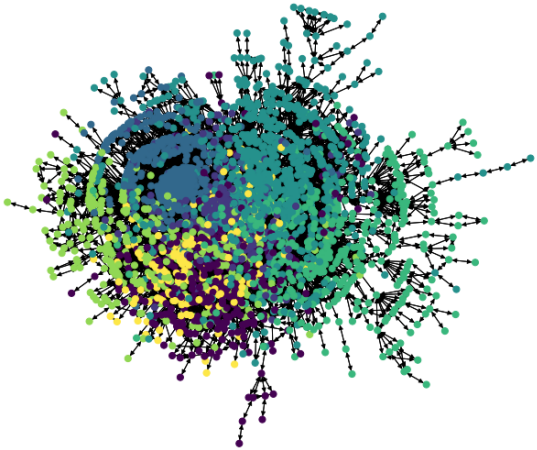
- **State-of-the-art** in **speech recognition**, exclusively for **time-ordered data**





Motivation

What if the data is structured but is **neither spatially nor temporally ordered** ?

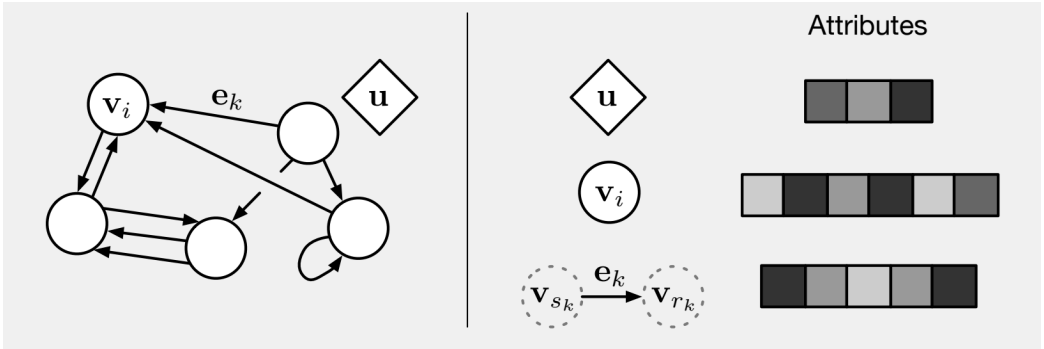


Social network: people and relationships

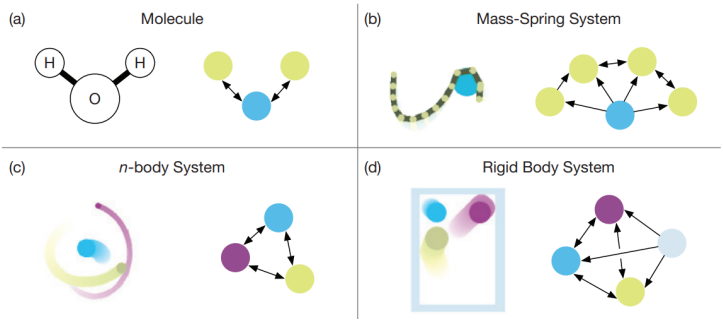
Referencing: papers and citation linkage

Graphs generalize concept of **locality** to **arbitrarily-ordered data**

- A set of **nodes**, $\{\boldsymbol{v_i}\}_{i=1}^{N_v}$ (e.g. person in social network, paper in an arXiv, etc.)
- A set of **edges**, $\{\boldsymbol{e_k}\}_{k=1}^{N_e}$ (e.g. friendship in social network, citation, etc.)
- A global state, $\boldsymbol{u}$, associated with one realization of the data (full network, full arXiv, etc.)



Graphs are often the natural choice to **represent correlations** in a physical data set



(a) **Nodes**: atoms (Z, A, etc.)
Edges: chemical bonds

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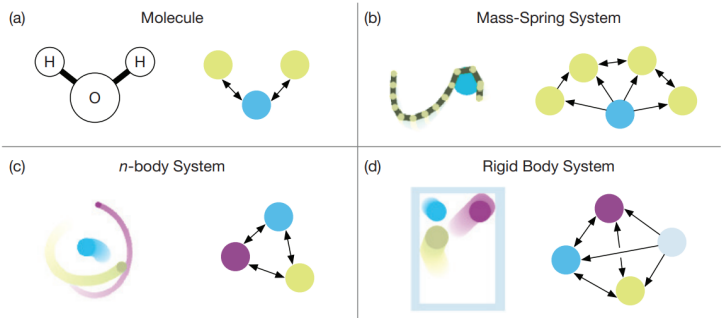

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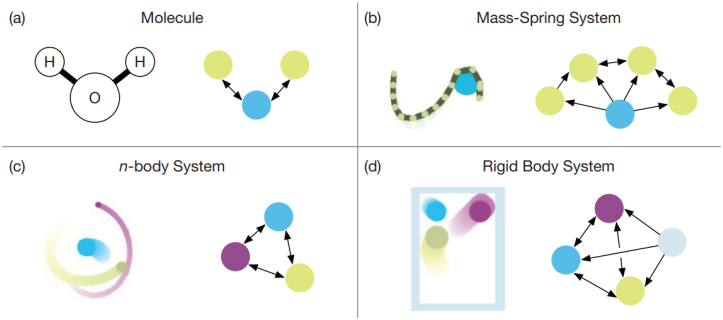

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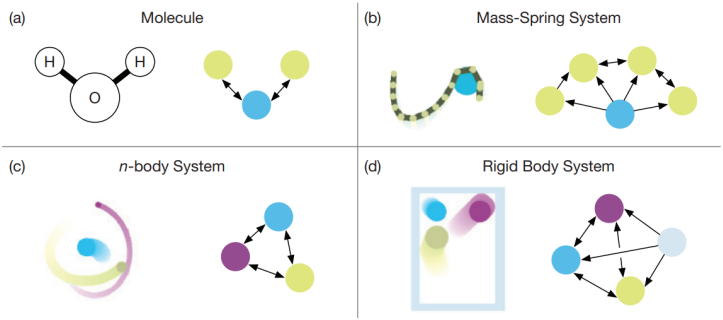

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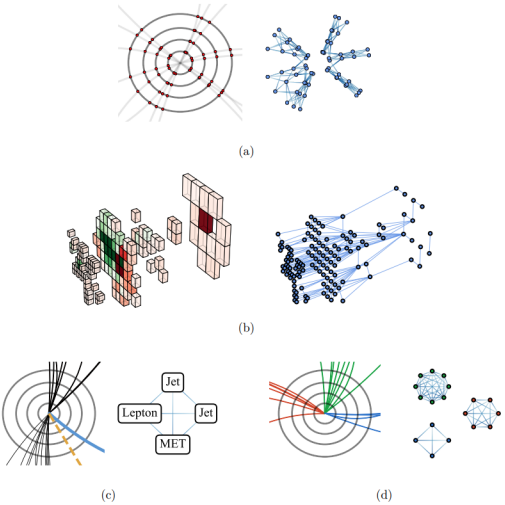

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Edges: hit connections (tracks)

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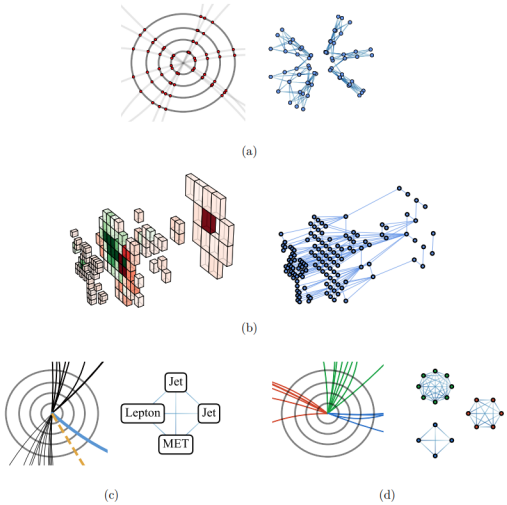

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Graphs | In HEP

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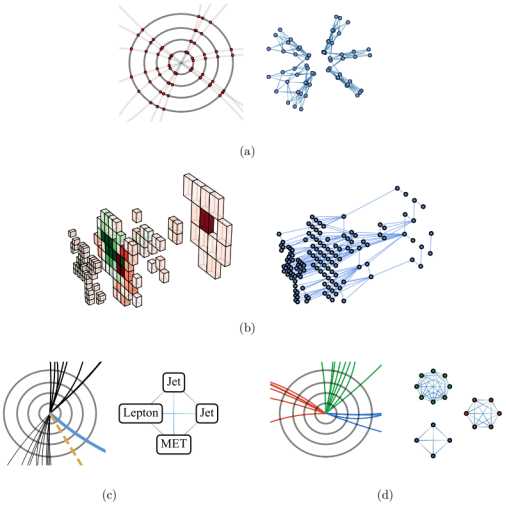

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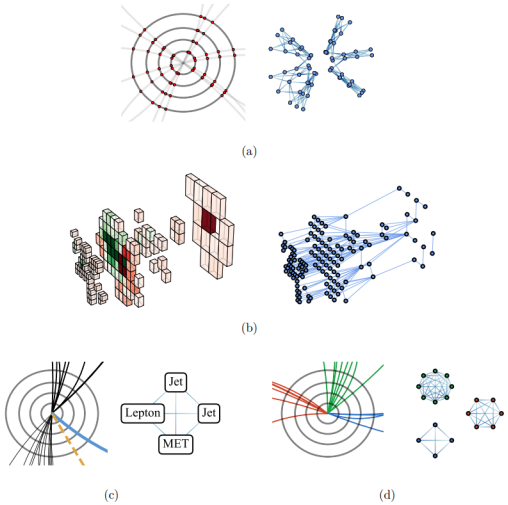

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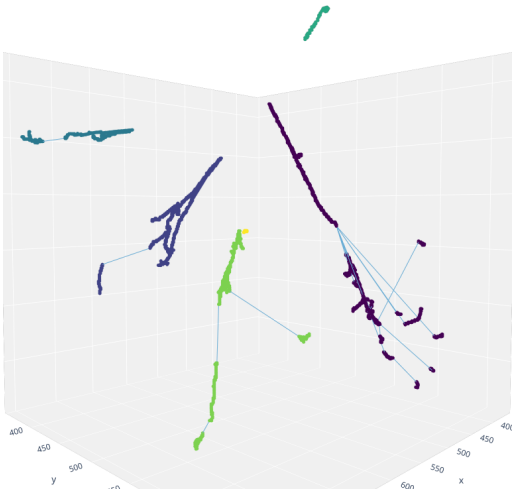

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(*) **Nodes**: particles
Edges: parentage or superstructure

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Karate Club

- **Nodes**: people in a club
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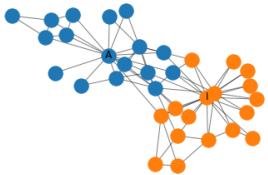

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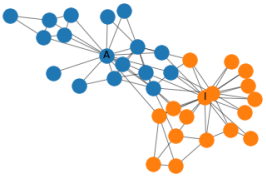
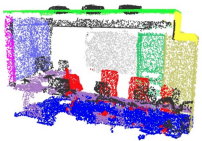


ShapeNet

- **Nodes**: point in cloud
- **Edges**: proximity
- Classify points into different categories



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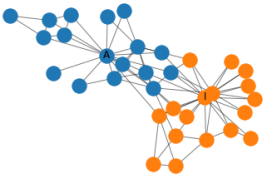

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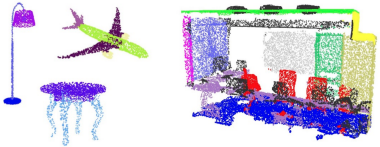
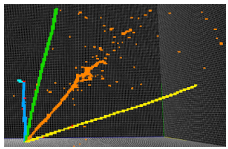


Particle classification

- **Nodes**: particles
- **Edges**: parentage
- Identify particle type (p, e, γ, μ, π)



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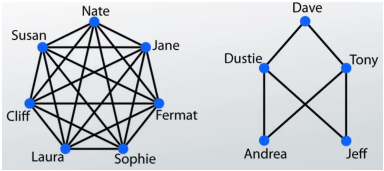
Link classification

- **Nodes**: people in a group
- **Edges**: potential links
- Are Nate and Laura friends, family, coworkers?



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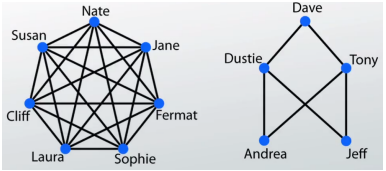

Scene comprehension

- **Nodes**: objects in scene
- **Edges**: all-to-all
- Is object A the same shape as B ? Is it bigger ?

Graphs

Task categories

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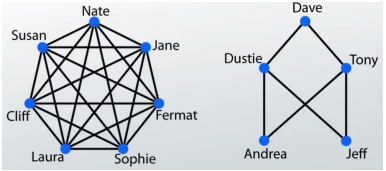

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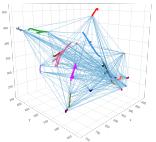
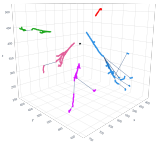
Particle clustering

- **Nodes**: particles
- **Edges**: all-to-all
- Is this edge a true parentage edge ?





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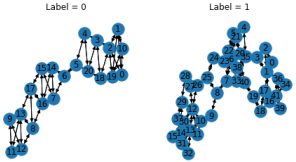
Enzyme classification

- **Nodes**: AA structures
- **Edges**: spatial proximity
- What is the purpose of this enzyme (protein) ?



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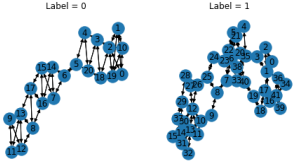
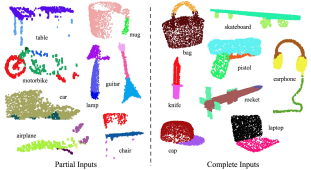


Point cloud classification

- **Nodes**: point in cloud
- **Edges**: proximity
- What class of object does it belong to ?



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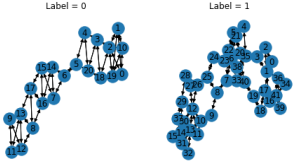

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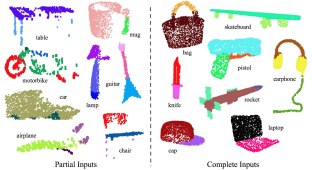
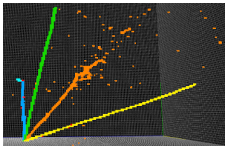


Interaction classification

- **Nodes**: particles
- **Edges**: parentage
- What class of interaction is this?

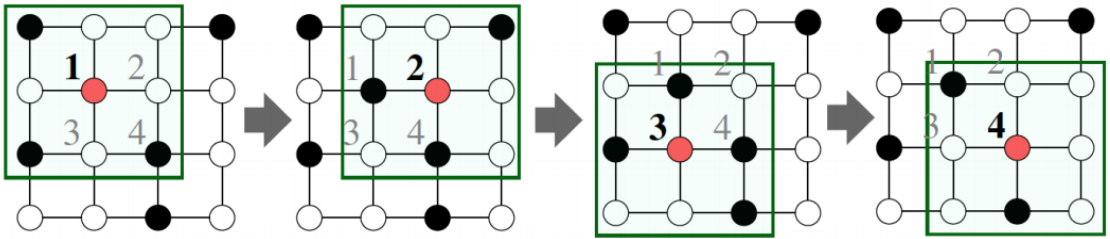


To perform the aforementioned tasks, the graph needs to develop **embeddings**, i.e. map the input features to a space in which the task can be performed.

The basic operation for CNNs is the **convolution layer**

- Aggregate a the pixel features within some distance by multiplying it by shared filter
- Formally: $\boldsymbol{x}_{i,j}^{(l+1)} = \sigma(\sum_{k \in \mathcal{N}(i)} \boldsymbol{w}_{j,k} \boldsymbol{x}_{k,j}^{(l)})$

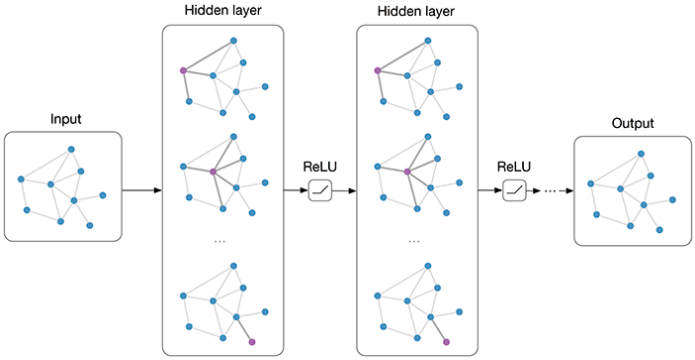
  with $x_{i,j}^{(l)}$ the j^{th} feature of pixel i at layer l and $w_{j,k}$ the k^{th} cell of filter j



Graph Convolutional Networks (GCNs) are an early implementation of GNNs which take:

- An (N, N_v) matrix, V, of **node features**
- An (N, N) **adjacency matrix**, A, only used for neighborhood aggregation

  NB: The adjacency matrix is a dense formulation of edges, in which $A_{ij} = 1$ if the corresponding edge $e_{\{k|i=s_k, j=r_k\}}$ exists in the graph, $A_{ij} = 0$ otherwise



GNNs don't have regular neighborhoods, but why not use the adjacency matrix?

$$h_i^{(l+1)} = \sigma(\sum_{j=1}^{N} A_{i,j} h_j^{(l)} W^{(l)}), \qquad \text{or} \quad H^{(l+1)} = \sigma(AH^{(l)}W^{(l)}), \tag{1}$$

where σ is an activation function, $W^{(l)}$ is an $(N_v^{(l-1)}, N_v^{(l)})$ **weight matrix shared across all nodes** (similar to to the convolution filters of CNNs).

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Two caveats:

- A must contain self-loops (otherwise no self-preservation): $\hat{A} = A + I$
- The nodes with more connections (higher degree) have larger features. That is not desirable, so divide by degree matrix $\hat{D}$ of $\hat{A}$.

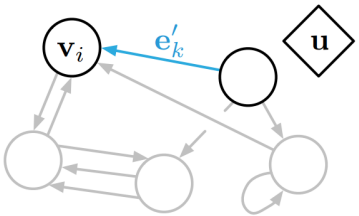
$$h_i^{(l+1)} = \sigma(\frac{1}{\hat{d}_i} \sum_{j=1}^{N} \hat{A}_{i,j} h_j^{(l)} W^{(l)}), \qquad \text{or} \quad H^{(l+1)} = \sigma(\hat{D}^{-1} \hat{A} H^{(l)} W^{(l)}), \tag{2}$$

The GCN neighborhood aggregation method, while elegant in its one-to-one similarity with pixel convolutions in CNN, is inherently limited:

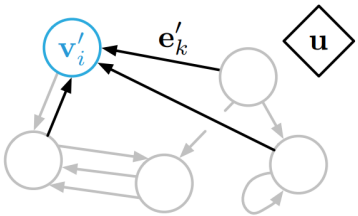
- It does not support edge-specific features
- It does not support explicit graph-specific features
- It does not support other neighborhood aggregation strategies than a simple sum

$\rightarrow$ How can we build features with a graph in all its complexity ?

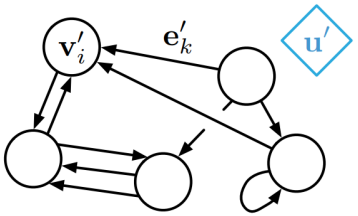
The most general for GNNs is called **message passing**



(a) Edge update



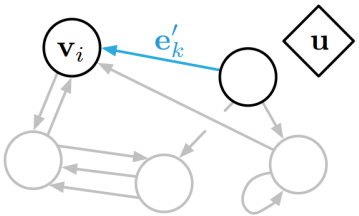
(b) Node update



(c) Global update

The most general for GNNs is called **message passing**

1. **Edge update**: fold adjacent node features and global features into an edge
   $\boldsymbol{e}'_k = \phi_e(\boldsymbol{e}_k, \boldsymbol{v}_{r_k}, \boldsymbol{v}_{s_k}, \boldsymbol{u})$, with ϕ_e a learnable function



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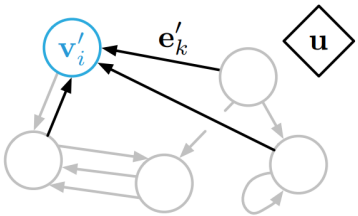

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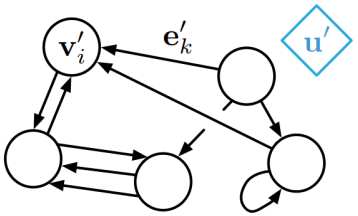

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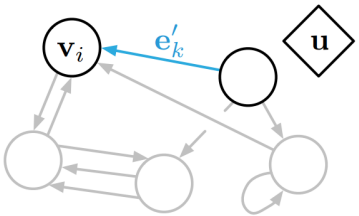

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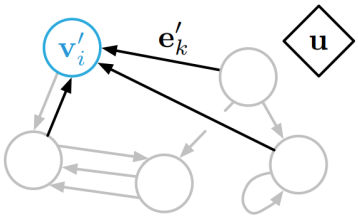

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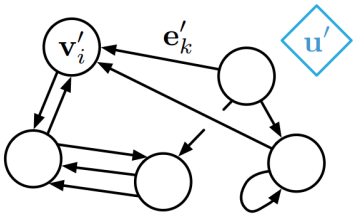

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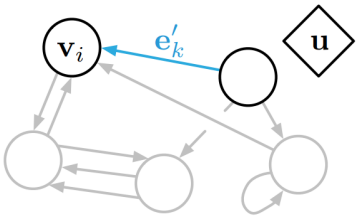
3. **Global update**: fold all node and edge features to update the global state
   $\boldsymbol{u}' = \phi_u(\rho_{e,u}(E'), \rho_{v,u}(V'), \boldsymbol{u})$, with ϕ_u a learnable function, $E' = \{\boldsymbol{e}_k\}_{k=1}^{N_e}$ and $E' = \{\boldsymbol{v}_i\}_{i=1}^{N_v}$



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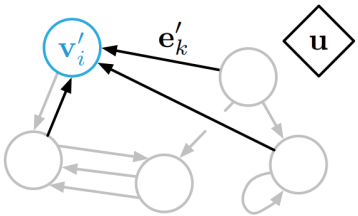

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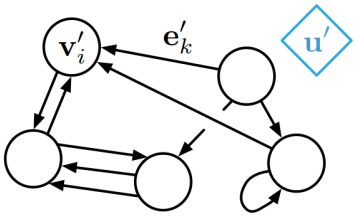
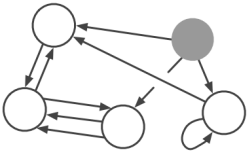
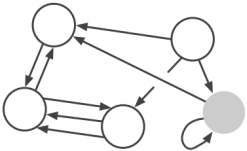


(c) Global update

The basic operation for GNNs is called **neighborhood aggregation** or **message passing**



$m = 0$



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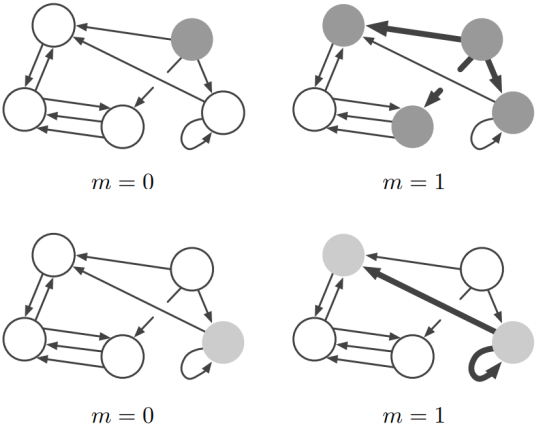

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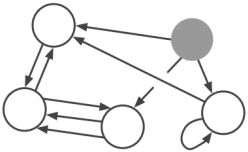
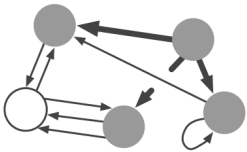
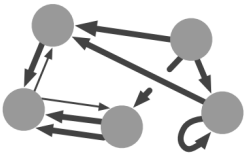


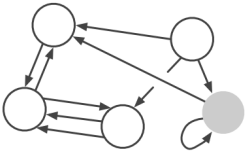
$m = 0$



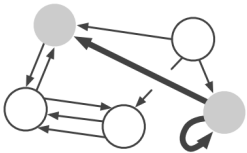
$m = 1$



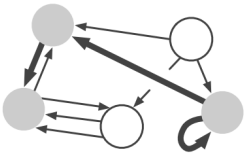
$m = 2$



$m = 0$



$m = 1$



$m = 2$

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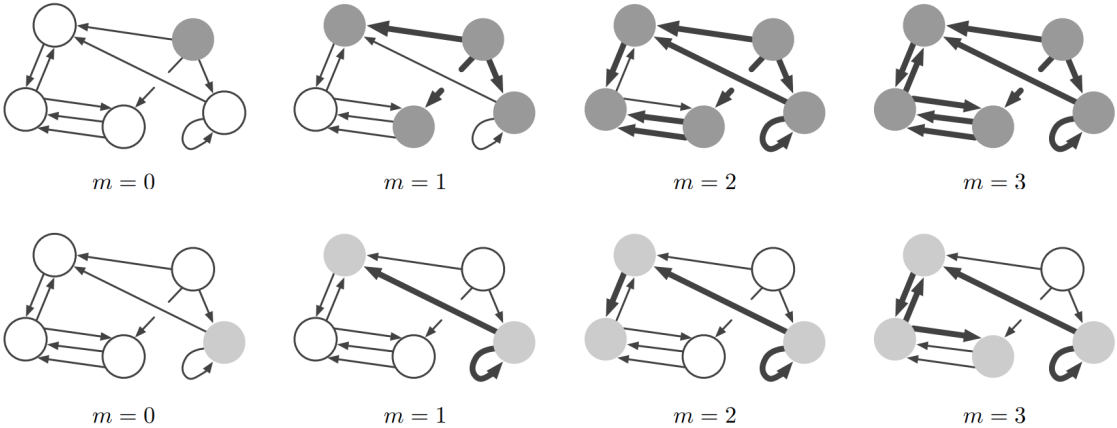
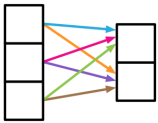
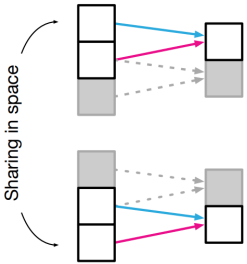


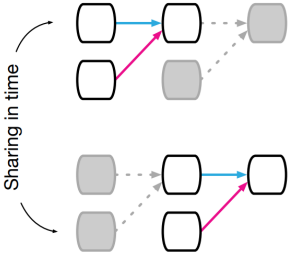
Component	Entities	Relations	Rel. inductive bias	Invariance
Fully connected	Units	All-to-all	Weak	-
Convolutional	Grid elements	Local	Locality	Spatial translation
Recurrent	Timesteps	Sequential	Sequentiality	Time translation
Graph network	Nodes	Edges	Arbitrary	Node, edge permutations



(a) Fully connected



(b) Convolutional



(c) Recurrent

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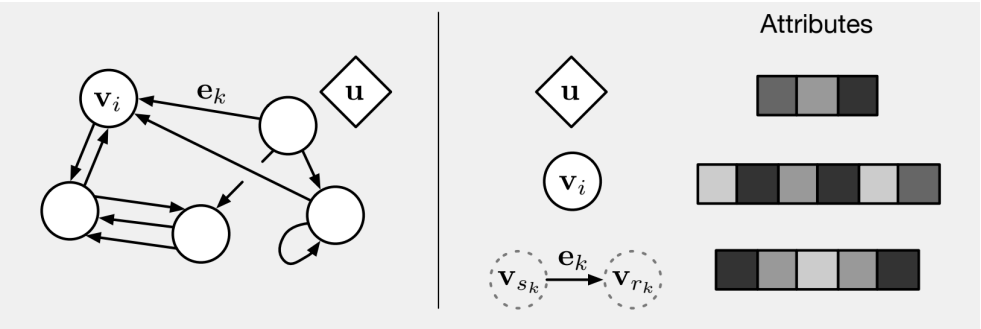

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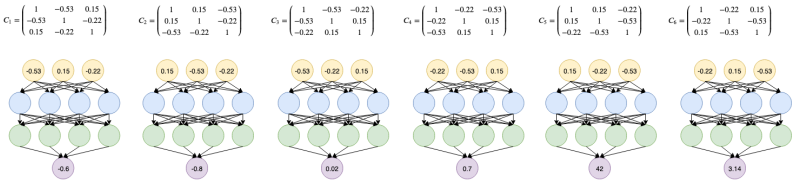
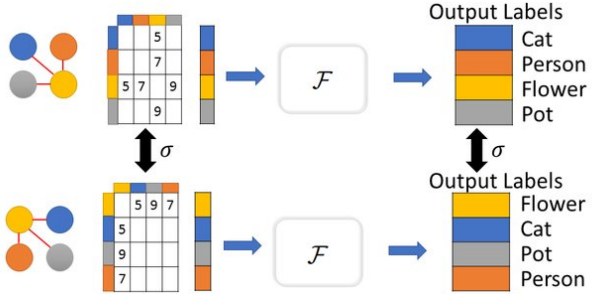
MLP



$$\exists \pi \in \mathfrak{S}_n, f(x_1, x_2, \ldots, x_M) \neq f(x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(M)})$$

GNN

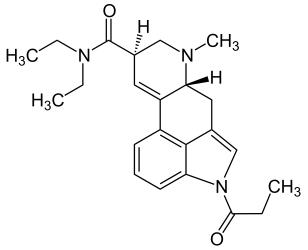


From nodes, sometimes the graph edges come naturally...

- Bonds on a molecule, springs in physical system, etc.

... and sometimes they do not:

- Point clouds, particle clustering, etc.



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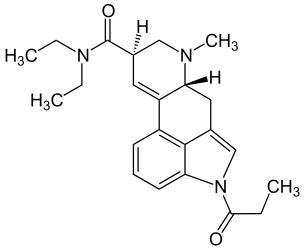

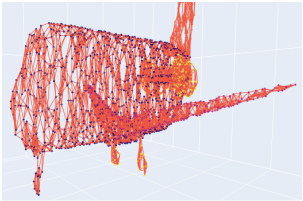

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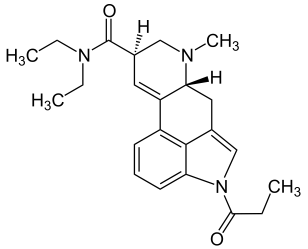

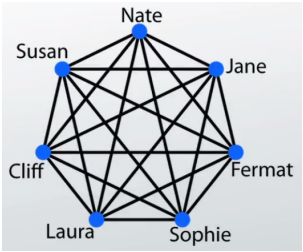

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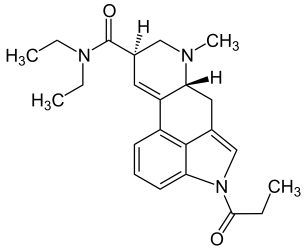

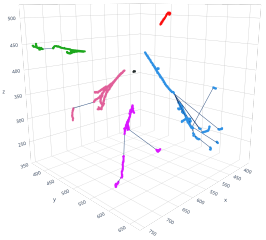

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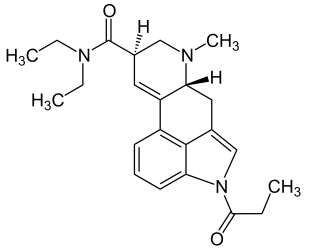
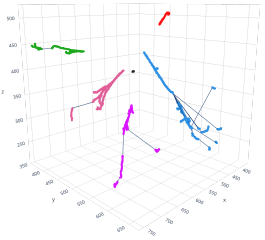
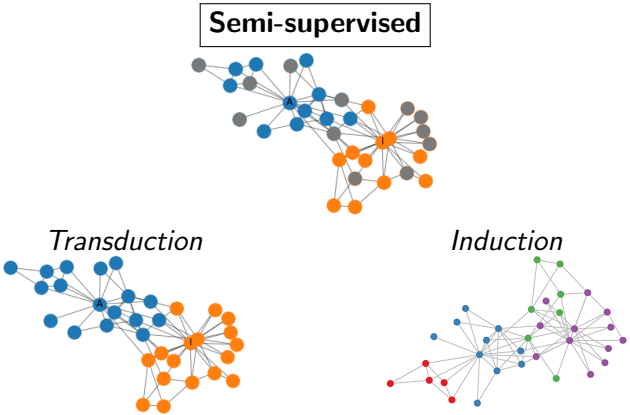
- Edges can also **dynamically** evolve during training





GNNs have the peculiarity of supporting either **transductive** of **inductive inference**

- **Semi-supervised** learning: some of the nodes in the input graph(s) are unlabeled



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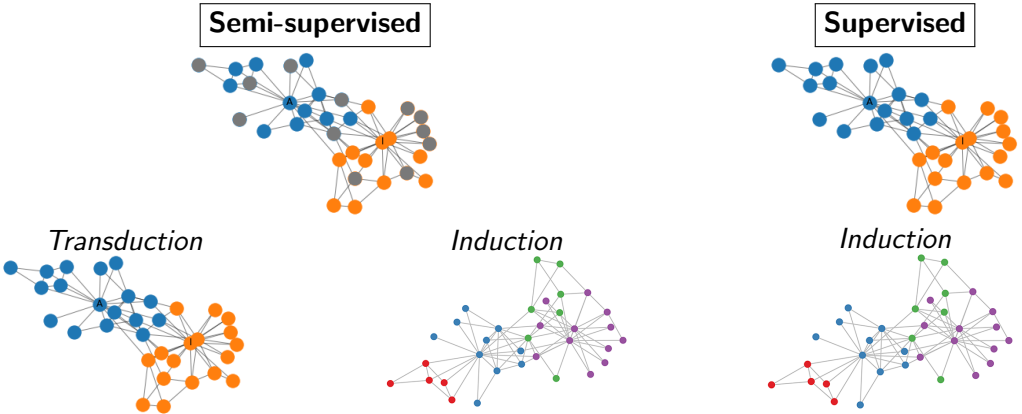
- **Supervised** learning: all of the nodes in the input graphs(s) are labeled



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- Recall from earlier: $\boldsymbol{u} = \phi_u(\rho_{e,u}(E'), \rho_{v,u}(V'))$

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  with ϕ_u a learnable function, $\rho_{e,u}$, $\rho_{v,u}$ edge and node feature aggregators, respectively
- The aggregators are typically one of sum, mean or max

After developing node (+edge) features, if one wants to infer graph-wide properties, the features must be pooled. The simplest method is **single-step aggregation**:

- Recall from earlier: $\boldsymbol{u} = \phi_u(\rho_{e,u}(E'), \rho_{v,u}(V'))$

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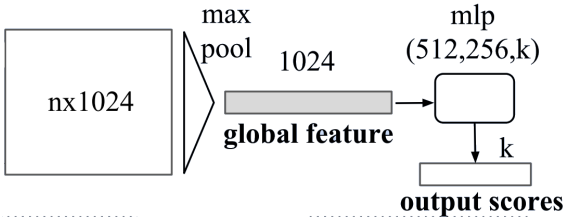
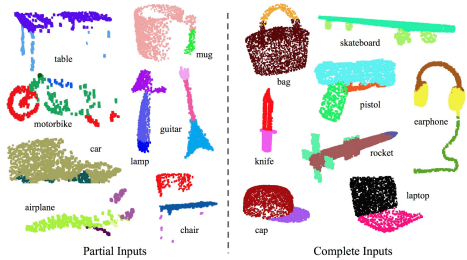
Example: **PointNet** used to classify 3D shapes (arXiv:1612.00593)





Single-step not the SOTA because it only convolves local neighborhood of nodes. As in CNN, one wants to progressively extract more / features. **Hierarchical pooling** iteratively uses:

- **Sampling**: reduce the number of nodes between layers
- **Grouping**: aggregate the features of the nodes that are gone

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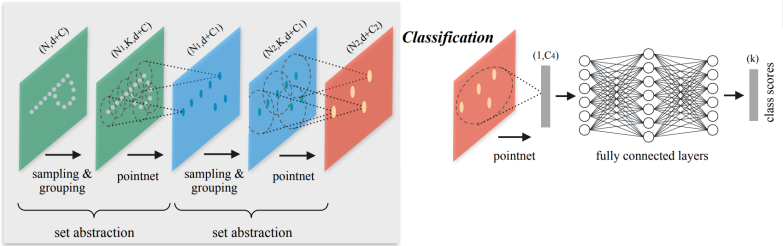
Example 1: PointNet++ for point cloud classification

- Iterative farthest point sampling
- Max-pool grouping over neighborhood of new nodes



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- **Sampling**: reduce the number of nodes between layers
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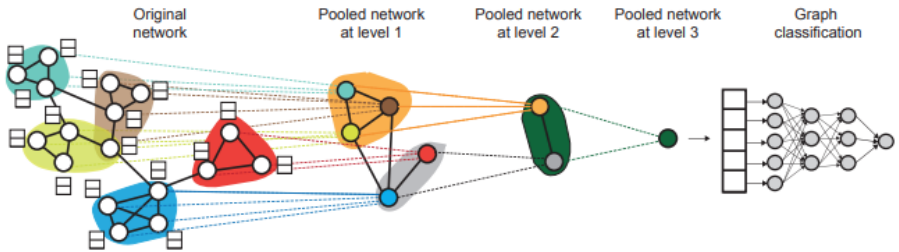
Example 2: DiffPool for arbitrary graph classification

- At each step, let the network learn a $(N_v^{(l)}, N_v^{(l+1)})$ **assignment matrix** $S^{(l)}$ (w/ GNN):
  $H^{(l+1)} = {S^{(l)}}^T H^{(l)}, \qquad A^{(l+1)} = {S^{(l)}}^T A^{(l)} S^{(l)}$



Example A: Social network | Task

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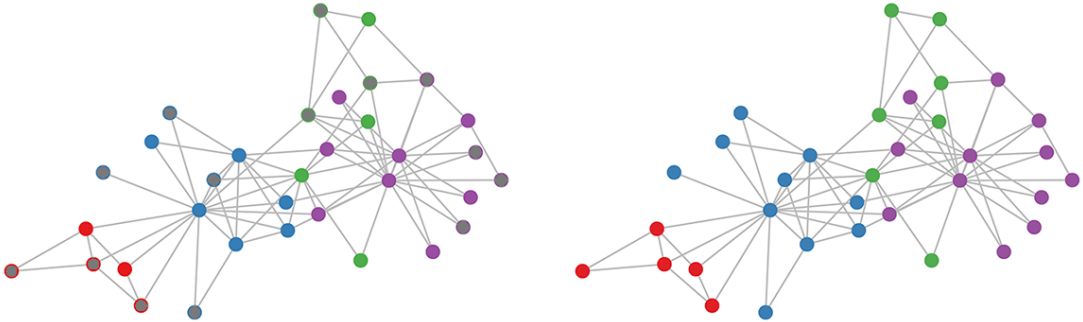
Dataset: **Zachary's Karate club**, famous early (70s) example of a social network problem

- Consists of $N = 34$ nodes (individuals), with no node features (no information)
- Has 78 edges, corresponding to pairs of people who talk to each other outside of the club
- The group splits (in this example four ways), who goes with in what group ?

Goal: Some nodes are known, some are unknown, classify unknown nodes (semi-supervised)



Embedding visualization | t-SNE

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An aside: how to represent point in a feature space of dimension > 3 ?

The t-distributed Stochastic Neighbor Embedding is a transformation which:

1. Computes the similarity between every pair of N points in d dimensions:
   $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}$, with $p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$, and σ_i adpatative to local density

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3. Defines the t-distributed (strong tails) similarity of points in the new space as
   $q_{ij} = \frac{(1+\|\mathbf{y}_i-\mathbf{y}_j\|^2)^{-1}}{\sum_k\sum_{l\neq k}(1+\|\mathbf{y}_k-\mathbf{y}_l\|^2)^{-1}}$

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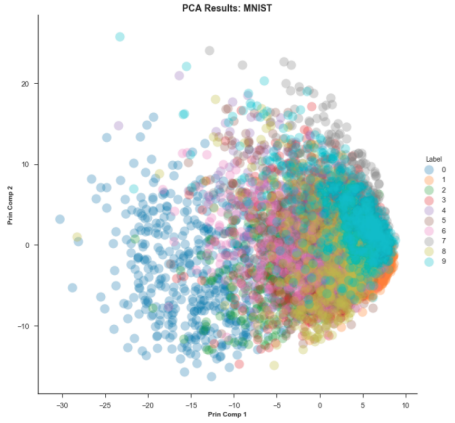
4. Minimize the KL-divergence (see Kazu day 1) between the two set of similarities using gradient decent (optimization)
   $\mathrm{KL}(P \parallel Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$

Embedding visualization | t-SNE

Fundamentally different approach (albeit much more complex) to PCA:

- PCA maximizes variance in the lower-dimensional space



Embedding visualization | t-SNE

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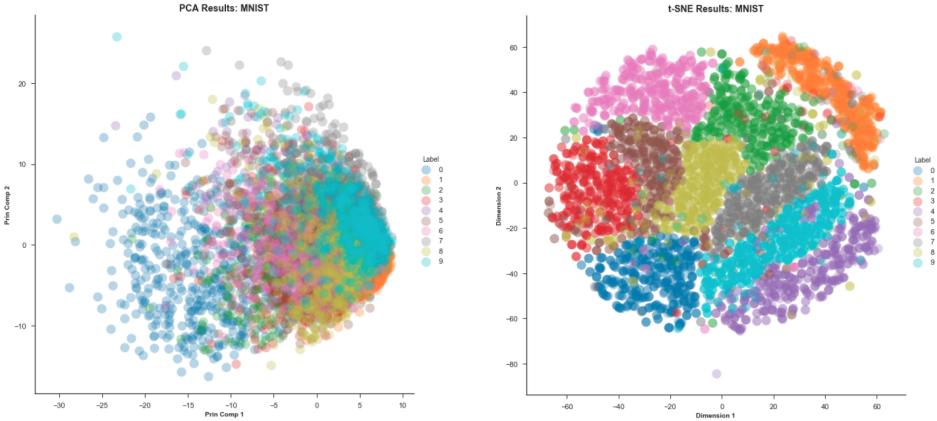
Fundamentally different approach (albeit much more complex) to PCA:

- PCA maximizes variance in the lower-dimensional space
- t-SNE preserves data point similarity (close in original space $\rightarrow$ close in lower dimension)

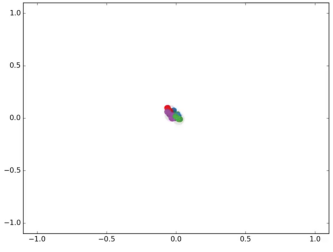


These are the steps of the feedforward network:

- Pass the nodes through two GCN layers
  1. Increase node features from 1 (blank) to 16
  2. Maintain 16 features in the convolution
- Pass the nodes features through a fully connected linear classification layer $(16 \to 4)$
- Apply the class-wise mean cross-entropy loss on node scores

$$L = -\frac{1}{N_c}\frac{1}{N}\sum_i \sum_c s_{i,c} \times \ln(s_{i,c}), \qquad s_i = \text{softmax}(x_i)$$

- Apply storchastic gradient decent 300 times



Watch the embeddings before the classification layer evolve: video

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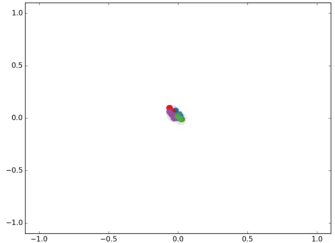
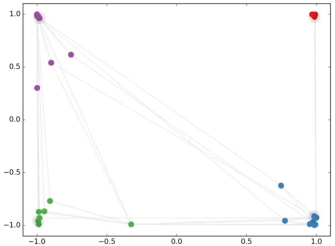
The GNN learns to separate classes in the feature hyperspace





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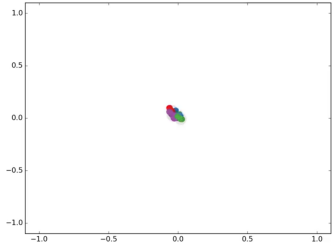
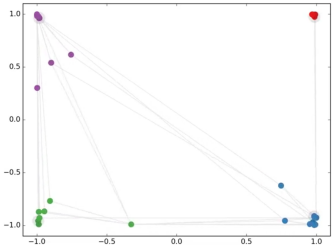
The GNN learns to separate classes in the feature hyperspace

Will use this technique for another task in the tutorial!

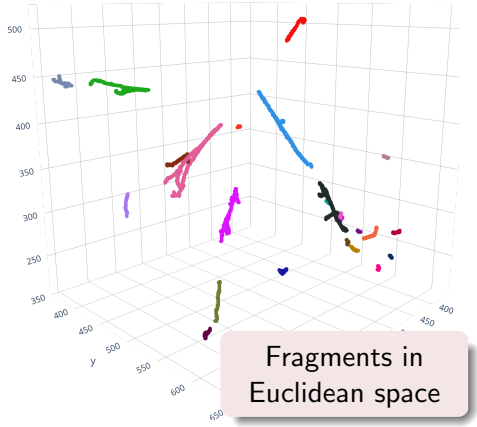




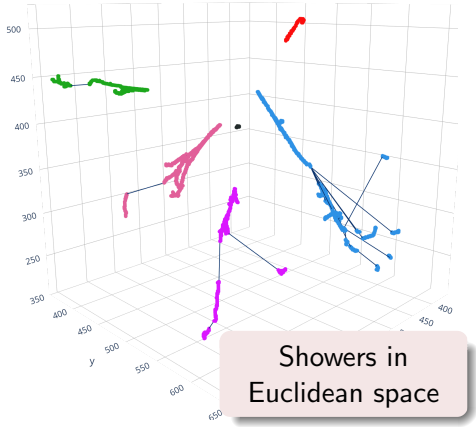
Example B: Clustering | Task

Here the goal is to cluster multiple particle traces into superstructures

- Nodes are particles, edges are connections.



Fragments in Euclidean space



Showers in Euclidean space

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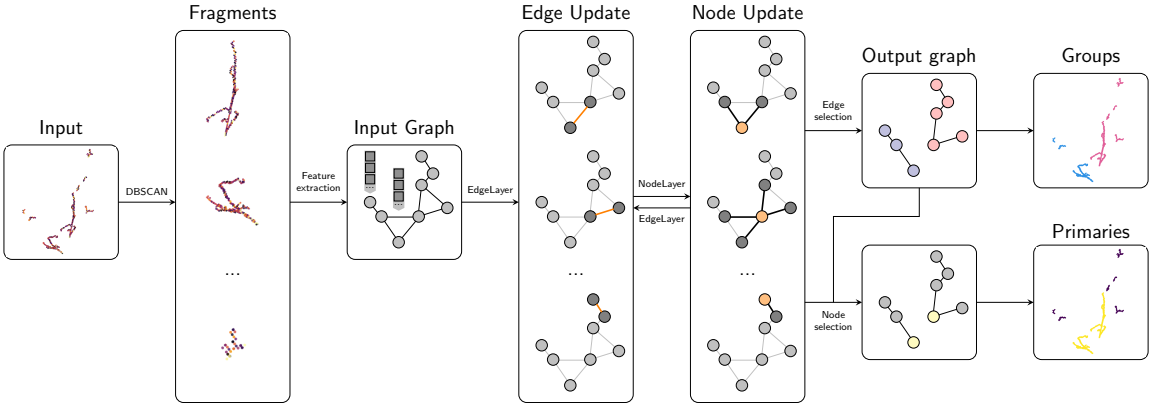


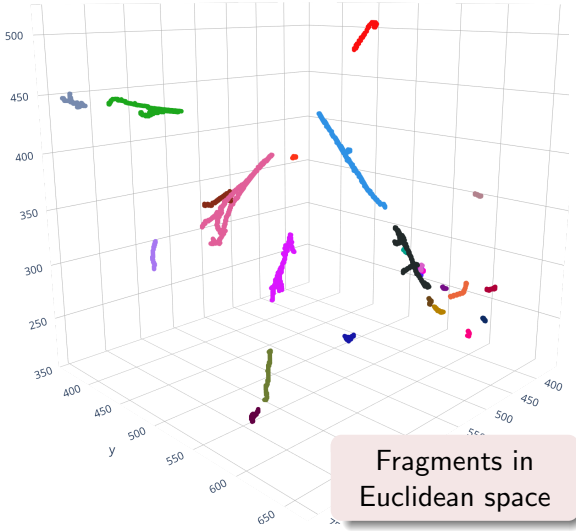
Paper: arXiv:2007.01335

Shower clustering

Network input

Input:

- Fragmented EM showers



Fragments in Euclidean space

Shower clustering

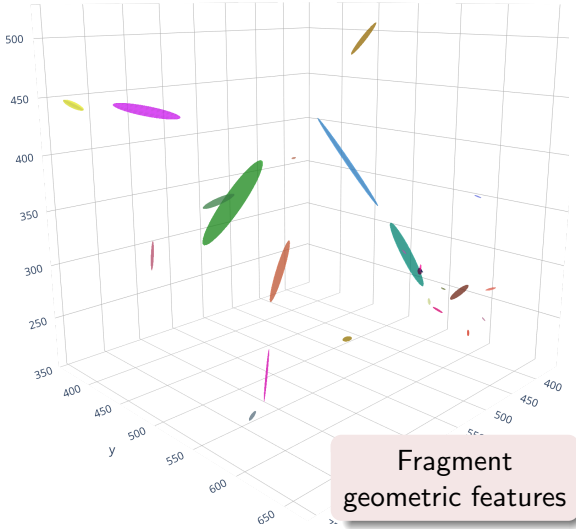
Network input

Input:

- Fragmented EM showers

Node features:

- Centroid
- Covariance matrix, PCA
- Start point, direction (PPN)



Fragment geometric features

Shower clustering

Network input

Input:

- Fragmented EM showers

Node features:

- Centroid
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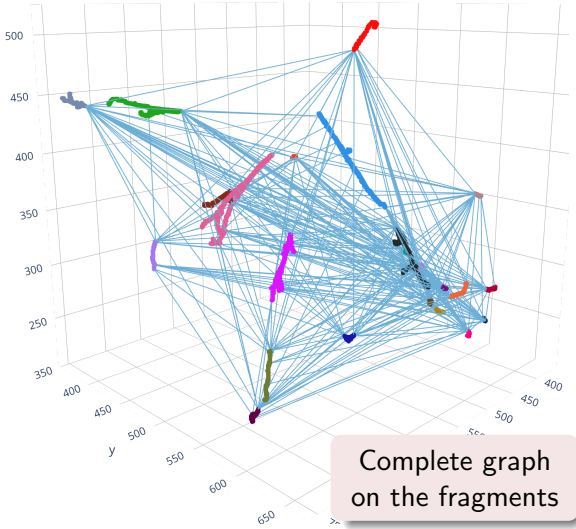
- Start point, direction (PPN)

Input graph:

- Connect every node with every other node (**complete graph**)



Complete graph on the fragments

Shower clustering

Network input

Input:

- Fragmented EM showers

Node features:

- Centroid
- Covariance matrix, PCA
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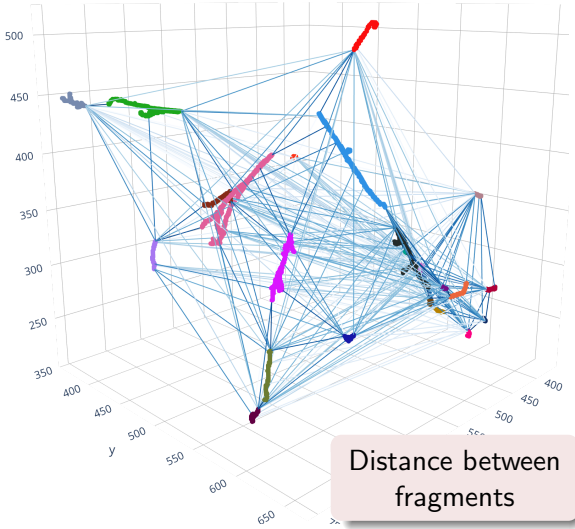
Input graph:

- Connect every node with every other node (**complete graph**)

Edge features:

- Displacement vector (+variations)
- Closest points of approach



Distance between fragments

Shower clustering

Edge classification

At each message passing step (MetaLayer: arXiv:1806.01261):

- **Edge update**

  $\boldsymbol{e}'_k = \text{MLP}(\boldsymbol{v}_{s_k}, \boldsymbol{v}_{r_k}, \boldsymbol{e}_k)$

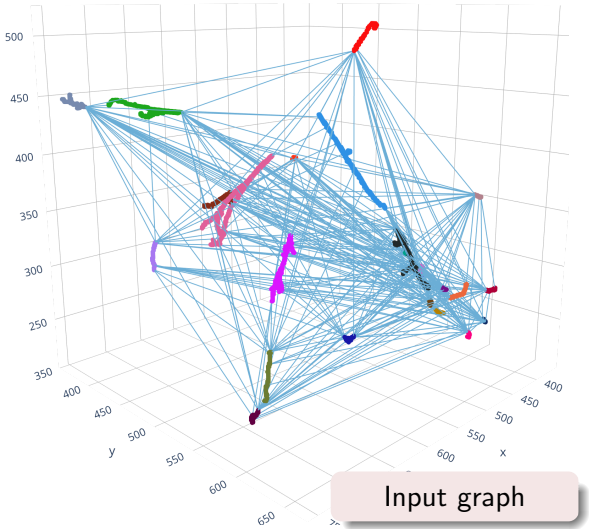
- **Node update**

  $\boldsymbol{m}_{ji} = \text{MLP}(\boldsymbol{v}_j, \boldsymbol{e}'_{\{k|s_k=j,r_k=i\}})$

  $\boldsymbol{v}'_i = \text{MLP}(\boldsymbol{v}_i, \square_{i\in\mathcal{N}(i)}\boldsymbol{m}_{ji})$

After $n = 3$ node+edge updates:

- Edge binary classification



Input graph

Shower clustering

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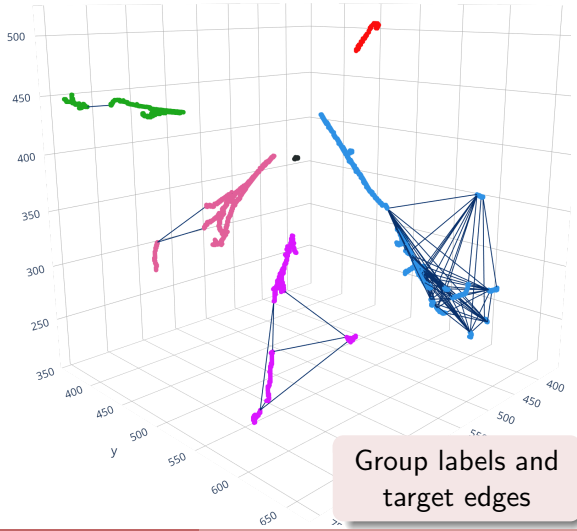
After $n = 3$ node+edge updates:

- Edge binary classification

Target:

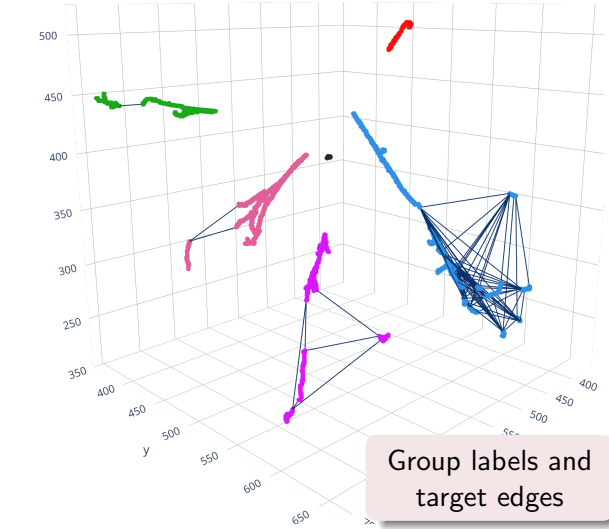
- Predict adjacency matrix $A_{ij} = \delta_{g_i,g_j}$ with $\boldsymbol{g}$ the true partition of the set
- Apply cross-entropy loss



Group labels and target edges

Shower clustering

Example



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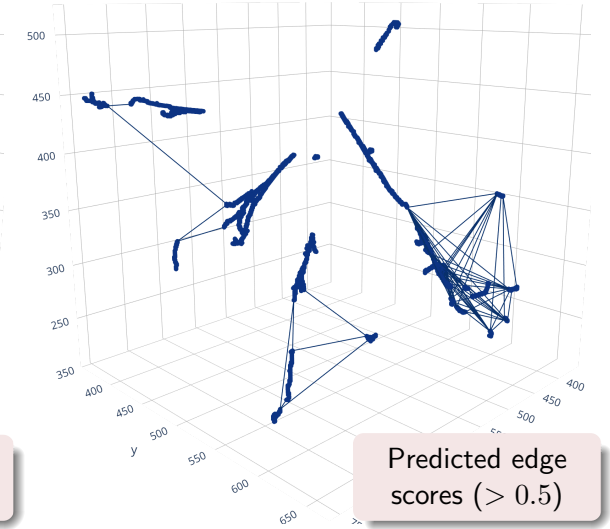
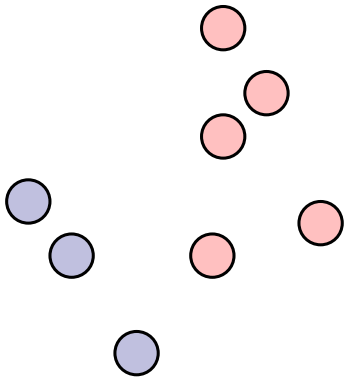


Predicted edge scores (> 0.5)

The network predicts a score matrix S, estimate of the true adjacency matrix A

- How to recover a set partition $\hat{g}$?

True partition



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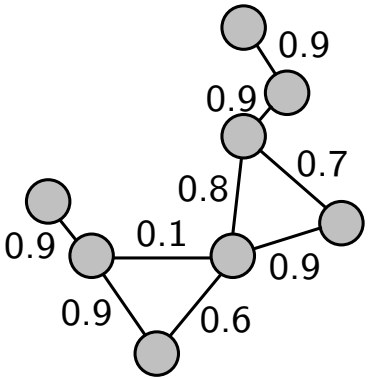
Edge scores



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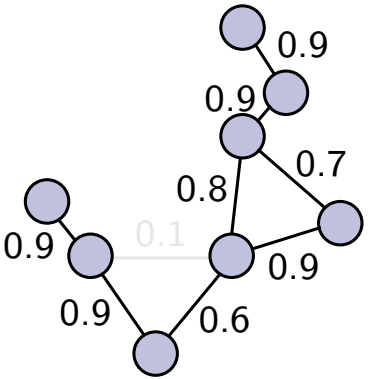
The network predicts a score matrix $\boldsymbol{S}$, estimate of the true adjacency matrix $\boldsymbol{A}$

- How to recover a set partition $\hat{\boldsymbol{g}}$?

We want the partition $\hat{\boldsymbol{g}}$ that minimizes the CE loss, given $\hat{A}_{ij} = \delta_{\hat{g}_i, \hat{g}_j}$, e.g.

$$L(S|g) = -\frac{1}{N_e} \sum_{(i,j)\in E} \delta_{g_i,g_j} \ln(s_{ij}) + (1 - \delta_{g_i,g_j}) \ln(1 - s_{ij})$$

Thresholded graph



$$L \simeq 3.92$$

The network predicts a score matrix $\boldsymbol{S}$, estimate of the true adjacency matrix $\boldsymbol{A}$

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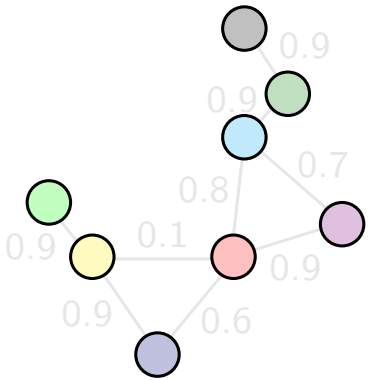
G is the set of all possible partitions

- Bell number, huge ($B_{20} \simeq 5 \times 10^{13}$), cannot brute force, how to optimize?
- Start with an empty graph

Empty graph



$L \simeq 15.35$

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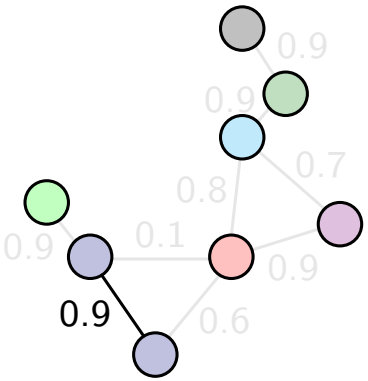
- Iteratively attempt to add most likely edges until edge score < 0.5

First edge



$L \simeq 13.15$

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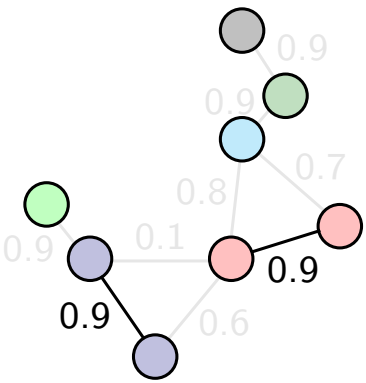
Second edge



$L \simeq 10.95$

The network predicts a score matrix $\boldsymbol{S}$, estimate of the true adjacency matrix $\boldsymbol{A}$

- How to recover a set partition $\hat{\boldsymbol{g}}$?

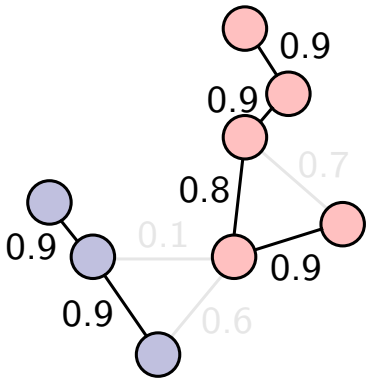
We want the partition $\hat{\boldsymbol{g}}$ that minimizes the CE loss, given $\hat{A}_{ij} = \delta_{\hat{g}_i, \hat{g}_j}$, e.g.

$$L(S|g) = -\frac{1}{N_e} \sum_{(i,j)\in E} \delta_{g_i,g_j} \ln(s_{ij}) + (1 - \delta_{g_i,g_j}) \ln(1 - s_{ij})$$

G is the set of all possible partitions

- Bell number, huge ($B_{20} \simeq 5 \times 10^{13}$), cannot brute force, how to optimize?
- Start with an empty graph
- Iteratively attempt to add most likely edges until edge score < 0.5

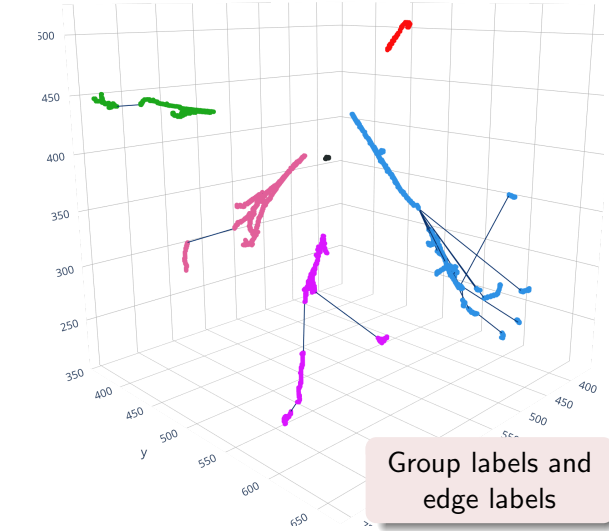
Optimized partition



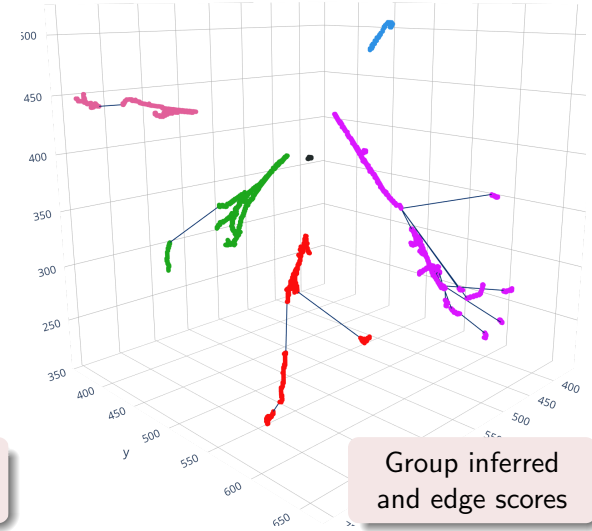
$$L \simeq 2.13$$

Shower clustering

Performance



Group labels and edge labels



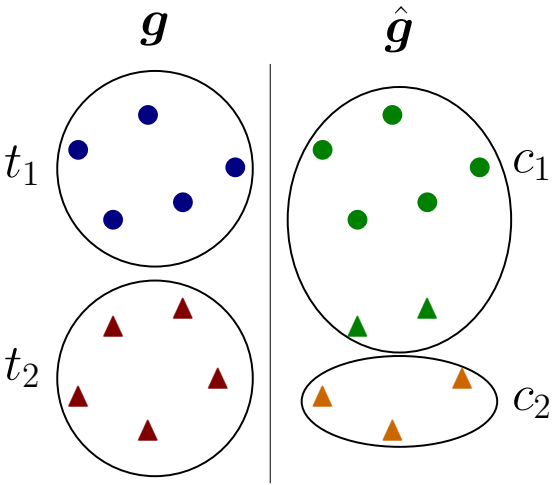
Group inferred and edge scores

Purity $= \frac{1}{N}\sum_{i=1}^{n_p} \max_j |c_i \cap t_j|$

- c_i predicted cluster
- t_j true cluster with highest count in c_i

Efficiency $= \frac{1}{N}\sum_{i=0}^{n_t} \max_j |c_j \cap t_i|$

- c_j pred. cluster with highest count in t_i
- t_i true cluster



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Purity $= \frac{1}{N}\sum_{i=1}^{n_p} \max_j |c_i \cap t_j|$

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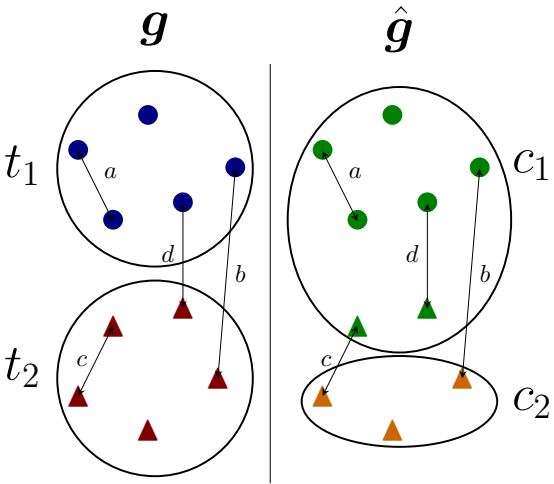
- c_j pred. cluster with highest count in t_i
- t_i true cluster

Adjusted Rand Index (ARI)

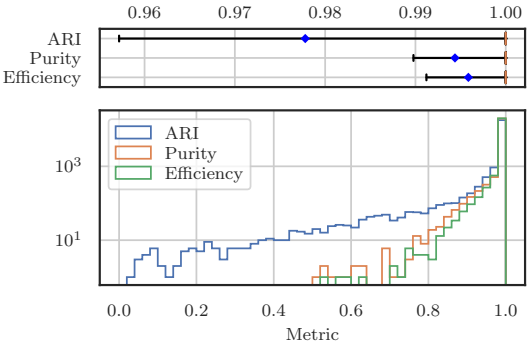
- Measure of overlap of prediction and truth, adjusted for random chance

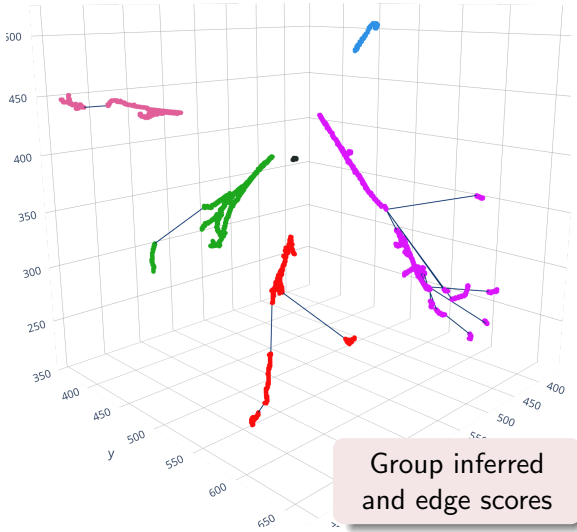
$\text{RI} = \frac{a+b}{a+b+c+d}$

$\text{ARI} = \frac{RI - E(RI)}{1 - E(RI)}$



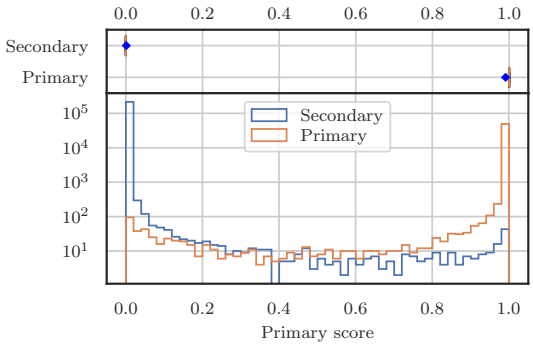
Shower clustering accuracy:

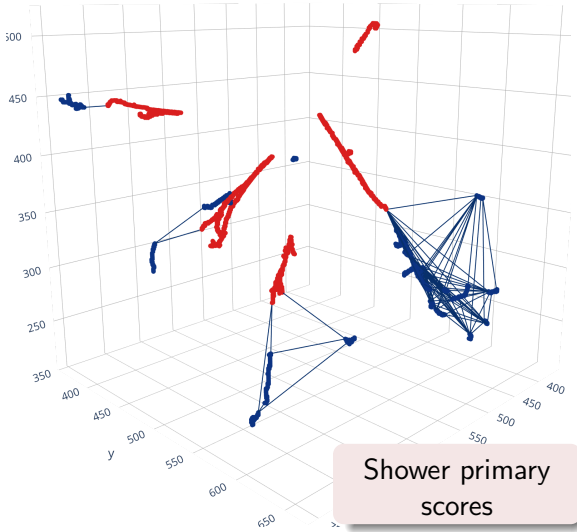




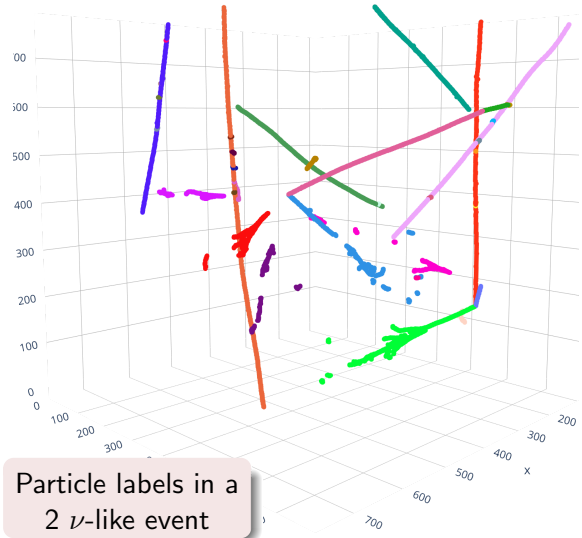
Group inferred and edge scores

Shower primary accuracy (**99.8 %**):





Shower primary scores



Particle labels in a 2 ν-like event

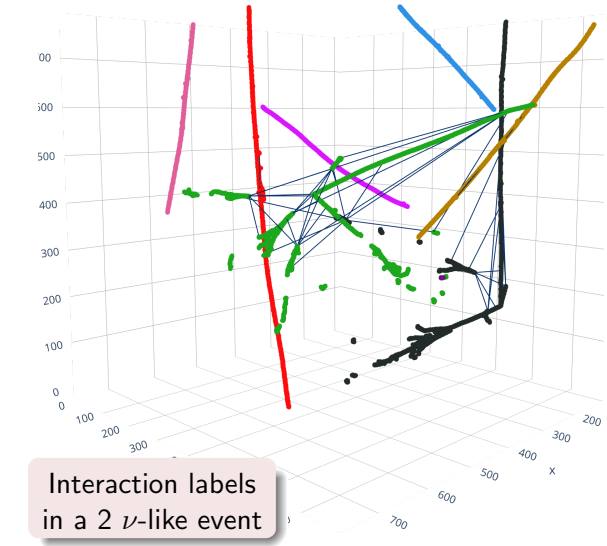
The shower clustering task can be extended to **interaction clustering**:

- Interaction group = particles that originate from the same vertex
- Fragment ID $\rightarrow$ Particle ID
- Particle ID $\rightarrow$ Interaction ID

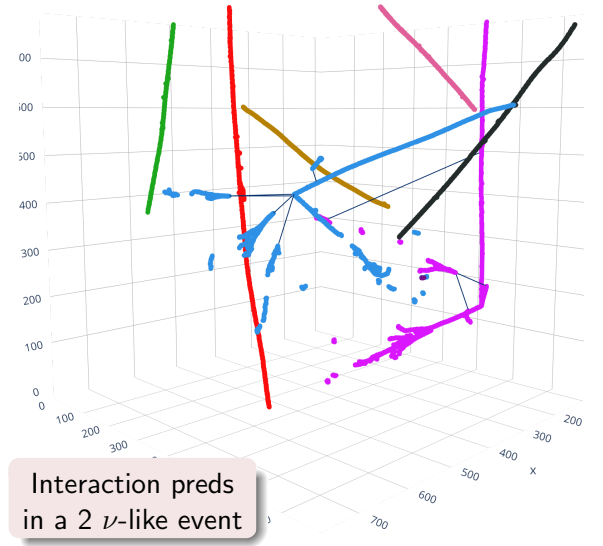
Useful to:

- Separate signal from background
- Resolve pileup

Interaction Clustering | Performance

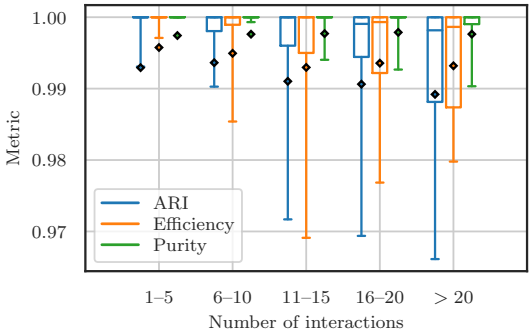


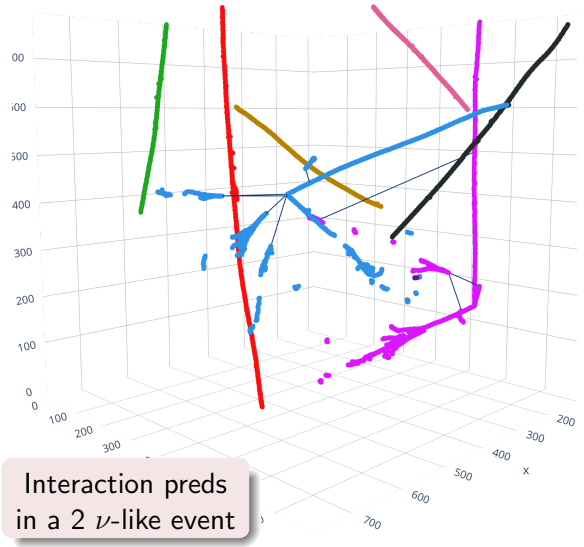
Interaction labels in a 2 ν-like event



Interaction preds in a 2 ν-like event

Interaction clustering performance:

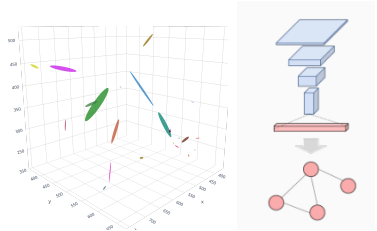


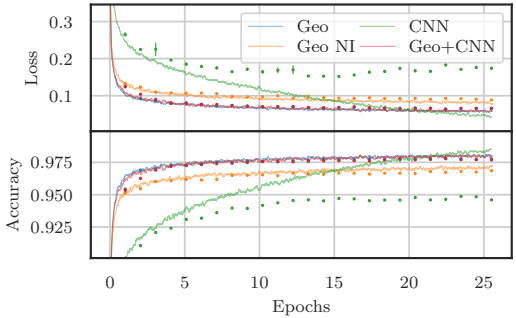


Interaction preds in a 2 ν-like event

A lot of work in optimizing the different components of the GNN chain:

- Feature extractor
  - Geometric (w/ or w/o PPN)
  - CNN



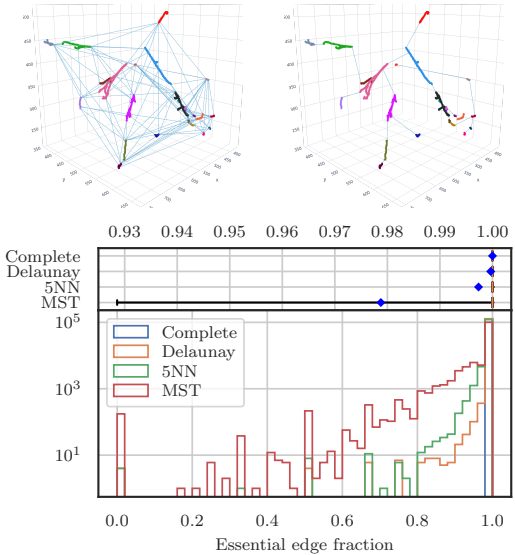


GNN Clustering

Optimization studies

A lot of work in optimizing the different components of the GNN chain:

- Feature extractor
  - Geometric (w/ or w/o PPN)
  - CNN
- Receptive field (graph)
  - Complete, Delaunay, MST, kNN



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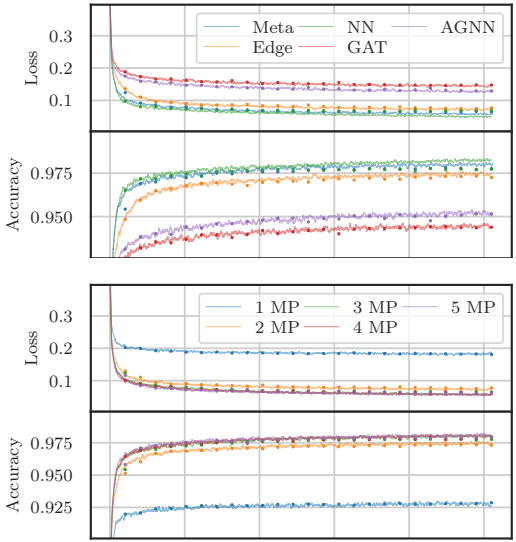
- Architecture
  - Node updater
  - Number of message passings



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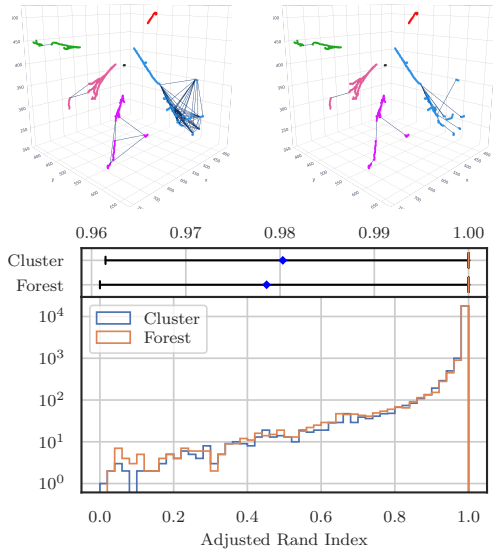
- Target adjacency matrix
  - Cluster graph
  - Forest



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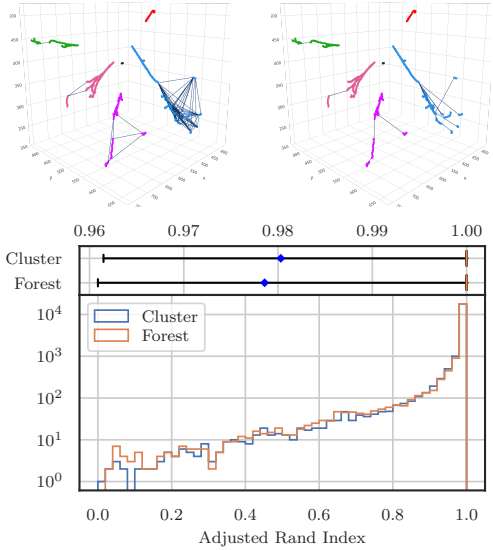


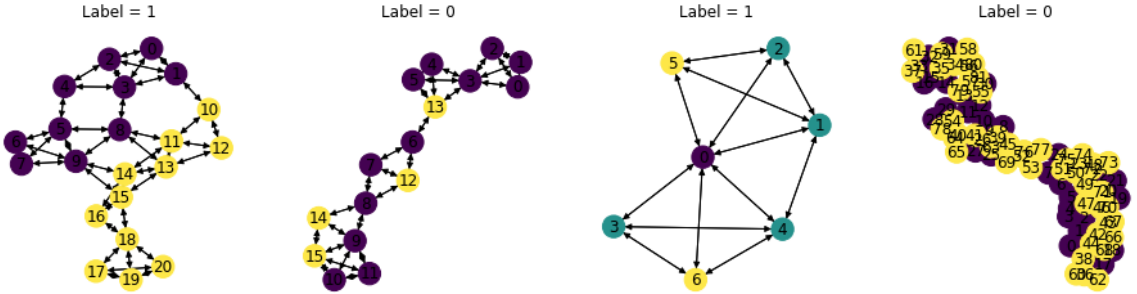
See paper: arXiv:2007.01335

Example C: Proteins | Task

Dataset: PROTEINS is a dataset of graph-encoded proteins

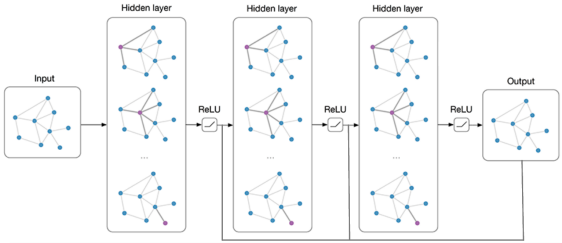
- There are 1113 graphs, one per protein
- The nodes are secondary structure elements (essentially turns, twists, folds, etc.)
- Edges connect adjacent structures (either in the chain, or in space)

Goal: Predict whether the protein is a enzyme, or not



For this example, there are two main ingredients:

- A 3-layer message passing function: **SAGEConv**
  - $x_i^{(l+1)} = W_1^{(l)} x_i^{(l)} + W_2^{(l)} \cdot \text{mean}_{j \in \mathcal{N}(i)} x_j^{(l)}$
- A linear layer combining the 3 node embeddings into a set of N_v' features
  - $x_i' = W'(x_i^{(1)}, x_i^{(2)}, x_i^{(3)})$



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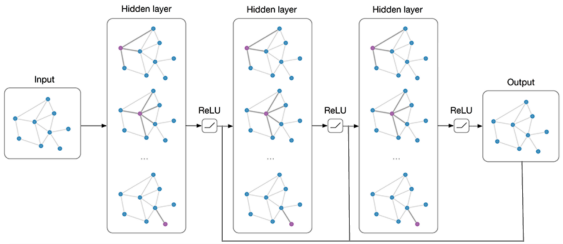
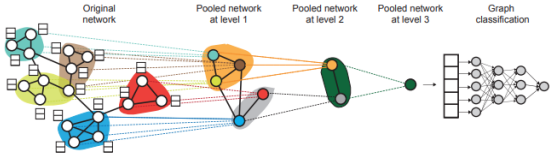
- A linear layer combining the 3 node embeddings into a set of N_v' features
  - $x_i' = W'(x_i^{(1)}, x_i^{(2)}, x_i^{(3)})$
- Two-layer graph pooling operation: **Diffpool**
  - First, reduce the number of nodes to N/4, then to N/16
- Aggregate the remaining node features to a 1D array
- Reduce to two features (one score for enzyme=NO, one for YES)





Given the 2-channel output of the network:

- The binary cross entropy loss is computed for each score pair:
  $-\frac{1}{N}(s_0 \ln(s_0) + s_1 \ln(s_1)), \qquad (s_0, s_1) = \mathsf{softmax}(x'_0, x'_1)$
- Update the model weights
- Repeat this for 10 epochs
  $\rightarrow$ Let's move to the notebook!

Conclusions

1. What are Graph Neural Networks (GNNs) good for ?
   - **Generalize** the concept of receptive field in CNNs and succession in RNNs to any **structured data**
   - Infer about objects in an ensemble, but also about **their correlations and superstructures**
2. How does information flow in a graph ?
   - GNNs are Neural Networks with a shared neighborhood aggregation rule: **message passing**
   - The adjacency matrix determines **information flow**
   - The message passing rule is extremely **flexible**... as long as it is **learnable**!

Thank you for your attention!