

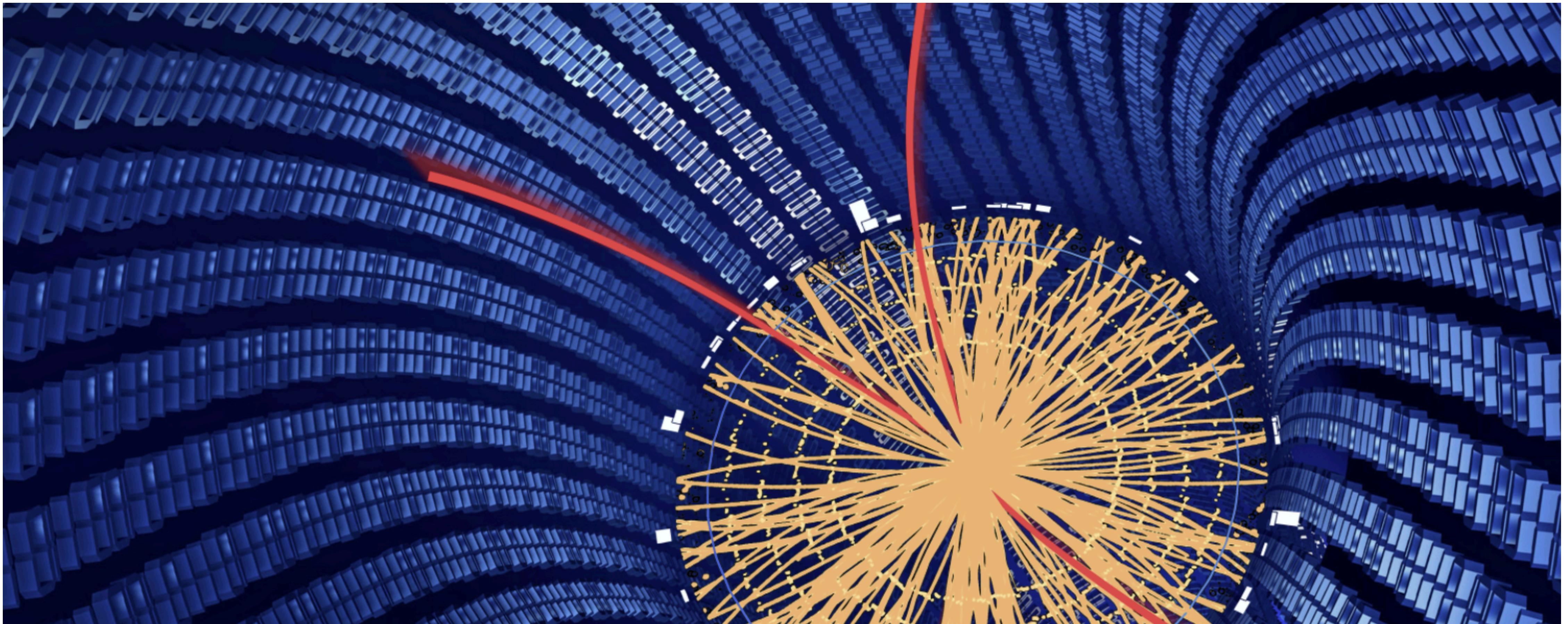
Graph neural networks

Maurizio Pierini



Outline

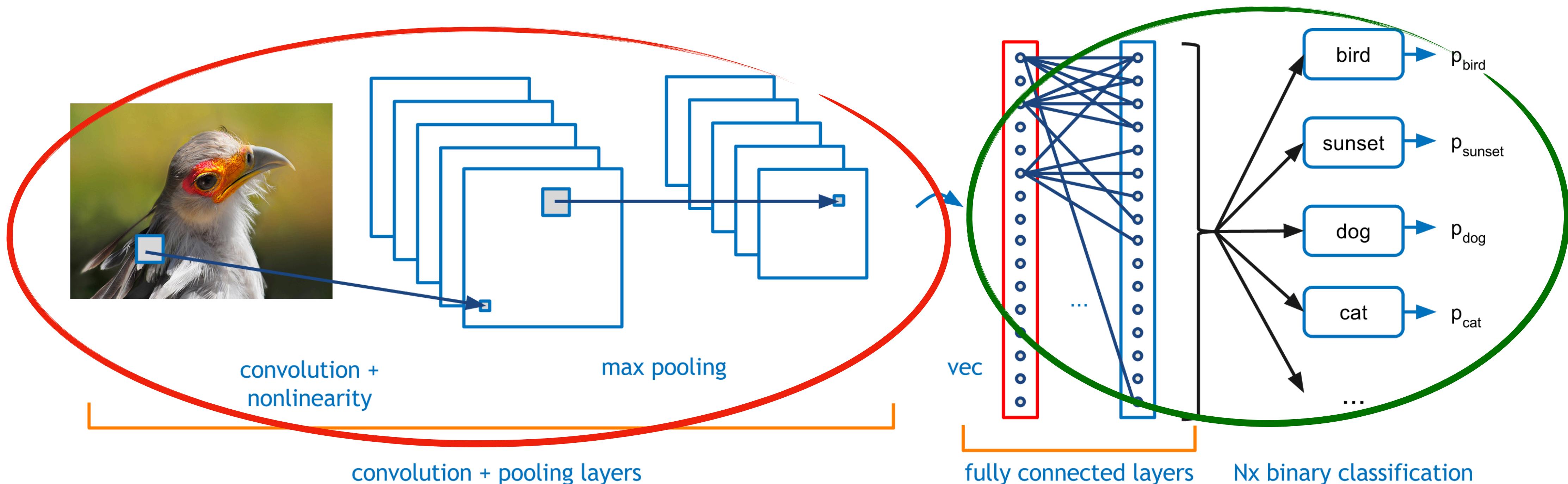
- *Deep Learning, Data representation and Graphs*
- *Message passing*
- *A few examples:*
 - *Edge Conv*
 - *Gated Graph Neural Networks*
 - *Interaction Networks*
 - *Distance-weighted NNs*
- *The GNN exercise* [NOT YET THERE]



Data Representation

Deep Neural Network in a nutshell

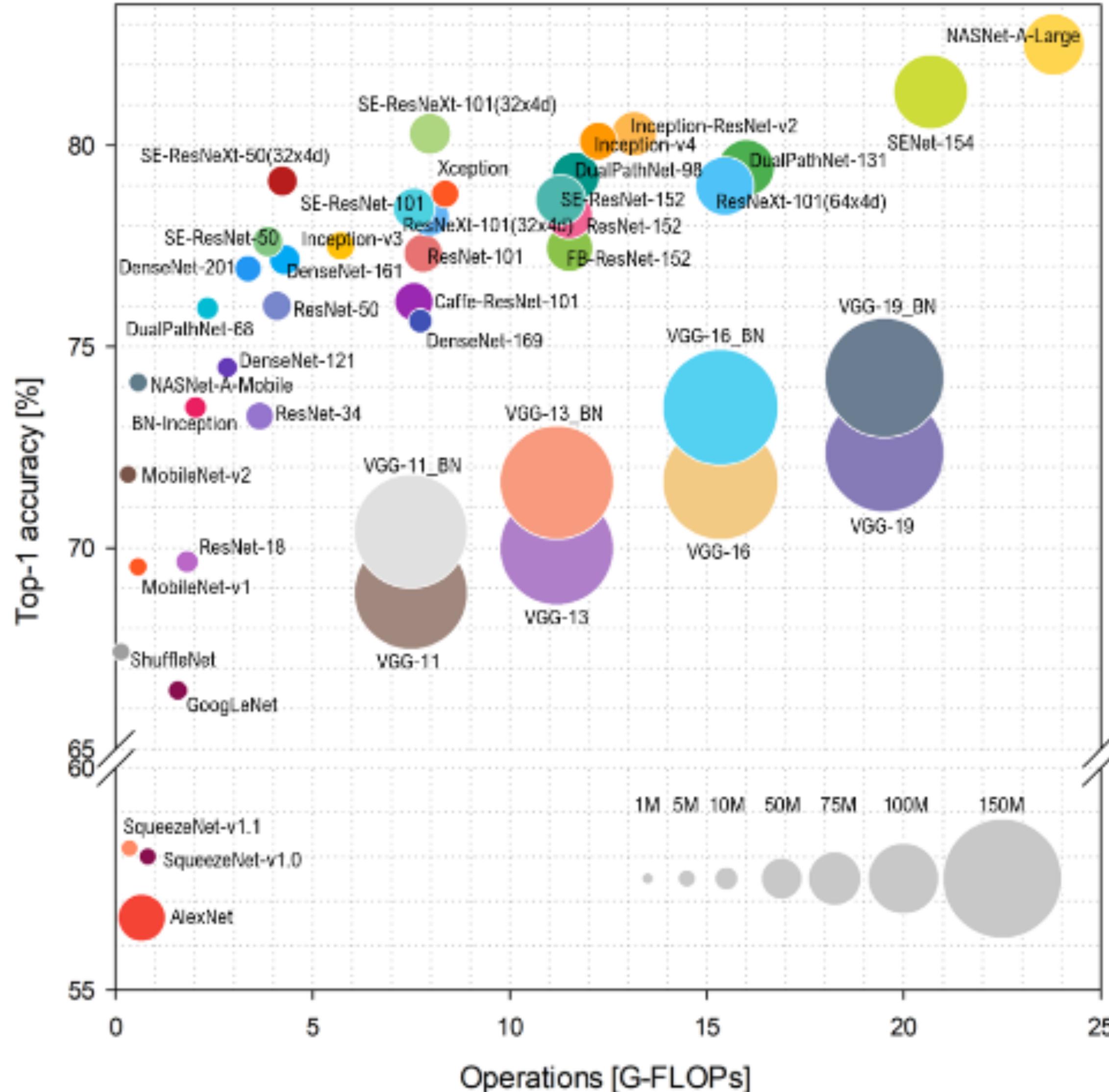
- DNNs typically rely on two phases:
 - **Feature engineering** from Raw Data. This is where new & exotic architectures (depending on data type) take the best out of your data



- **Task solving:** start from engineered features and solve the task (classification, regression, etc.)

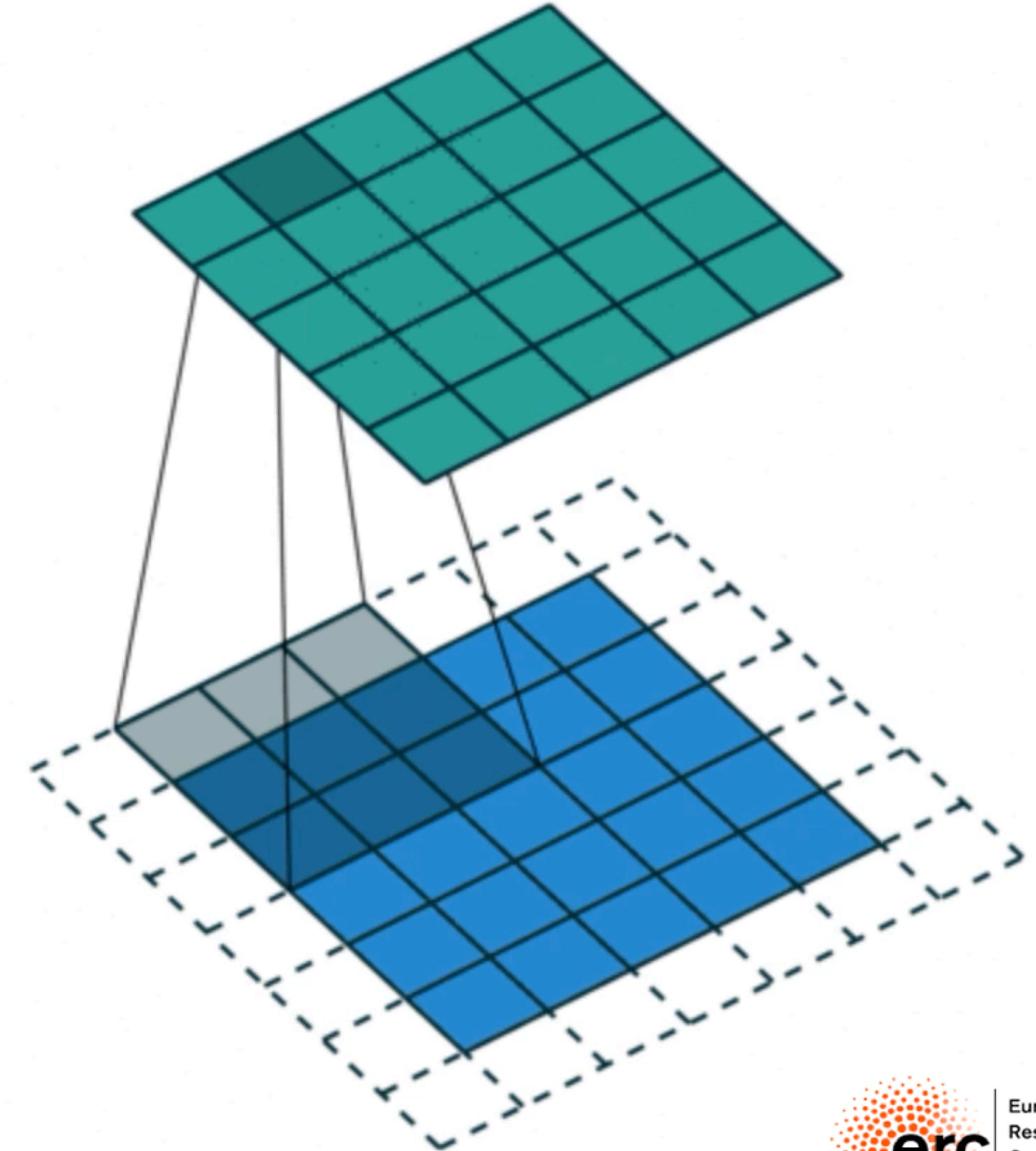
Deep Learning & Computing Vision

- *The most evident success of Deep Learning is computing vision with Convolutional NNs*
- *A kernel scans an array of pixels*
- *The network is translation invariant*
- *The network knows which pixels are near each other and learns from there*



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- *Paradigm applied successfully to many scientific problems*
- *Exoplanet detection*
- *Frequency-domain analysis of Gravitational Interferometer data*
- *Neutrino detection*
- *etc...*

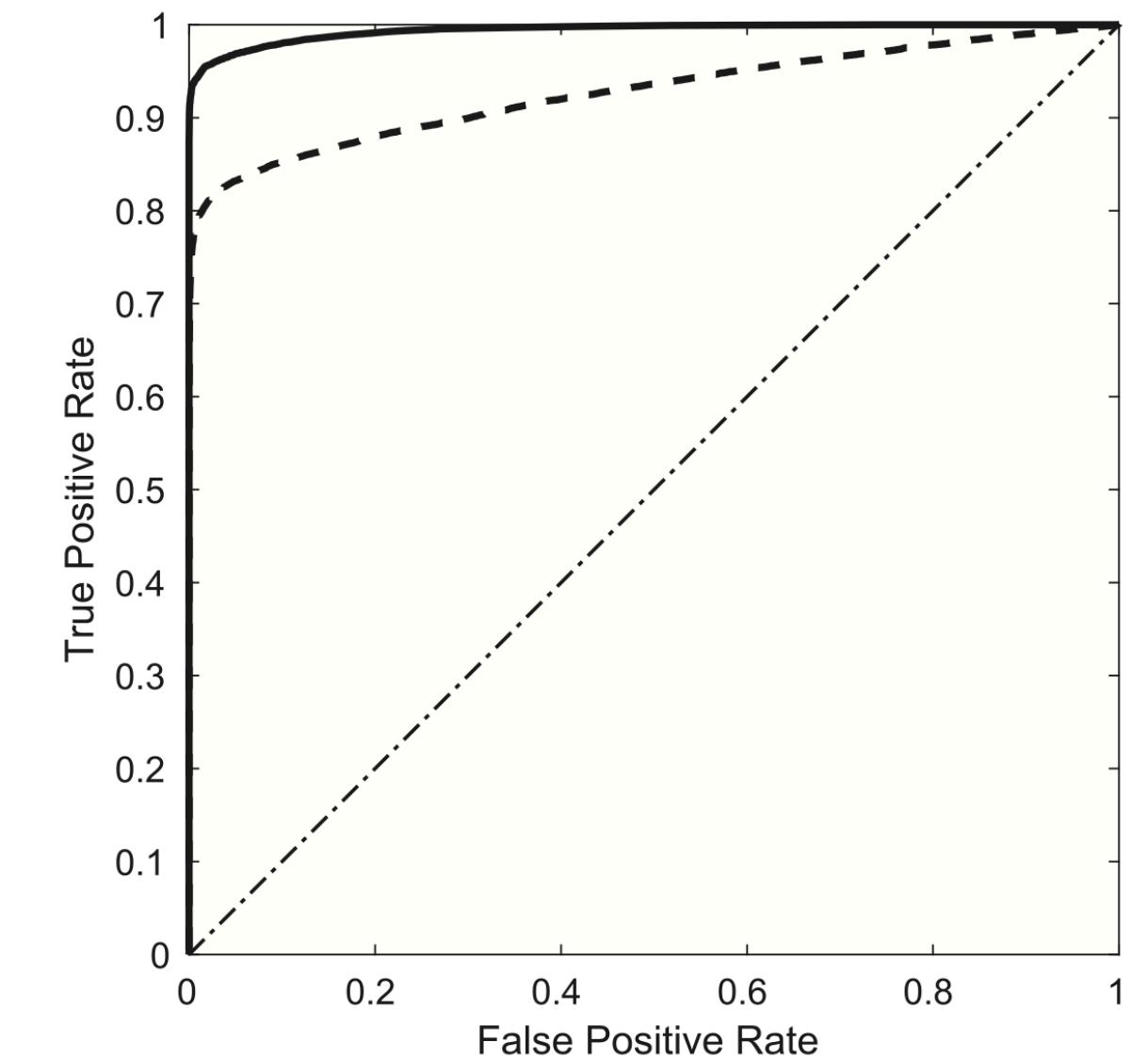
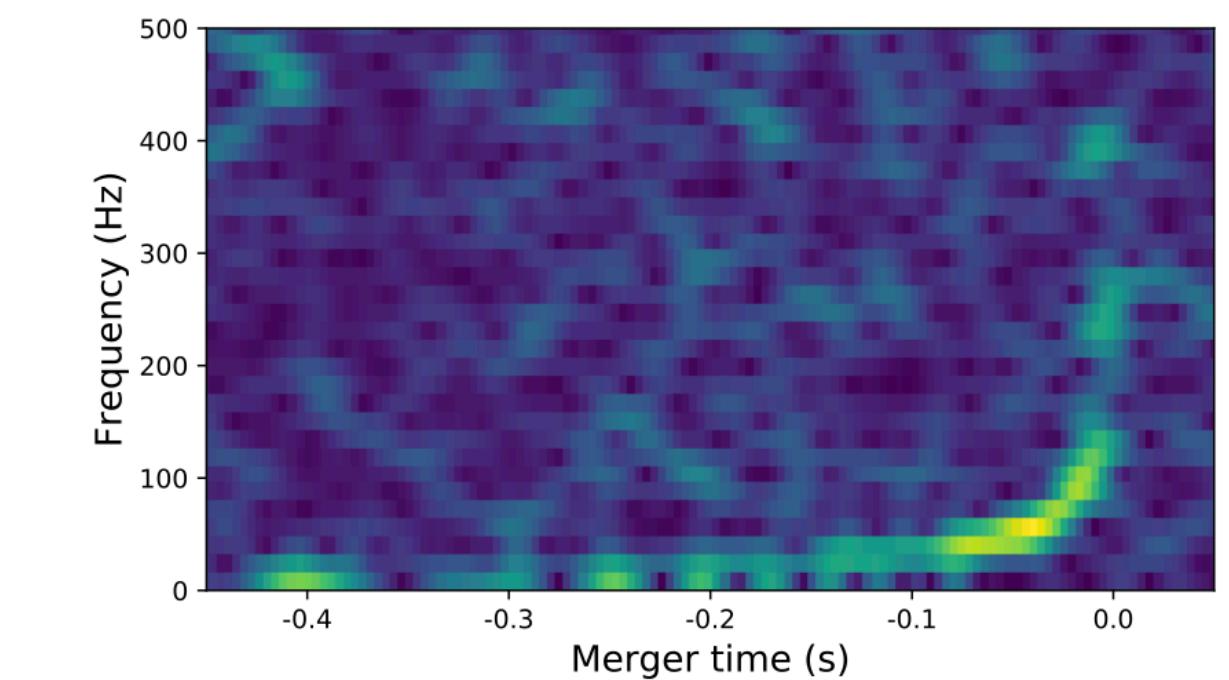
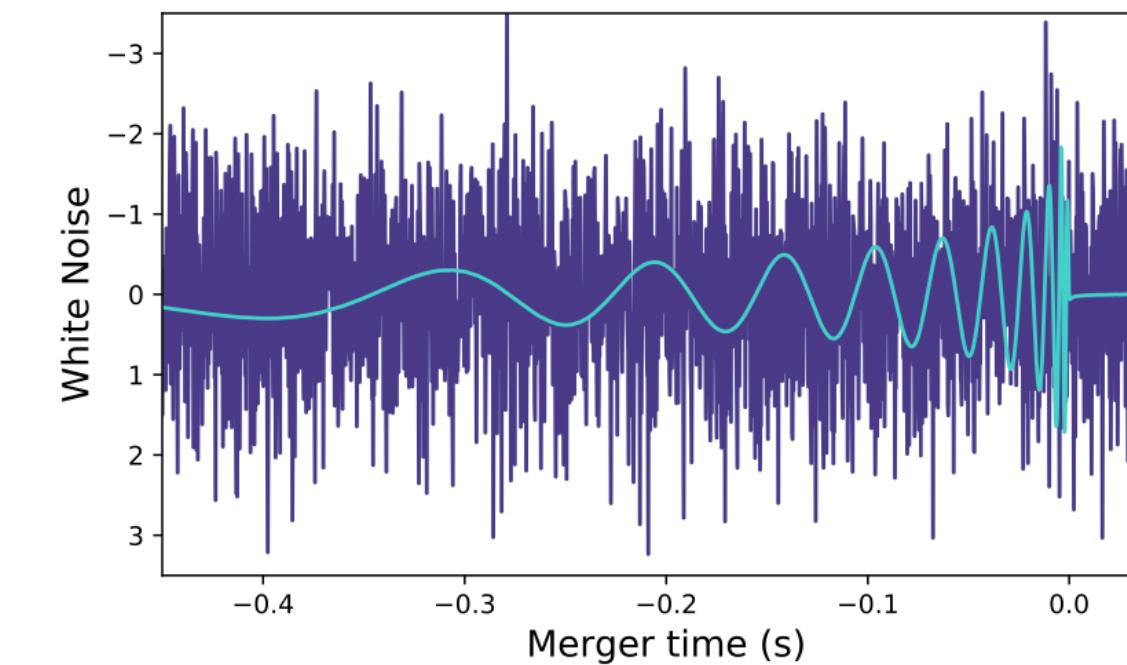
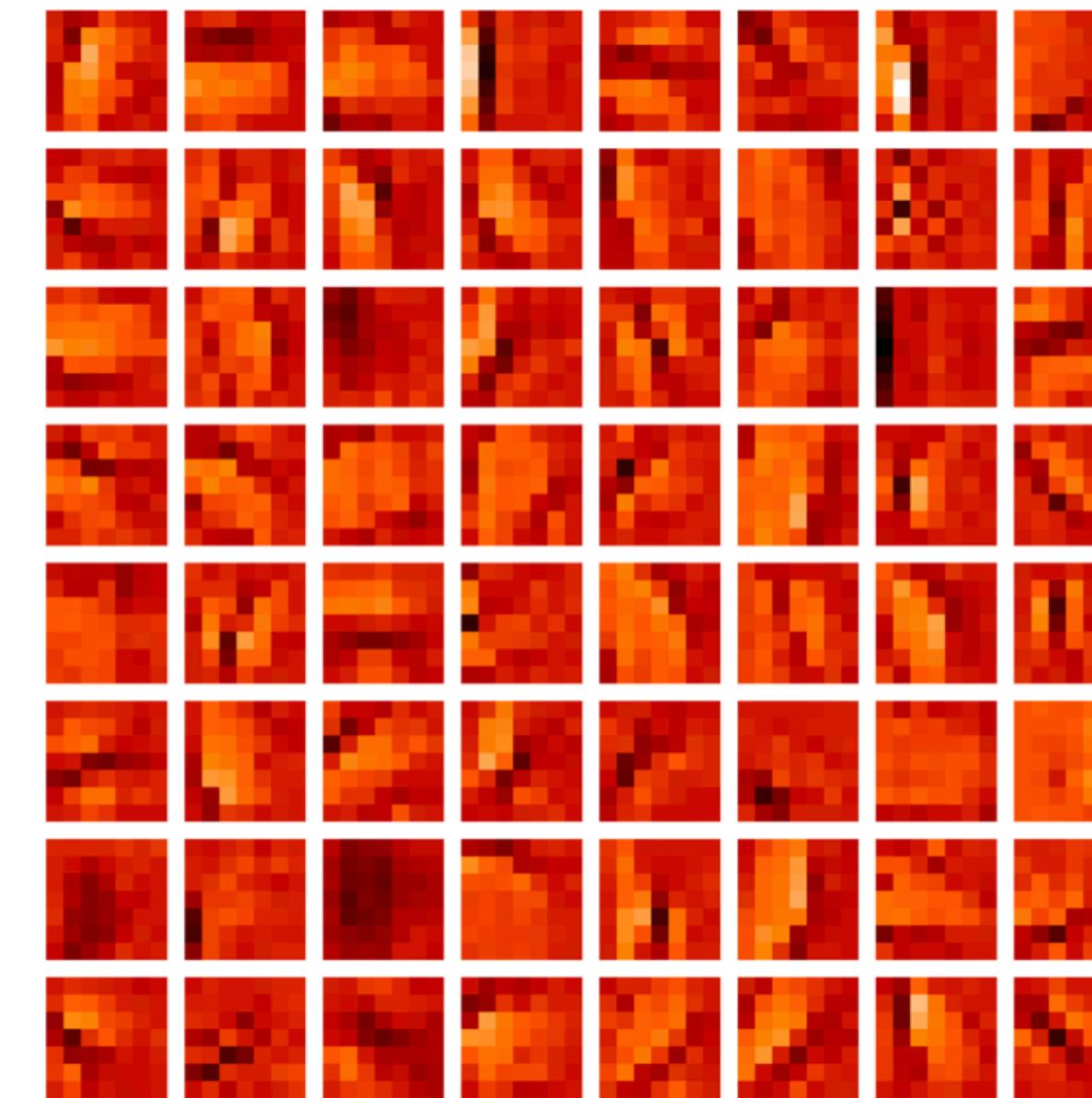
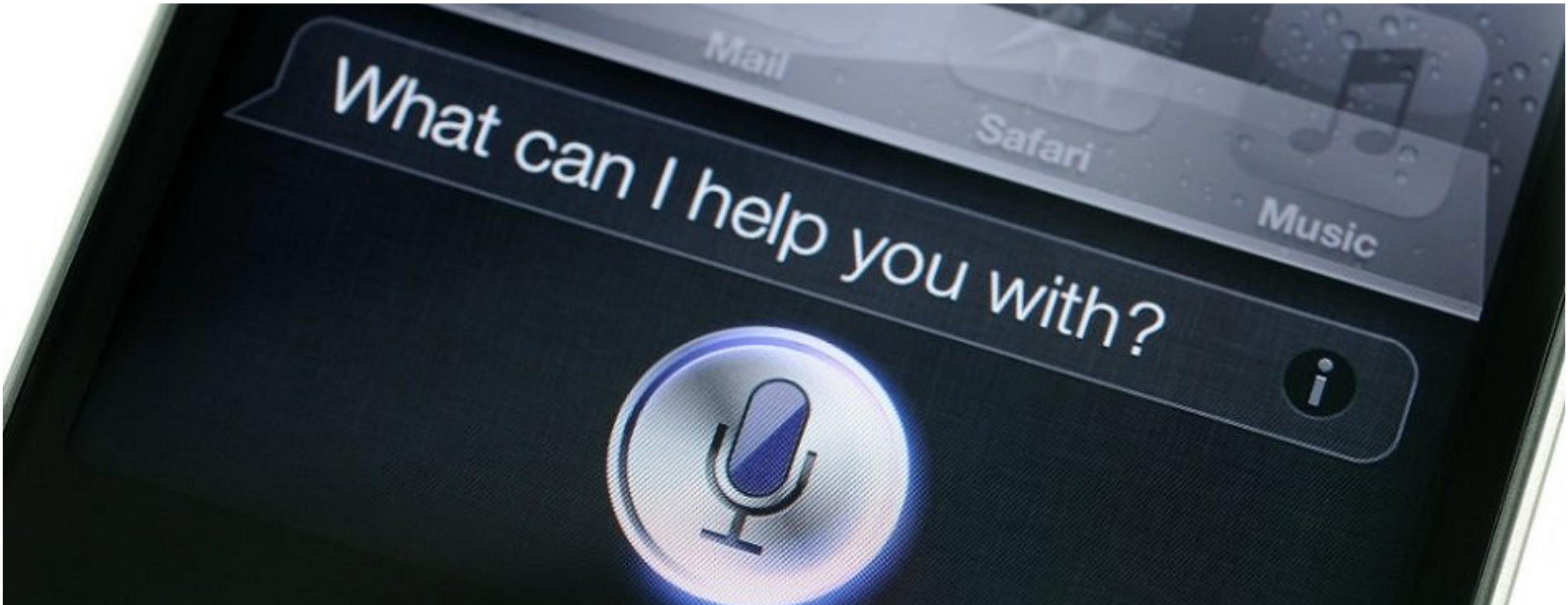


Figure 2. Receiver Operating Characteristic (ROC) curve for the neural network and the data set presented in this work. The dashed line represents the performance of the BLS preceded by a high-pass filter. The dotted-dashed line is the so-called “no-discrimination” line, corresponding to random guess.

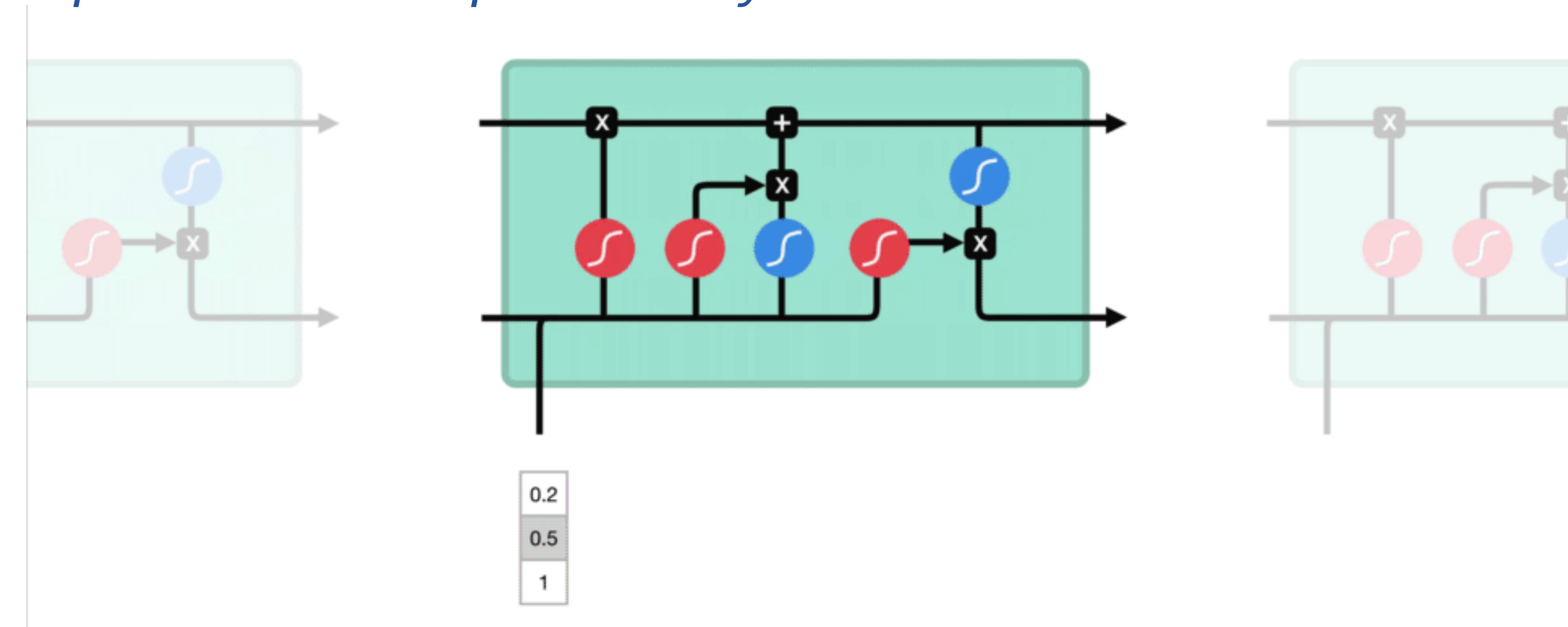
Deep Learning & Natural Language

- *Natural language processing is another big success of Deep Learning*
- *Based on recurrent neural networks*
 - *data ordered (time sequence, words in sentence, etc.)*
 - *data processed sequentially*



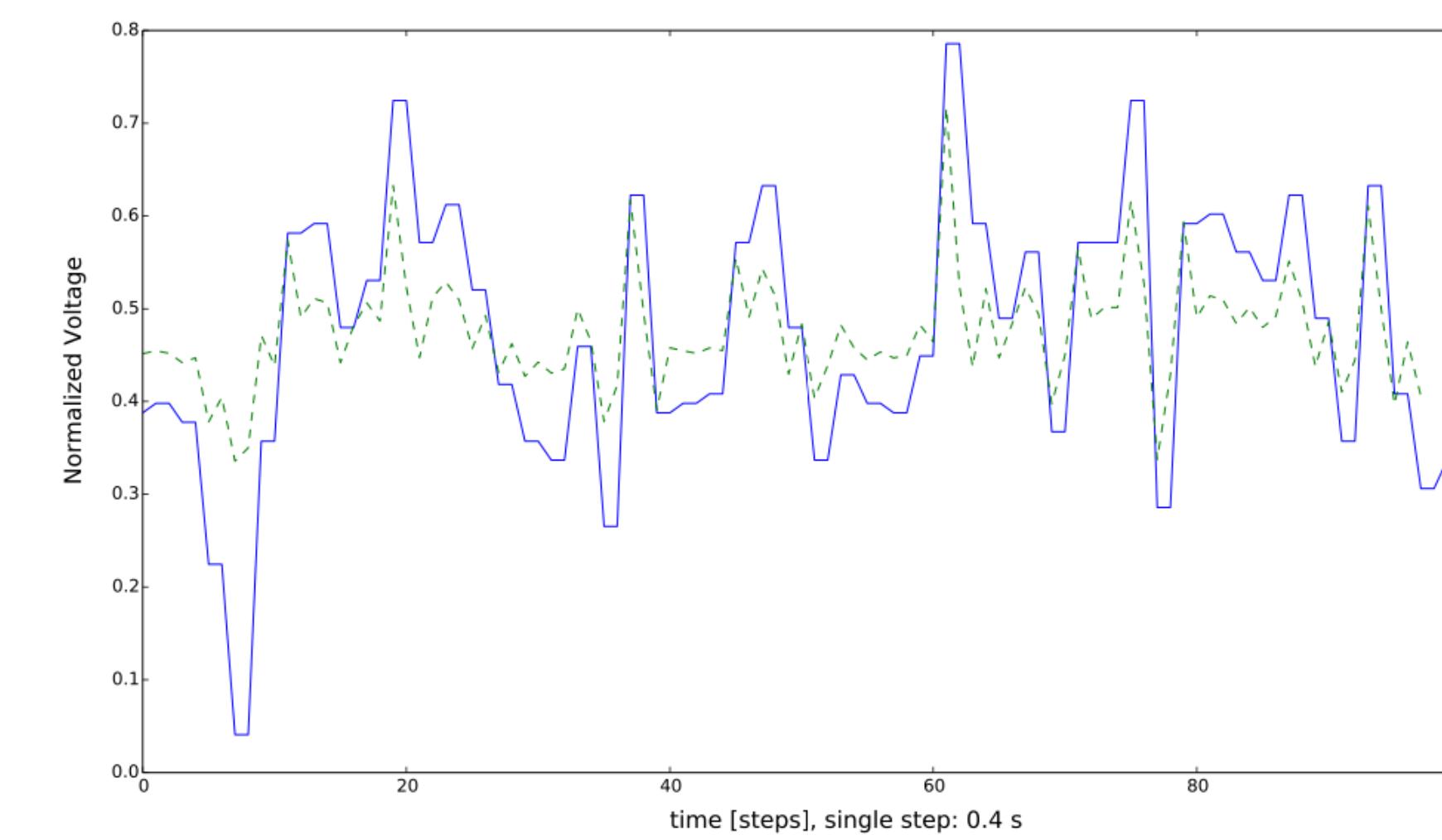
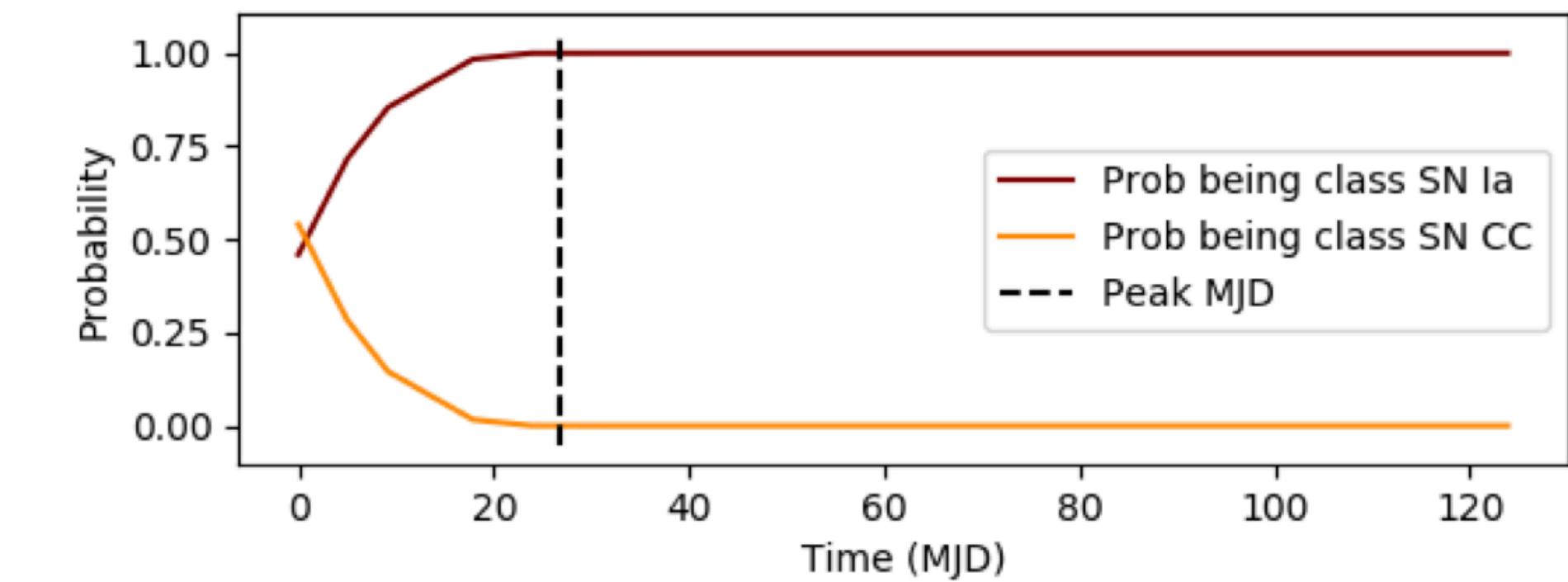
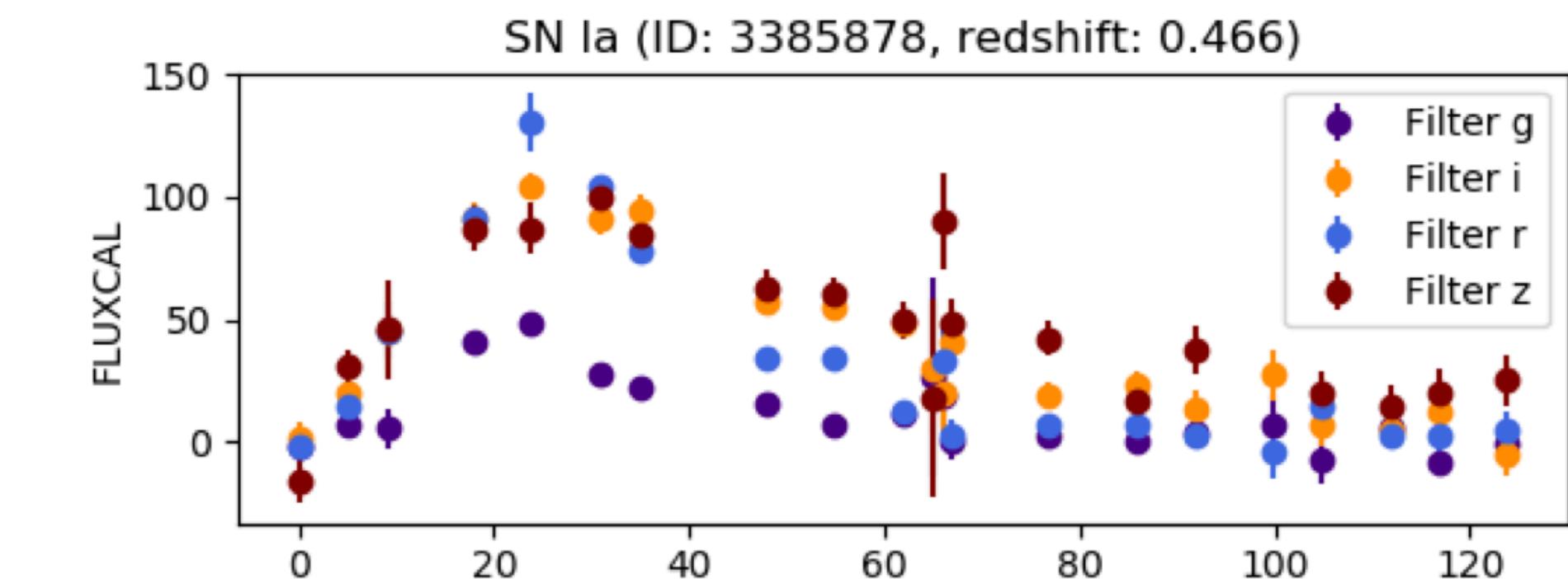
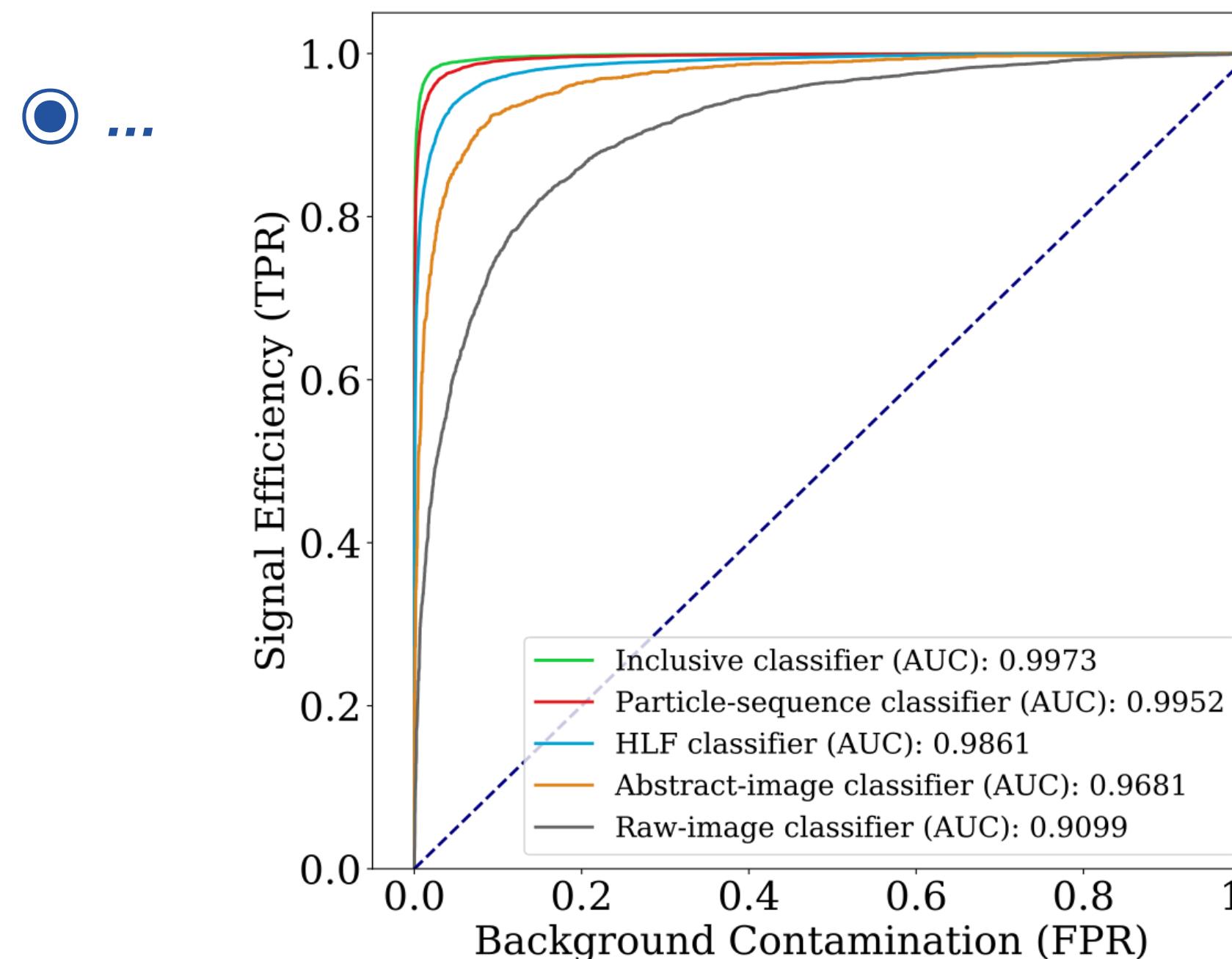
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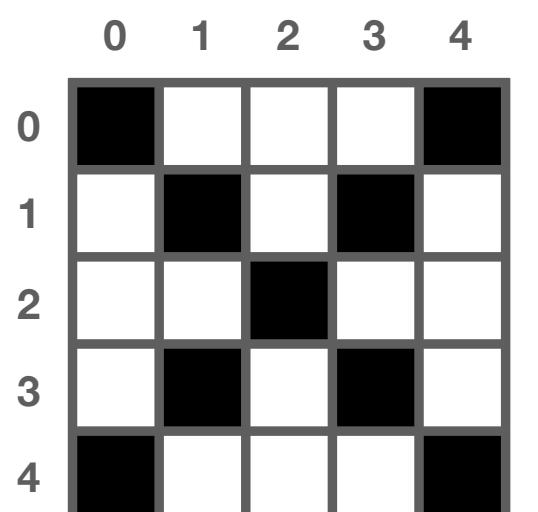
RNN in Science

- RNNs can be used to monitor time sequences and look for transient events
- Supernovae detection
- Monitoring LHC magnets
- Event classification at LHC

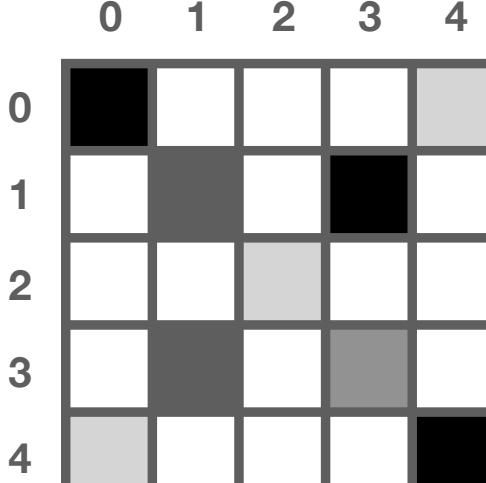


What about irregular data?

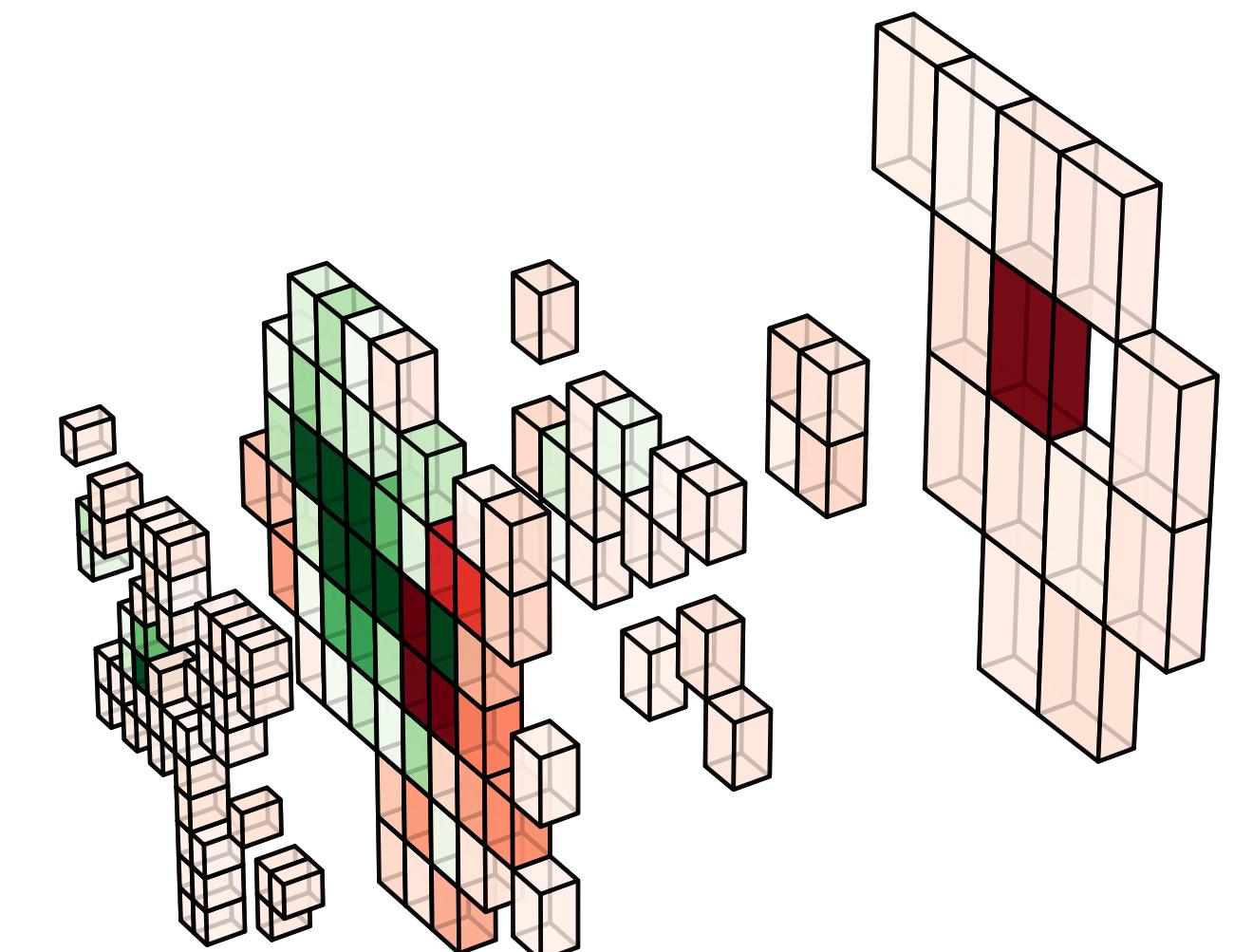
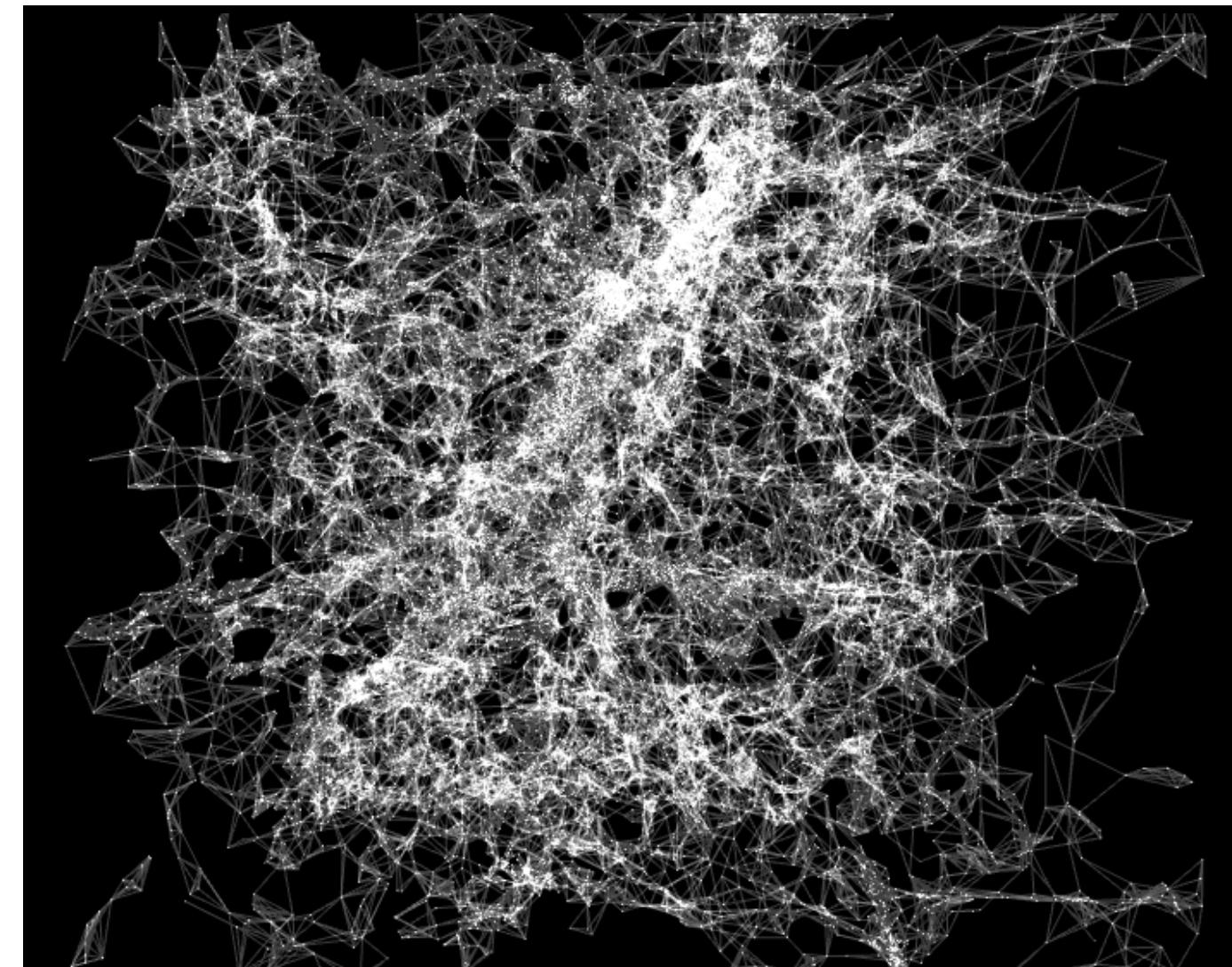
- Unfortunately, many scientific domains deal with data which are not regular arrays (neither images nor sequences)
 - Galaxies or star populations in sky
 - Sensors from HEP detector
 - Molecules in chemistry
- These data can all be seen as sparse sets in some abstract space
- each element of the set being specified by some array of features
- geometrical coordinates could be some of these features



| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 1 | 1 | 2 | 3 | 3 | 4 | 4 |
| 0 | 4 | 1 | 3 | 2 | 1 | 3 | 0 | 4 |

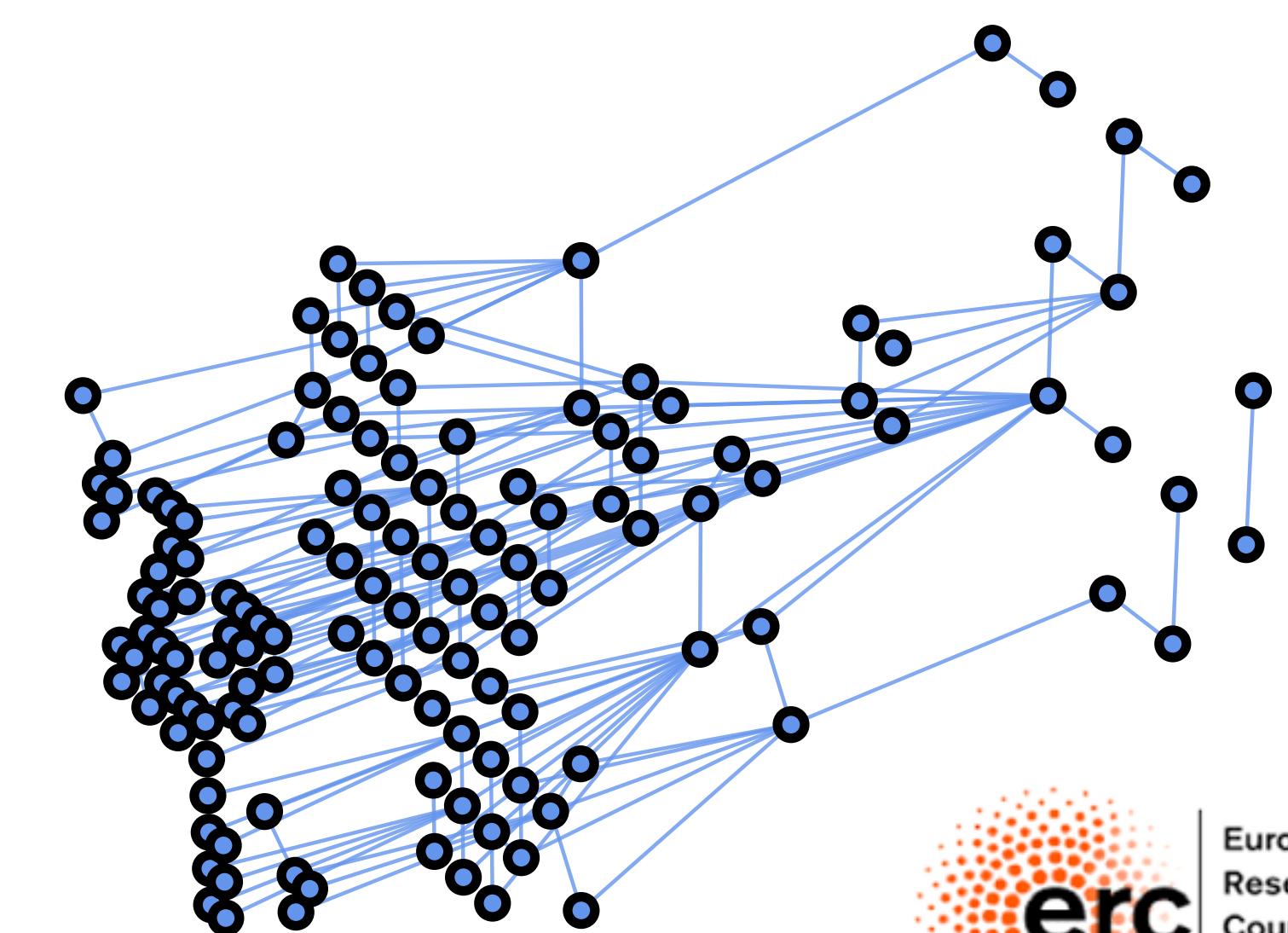
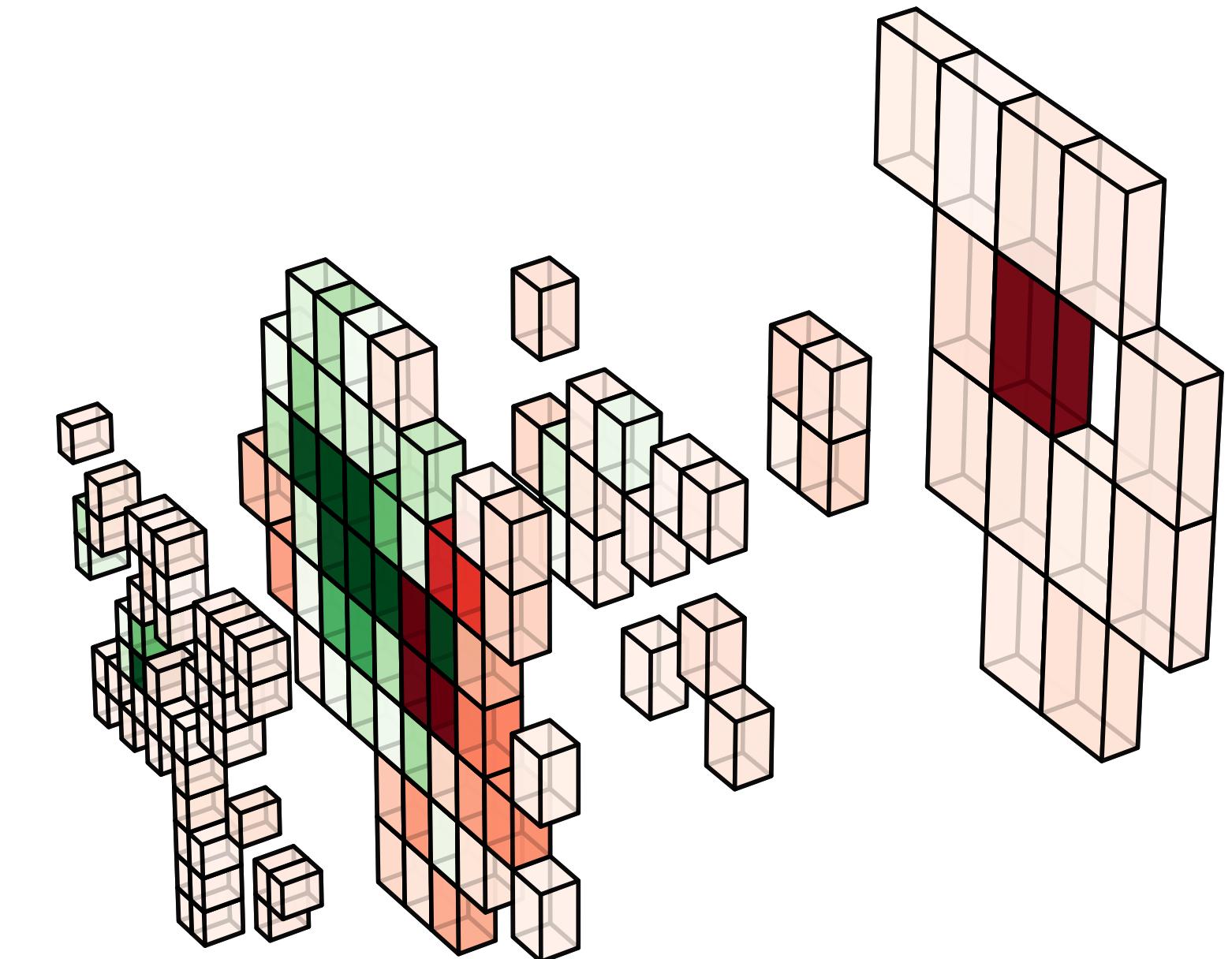


| | | | | | | | | |
|------|------|------|------|------|------|------|------|------|
| 0 | 0 | 1 | 1 | 2 | 3 | 3 | 4 | 4 |
| 0 | 4 | 1 | 3 | 2 | 1 | 3 | 0 | 4 |
| 1.00 | 0.25 | 0.75 | 1.00 | 0.25 | 0.75 | 0.50 | 0.25 | 1.00 |



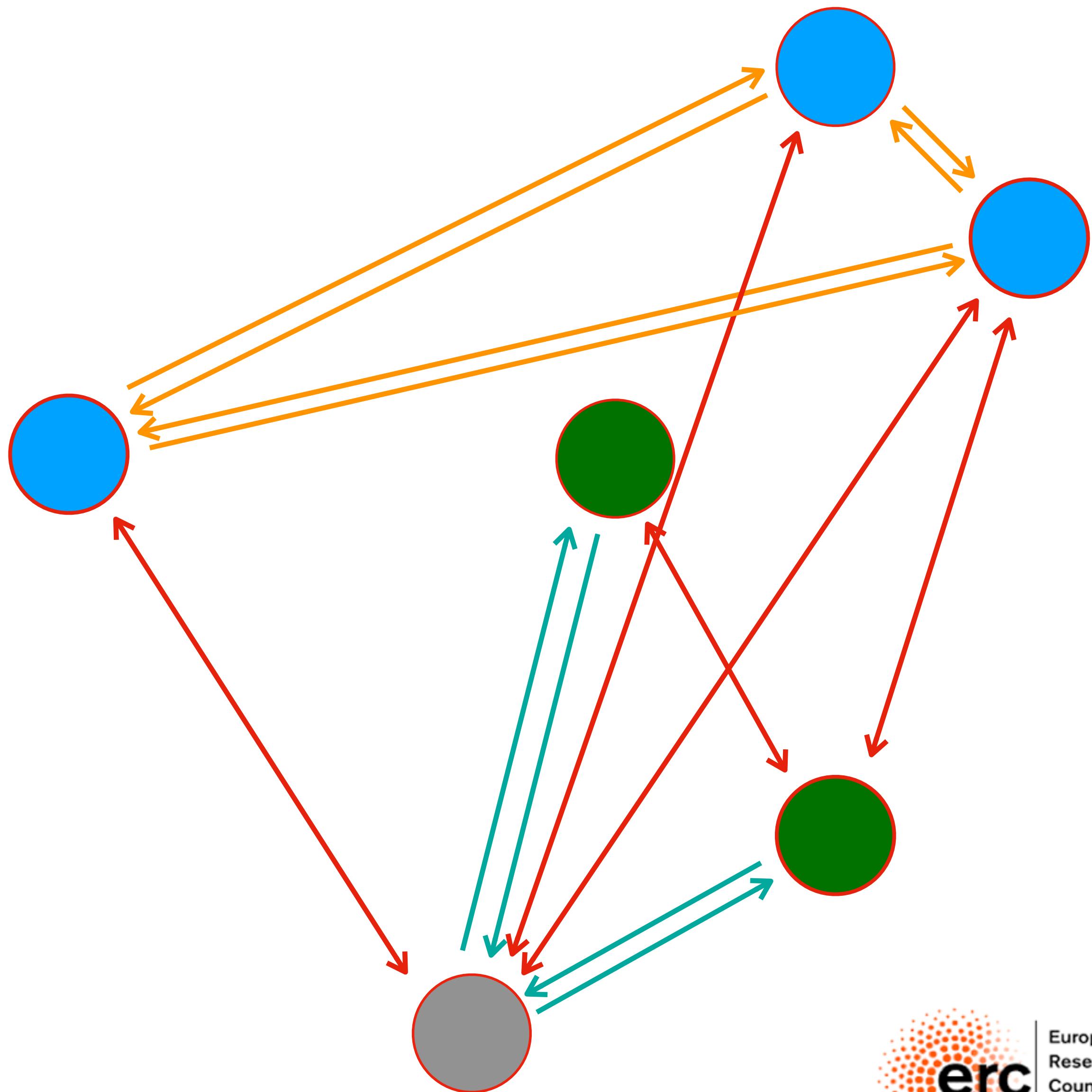
From Sets to Graphs

- Given such a set, we want to generalise the image representation as regular array that is fed to a CNN
 - Once that is done, we can generalise CNN itself
 - For images, a lot of information is carried by pixels being next to each other. A metric is intrinsic in the data representation as image
 - With a set, we need to specify a metric that tell us who is close to who in the abstract space of features that we have at hand
 - SOLUTION: connect elements of sets and learn (e.g., with a neural network) from data which connections are relevant



Building the Graph

- Each element of your set is a vertex V
- Edges E connect them
- Edges can be made directional
- Graphs can be fully connected (N^2)
- Or you could use some criterion (e.g., nearest k neighbours in some space) to reduce number of connections
- if more than one kind of vertex, you could connect only V s of same kind, of different kind, etc
- The (V, E) construction is your graph. Building it, you could enforce some structure in your data
- If you have no prior, then go for a directional fully connected graph

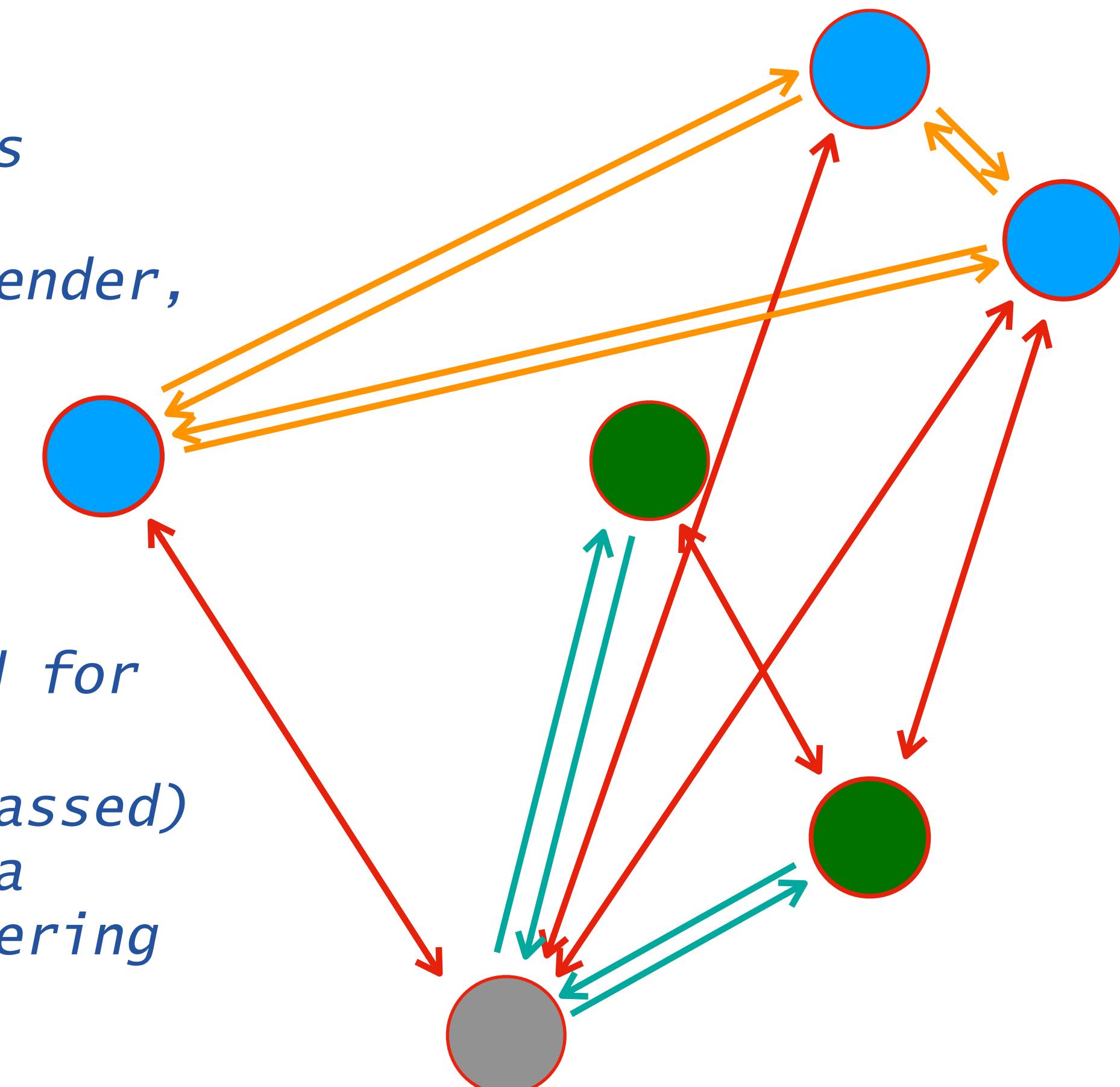




message Passing

Learning from Graph: an example

- Imagine a concrete example: given a social-media user, who will she vote for at the next elections?
- The graph here comes from social-media connections
- The features are what we know for a given user (gender, age, education, etc.)
- We want to gather information on someone from the social network of that person
 - we might know who some of her connections voted for
- We will use NNs to model the influence (message passed) of each user on her connection and learn from data which are the relevant connections. We are engineering features
- A final classifier will give us the answer we want
- You might become president with this + target pressure (ads, fake news, etc.)



Learning from Graph: an example

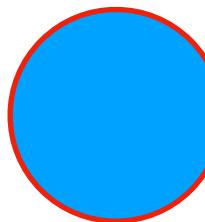
- Imagine a concrete example: given a social-media user, who will she vote for at the next elections?
- The graph here comes from social-media connections
- The features are what we know for a given user (gender, age, education, etc.)
- We want to predict the user's political affiliation based on her social connections
- We will use NNs to model the influence (message passed) of each user on her connection and learn from data which are the relevant connections. We are engineering features
- A final classifier will give us the answer we want
- You might become president with this + target pressure (ads, fake news, etc.)



Graph networks

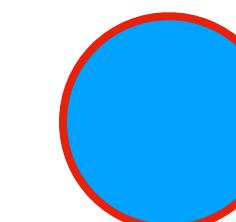
- *Graphs Nets are architectures based on an abstract representation of a given dataset*

$$\mathbf{v}_3 = (f_3^1, f_3^2, \dots, f_3^k)$$

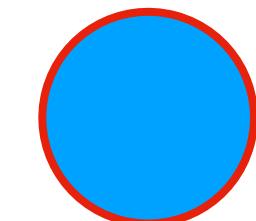


- ***Each example in a dataset is represented as a set of vertices***

$$\mathbf{v}_1 = (f_1^1, f_1^2, \dots, f_1^k)$$

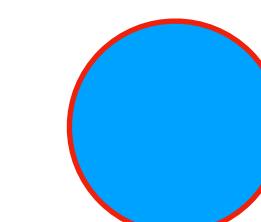


$$\mathbf{v}_4 = (f_4^1, f_4^2, \dots, f_4^k)$$

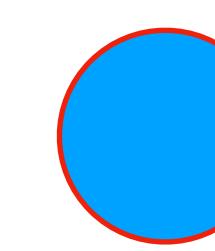
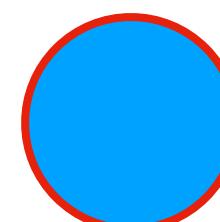


- ***Each vertex is embedded in the graph as a vector of features***

$$\mathbf{v}_2 = (f_2^1, f_2^2, \dots, f_2^k)$$



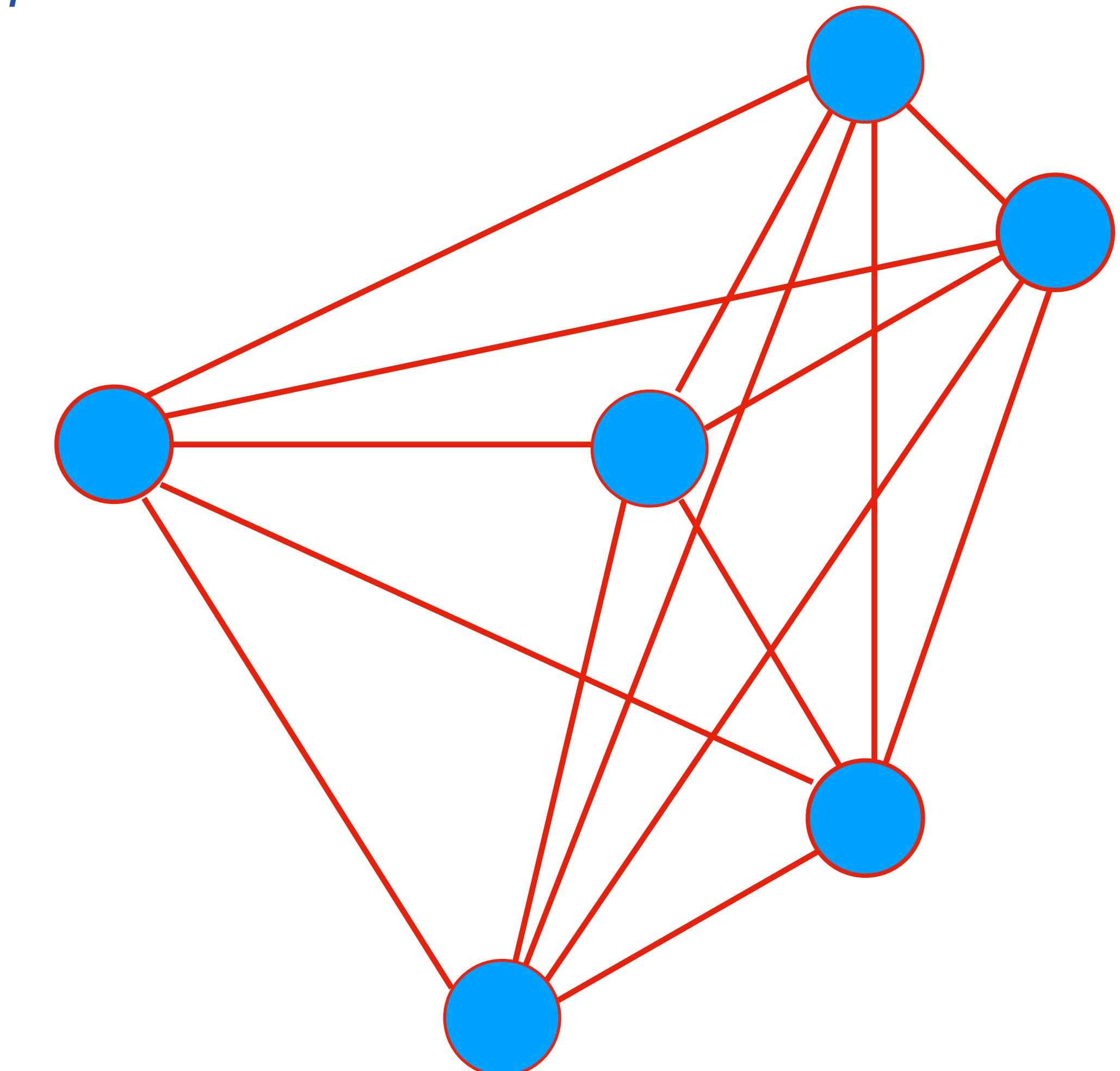
$$\mathbf{v}_5 = (f_5^1, f_5^2, \dots, f_5^k)$$



$$\mathbf{v}_6 = (f_6^1, f_6^2, \dots, f_6^k)$$

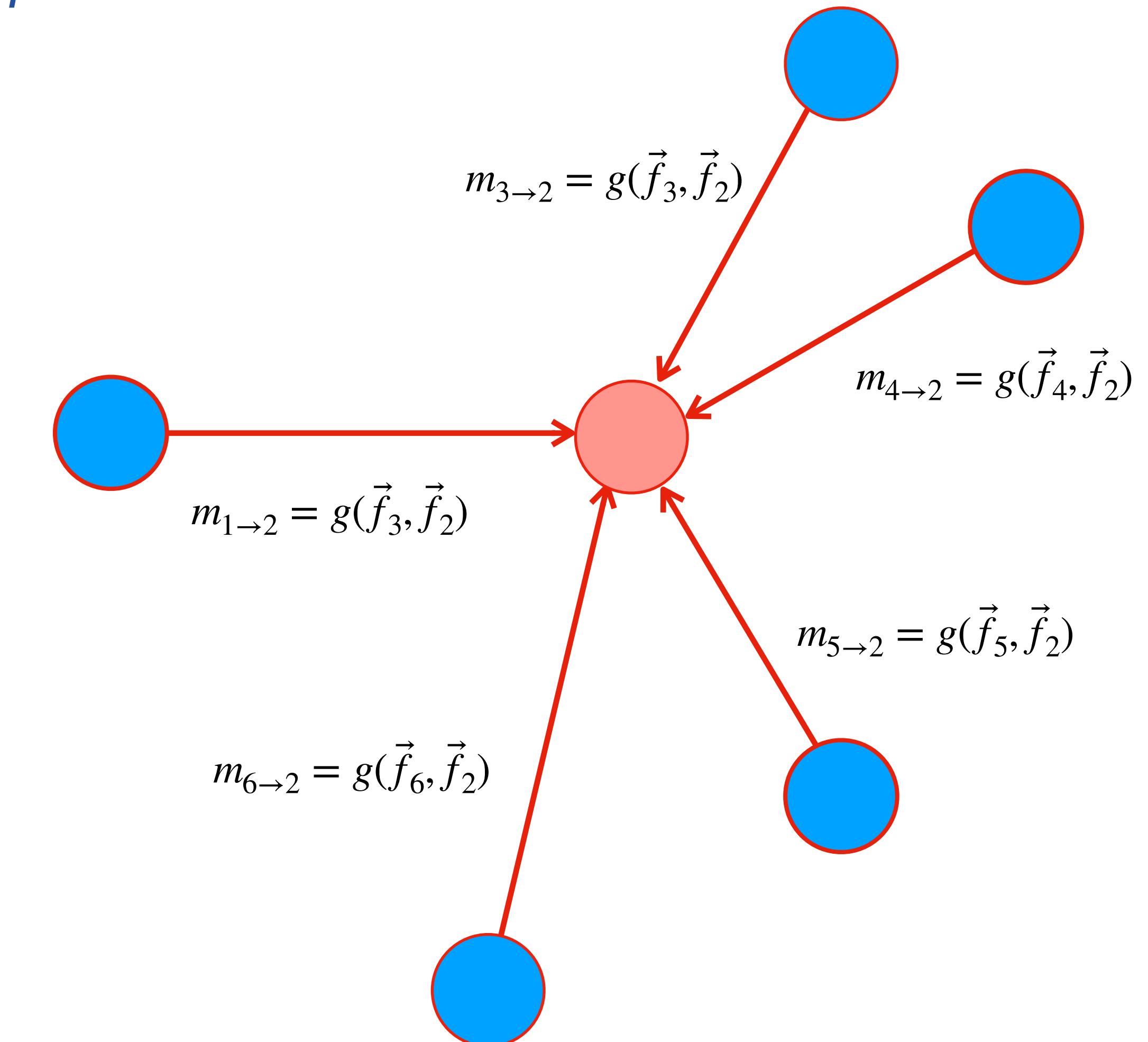
Graph networks

- Graphs Nets are architectures based on an abstract representation of a given dataset
- Each example in a dataset is represented as a set of vertices
- Each vertex is embedded in the graph as a vector of features
- Vertices are connected through links (edges)



Graph networks

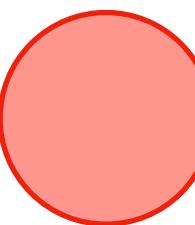
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- **Messages are passed through links and aggregated on the vertices**



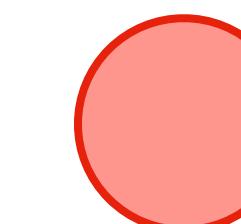
Graph networks

- Graphs Nets are architectures based on an abstract representation of a given dataset
- Each example in a dataset is represented as a set of vertices
- Each vertex is embedded in the graph as a vector of features
- Vertices are connected through links (edges)
- Messages are passed through links and aggregated on the vertices
- A new representation of each node is created, based on the information gathered across the graph

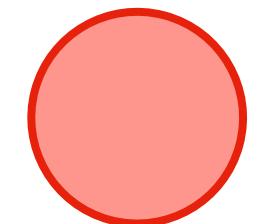
$$\mathbf{v}'_3 = \vec{f}'_3(m_{1 \rightarrow 3}, \dots, m_{6 \rightarrow 3})$$



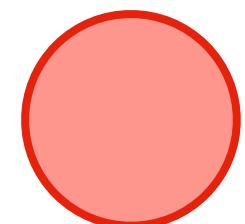
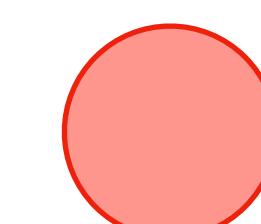
$$\mathbf{v}'_1 = \vec{f}'_1(m_{2 \rightarrow 1}, \dots, m_{6 \rightarrow 1})$$



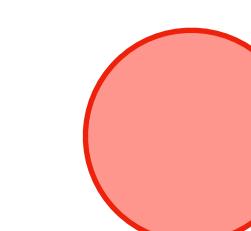
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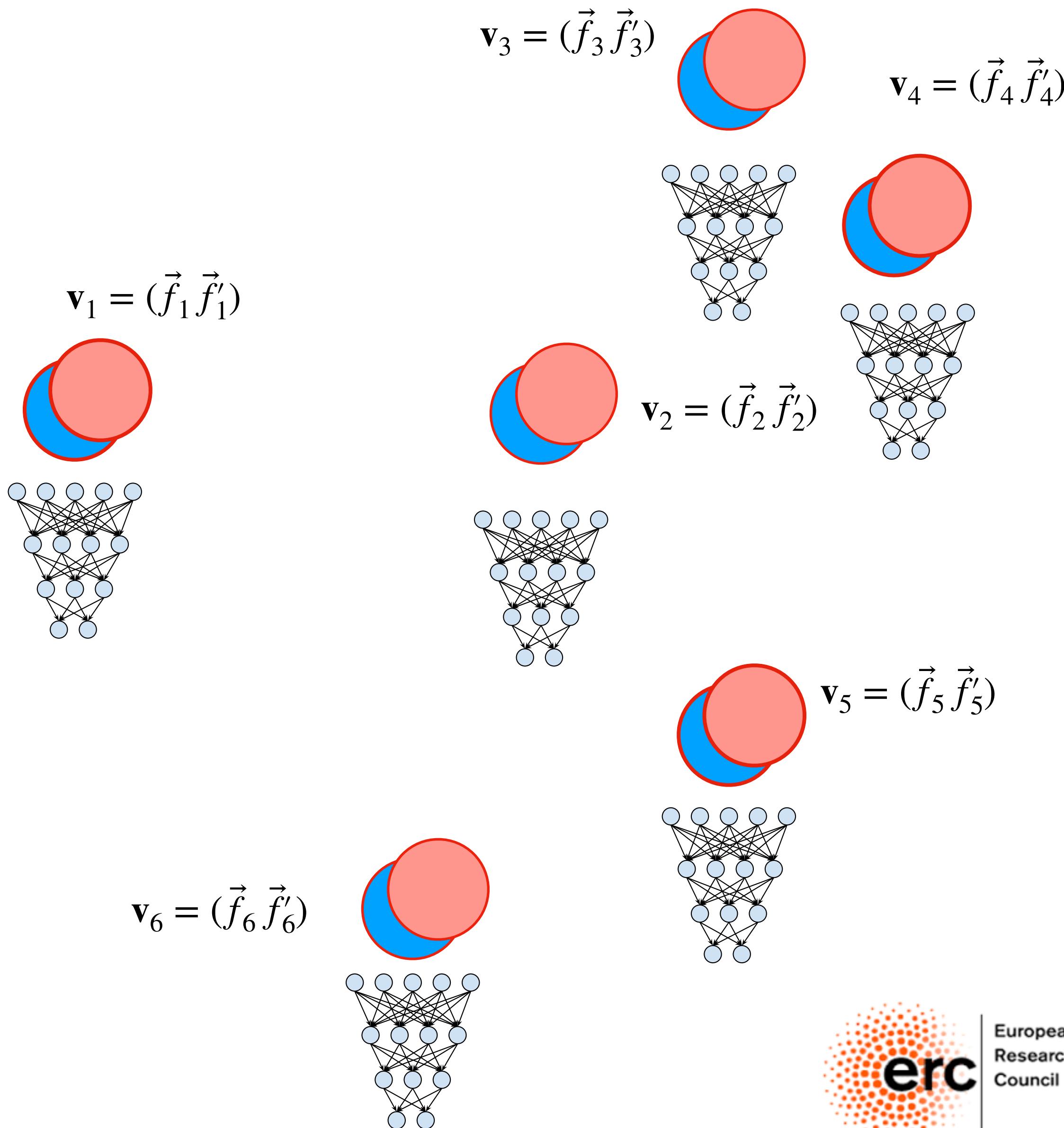
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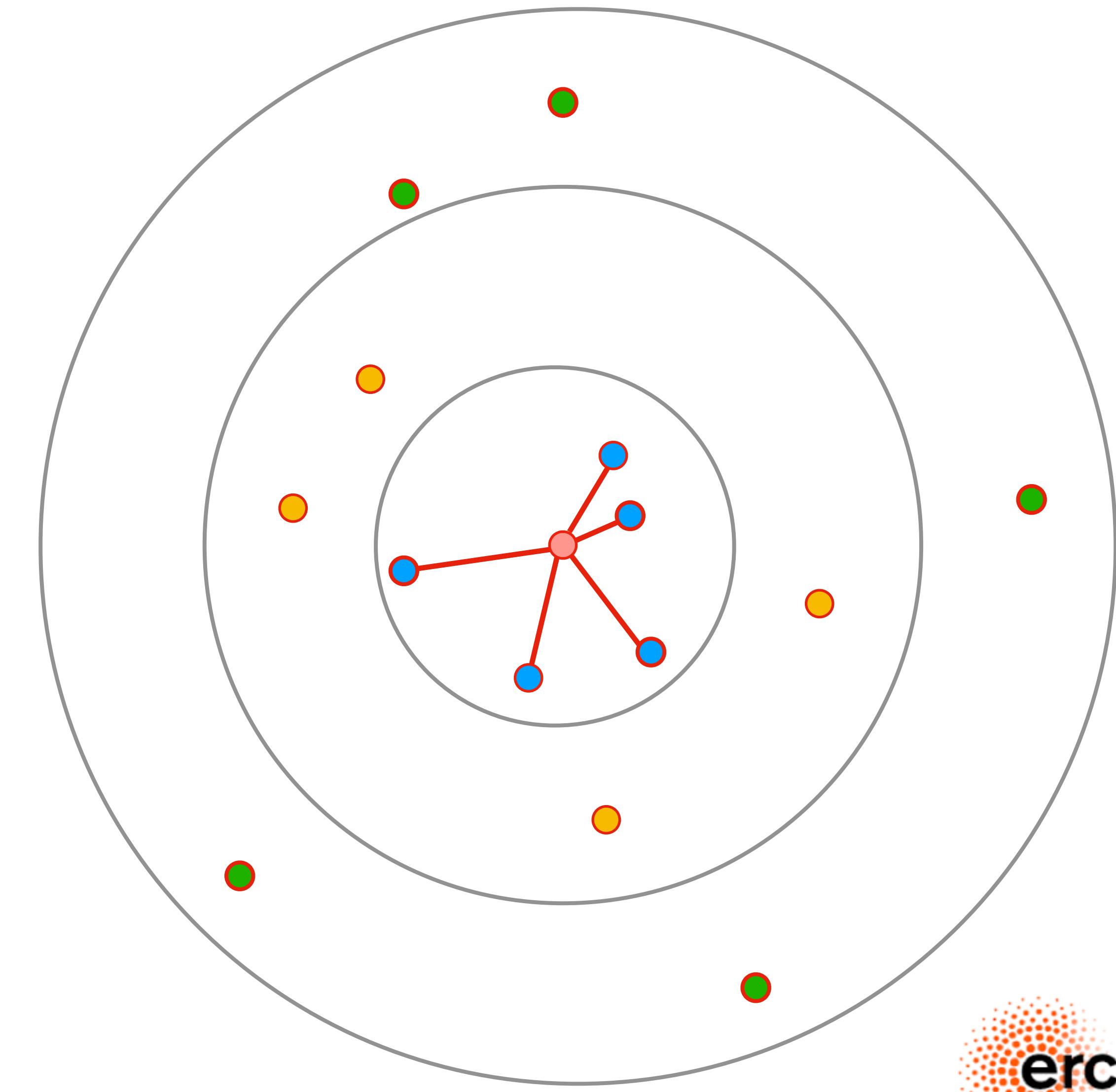
The inference step

- *The inference step usually happens on each vertex*
- *But, depending on the problem, it might happen across the graph*
- *Usually, this is done with a DNN taking*
 - *the initial features f_i*
 - *the learned representation f'_i*
 - *[optional] some ground-truth label (for classifiers)*



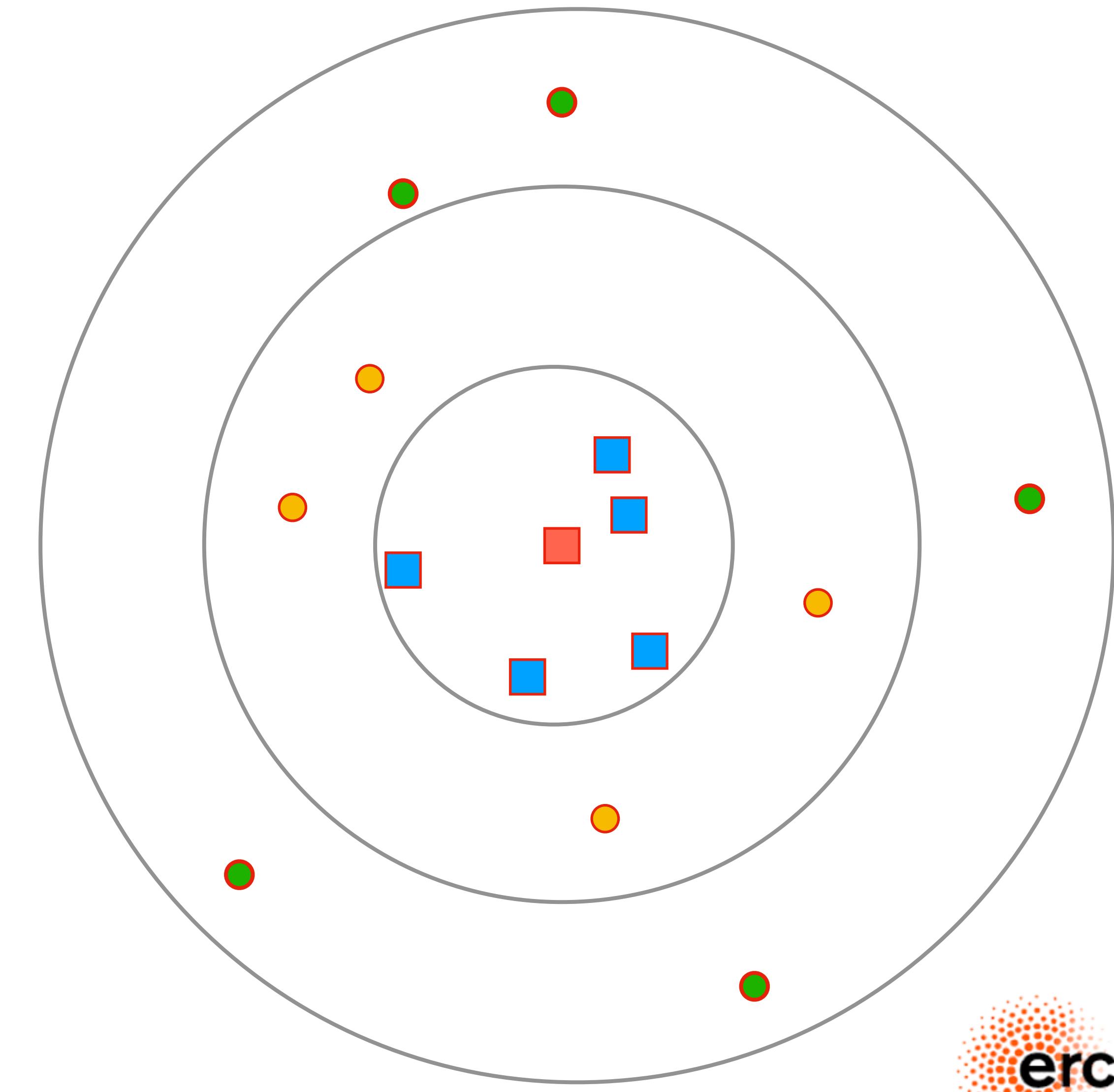
...and repeat

- Once message is passed, aggregated at each vertex V and processed, it creates a new representation of each vertex
- You could start from coordinates in real space + some feature
- Build function of them
- Build functions of functions of them
- At each step, you improve knowledge on your vertex V



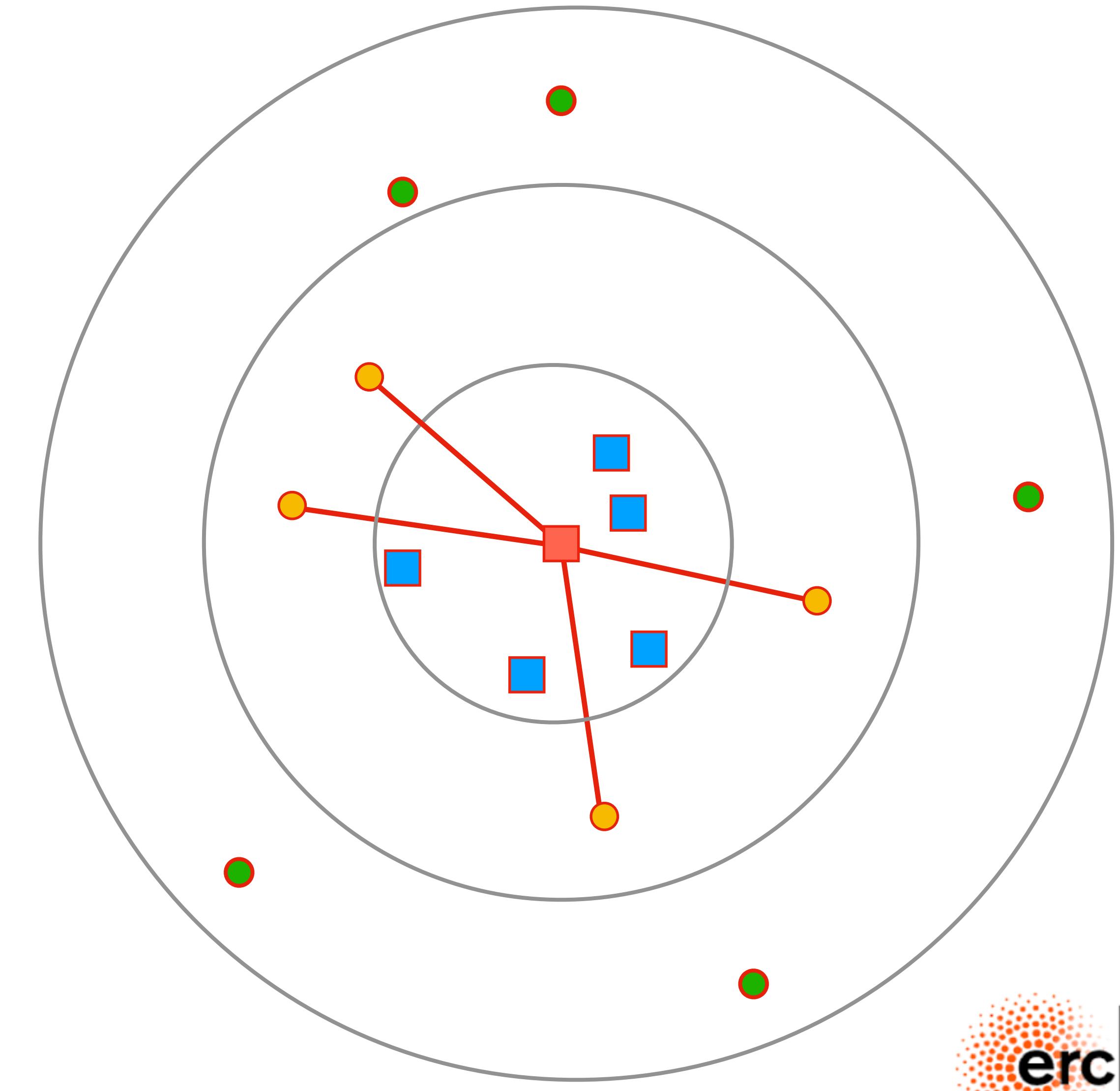
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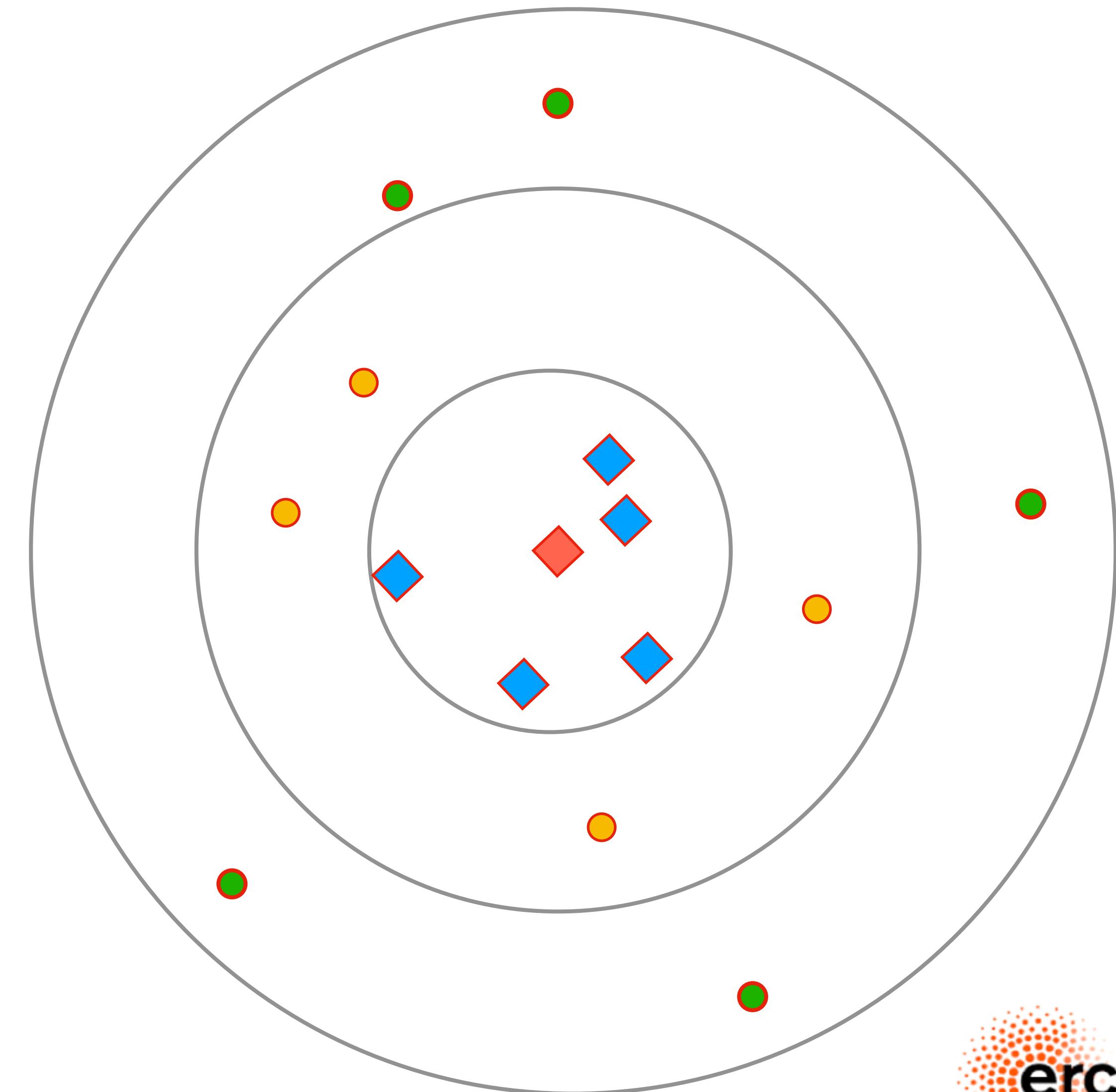
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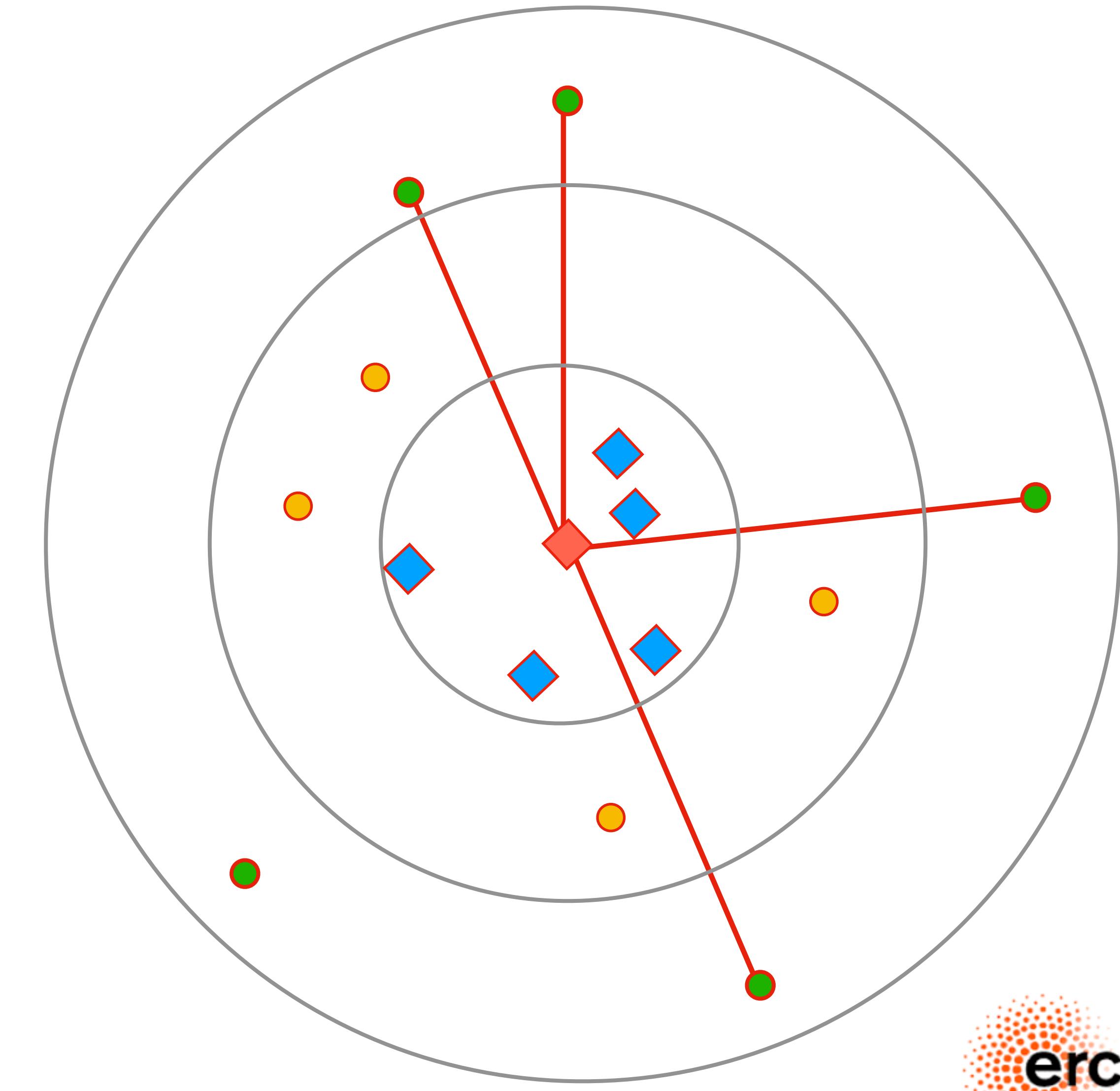
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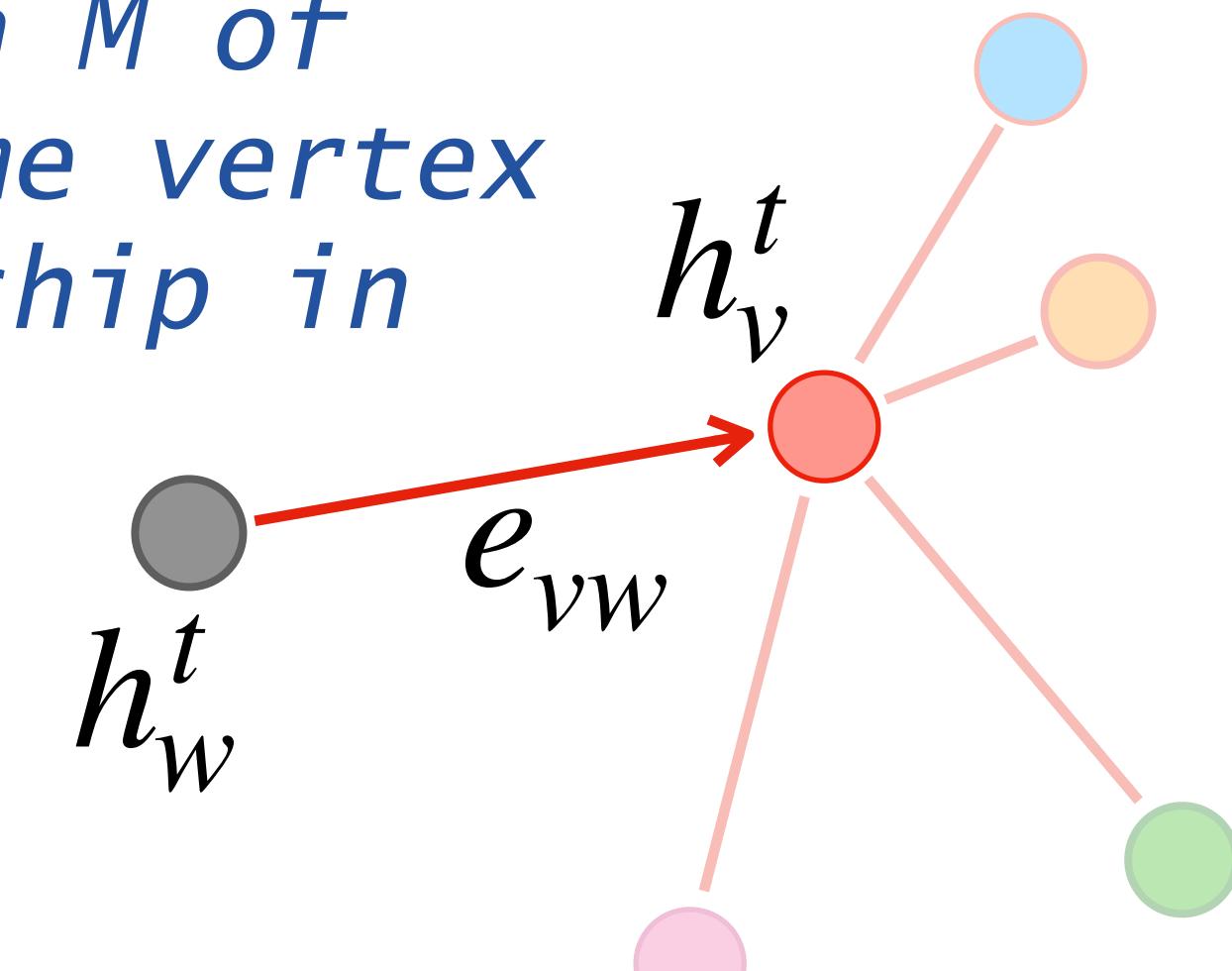
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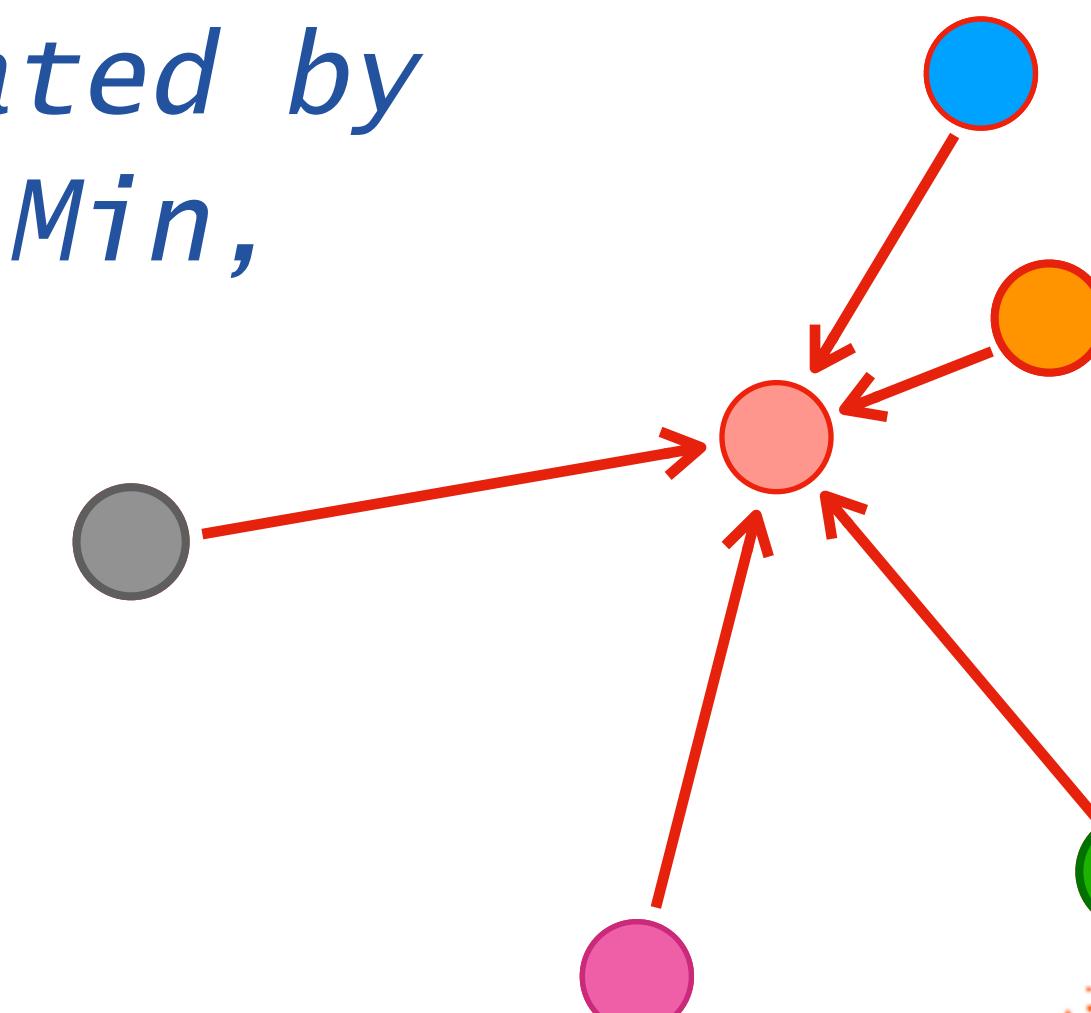
- Your message at iteration t is some function M of the sending and receiving features, plus some vertex features (e.g., business relation vs friendship in social media)

$$M_t(h_v^t, h_w^t, e_{vw})$$



- The message carried to a vertex v is aggregated by some function (typically sum, but also Max, Min, etc.)

$$m_v^{t+1} = \sum_{w \in G(v)} M_t(h_v^t, h_w^t, e_{vw})$$



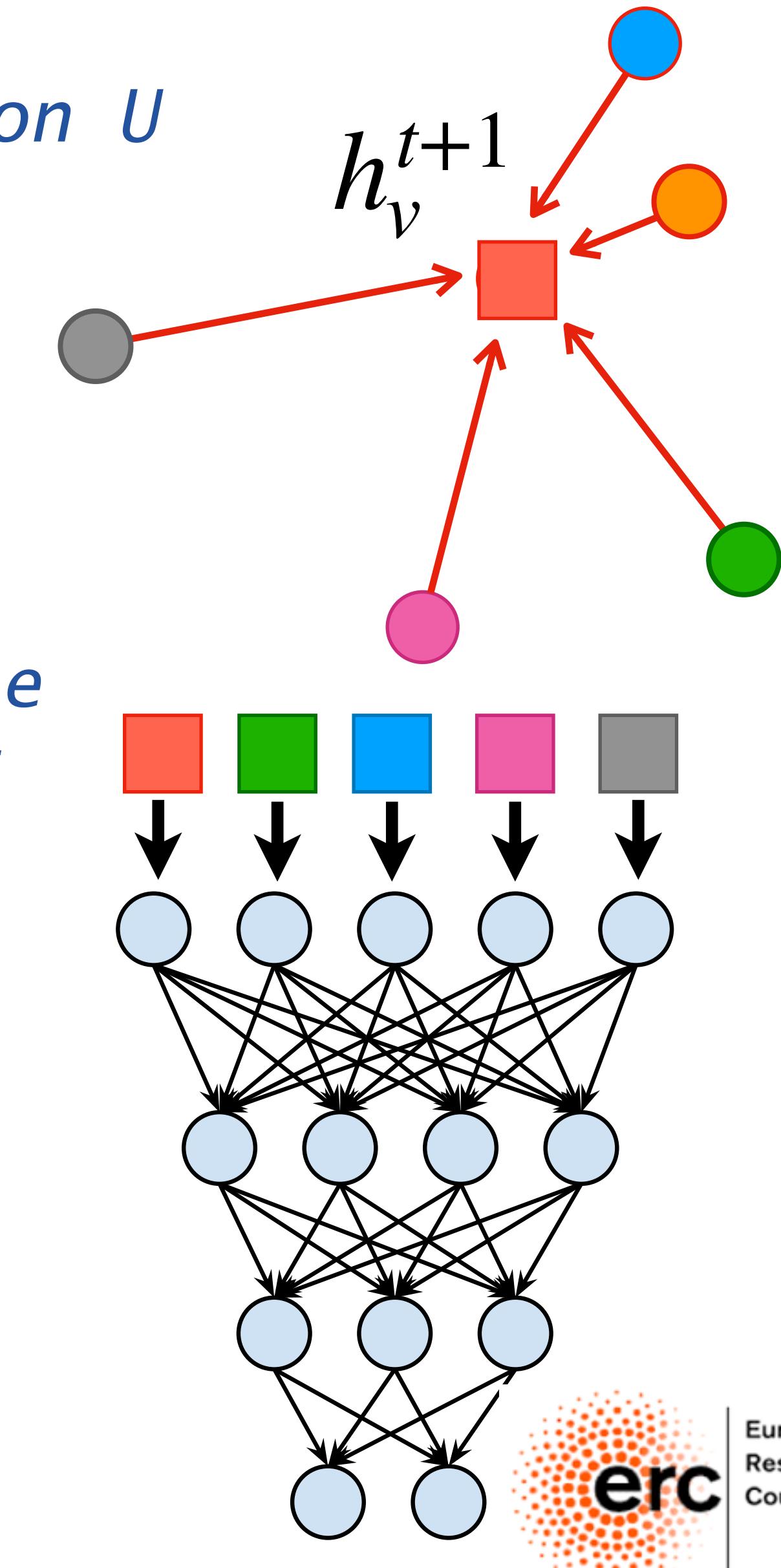
with equations...

- The state of vertex v is updated by some function U of the current state and the gathered message

$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

- After T iterations, the last representations of the graph vertices are used to derive the final output answering the question asked (classification, regression, etc.), typically through a NN

$$\hat{y} = R(h_v^T \mid v \in G)$$

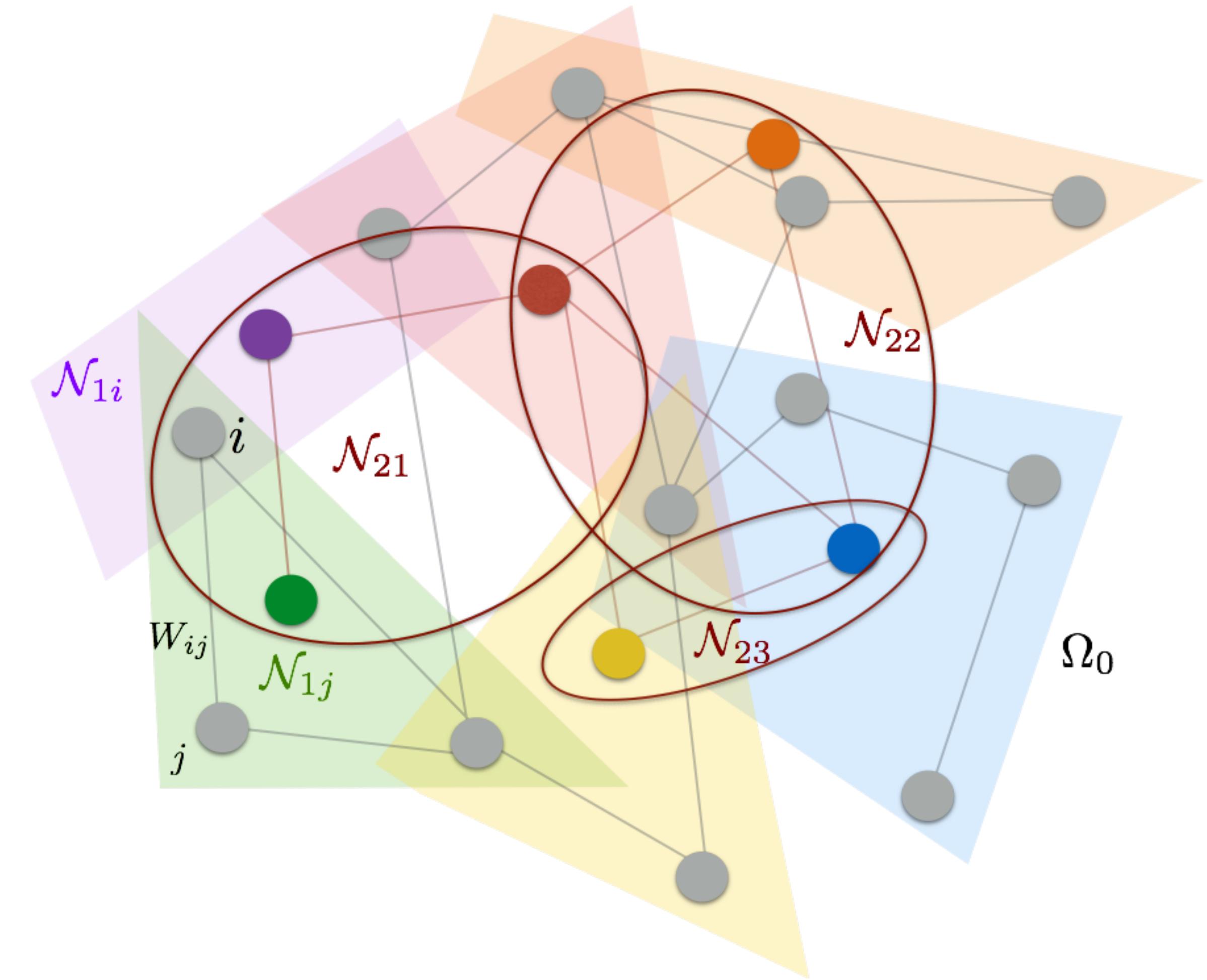


Learning message

- Typically, the M , U , and R functions are learned from data
- Expressed as neural networks (fully connected NNs, recurrent NNs, etc.)
- Which networks to use depends on the specific problem, as much as the graph-building rules
- But you could inject domain knowledge in the game
 - You might know that *SOME* message is carried by some specific functions (e.g., Newton's law for N-body system simulation)
 - You could then use analytic functions for some message
 - You could still use a learned function for other messages
- The trick is dealing with differentiable functions not to spoil your back propagation
- Graph networks become a tool for probabilistic programming

A little bit of History

- (*in this millennium*) Graph networks started (as often it is the case) with a Yann LeCun et al. paper
- They tried to generalise CNNs beyond the regular-array dataset paradigm
- They replaced the translation-invariant kernel structure of CNNs with hierarchical clustering



<https://arxiv.org/abs/1312.6203>

A little bit of History

- The idea of message passing can be tracked to a '15 paper by Duvenaud et al.
- The paper introduces “a convolutional neural network that operates directly on graphs”
- Language is different, but if you look at the algorithm it is pretty much what we discussed (for specific network architecture choices)

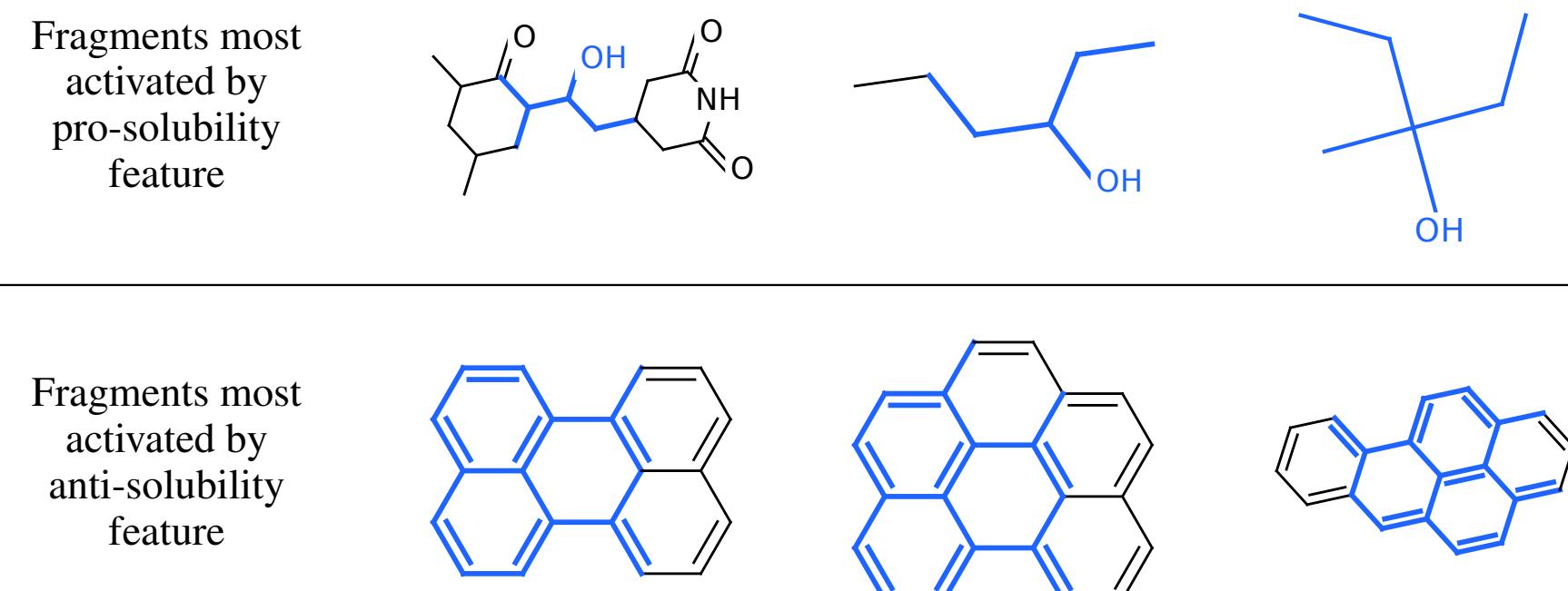
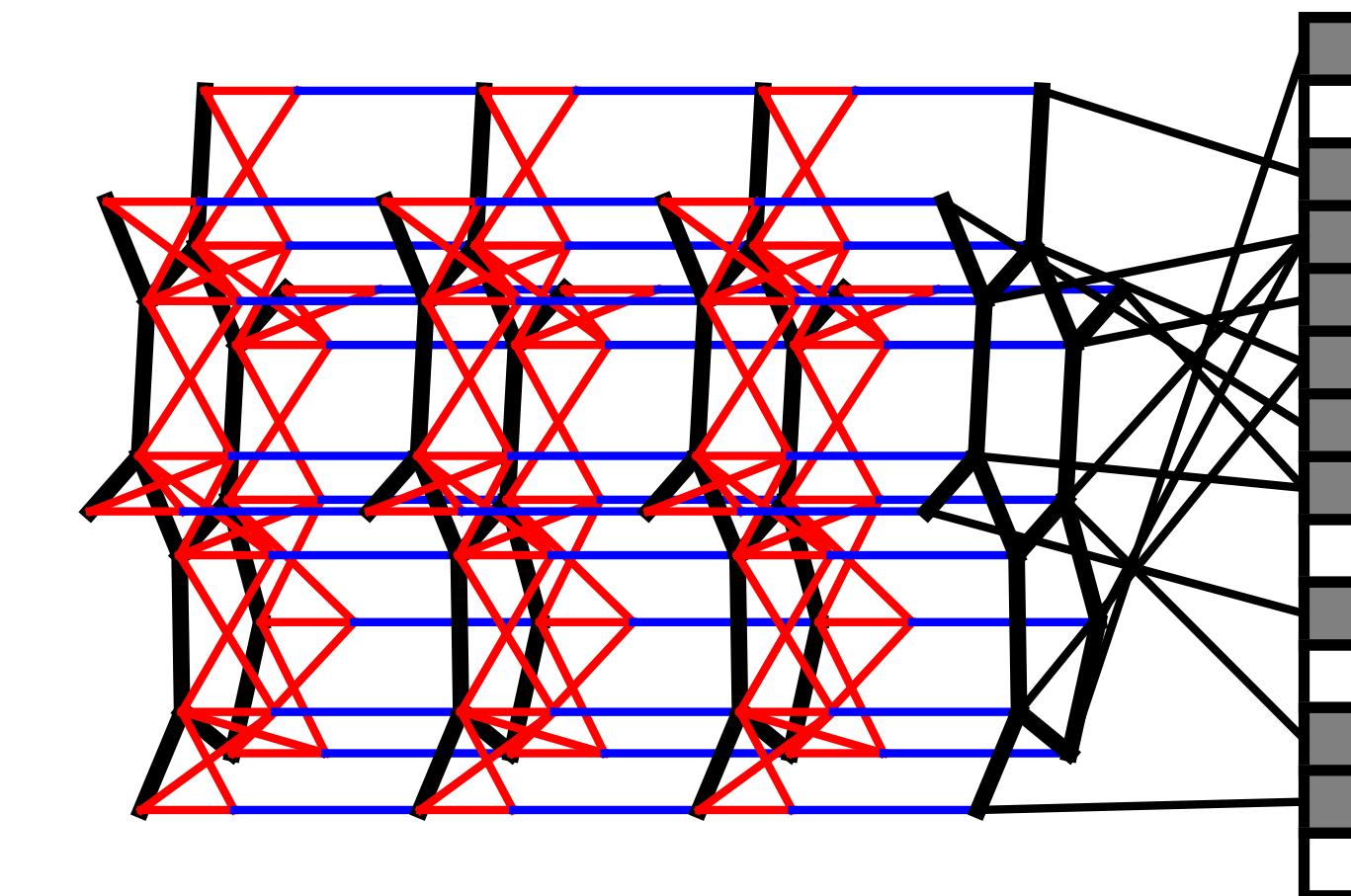


Figure 4: Examining fingerprints optimized for predicting solubility. Shown here are representative examples of molecular fragments (highlighted in blue) which most activate different features of the fingerprint. Top row: The feature most predictive of solubility. Bottom row: The feature most predictive of insolubility.

<https://arxiv.org/pdf/1509.09292.pdf>



Algorithm 2 Neural graph fingerprints

```

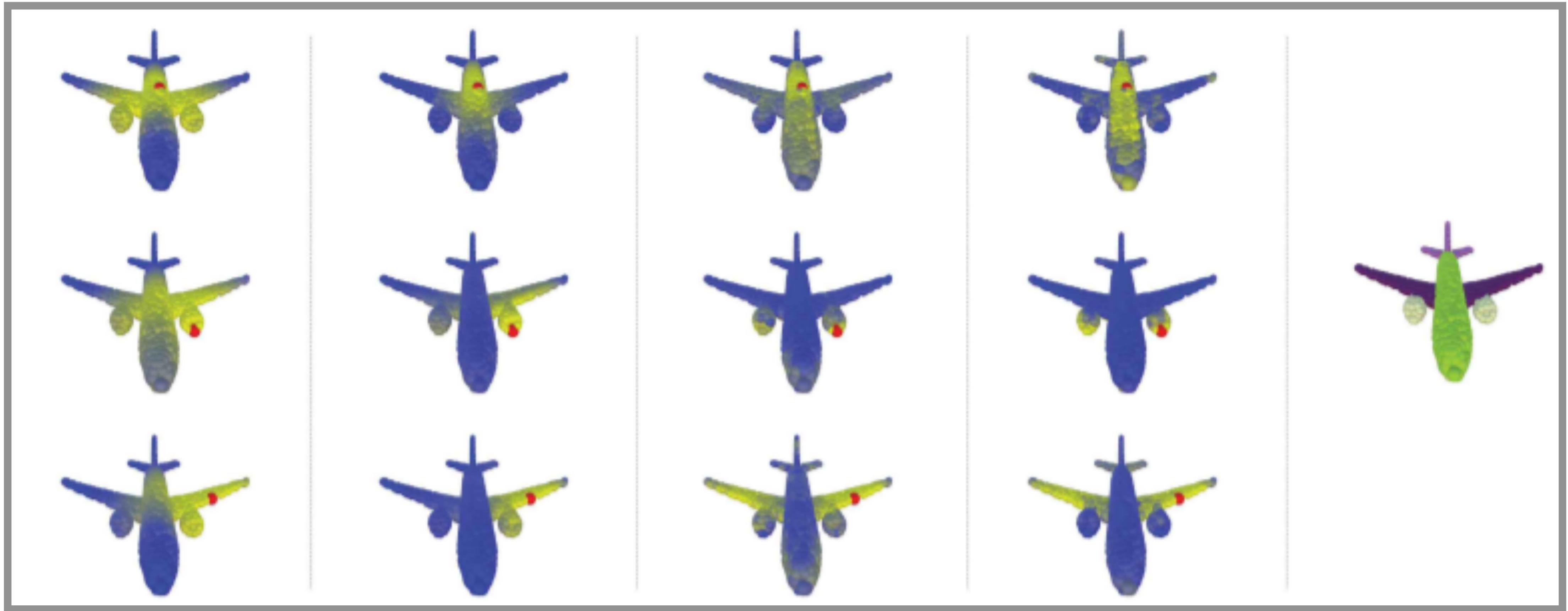
1: Input: molecule, radius  $R$ , hidden weights  $H_1^1 \dots H_R^5$ , output weights  $W_1 \dots W_R$ 
2: Initialize: fingerprint vector  $\mathbf{f} \leftarrow \mathbf{0}_S$ 
3: for each atom  $a$  in molecule
4:    $\mathbf{r}_a \leftarrow g(a)$             $\triangleright$  lookup atom features
5: for  $L = 1$  to  $R$             $\triangleright$  for each layer
6:   for each atom  $a$  in molecule
7:      $\mathbf{r}_1 \dots \mathbf{r}_N = \text{neighbors}(a)$ 
8:      $\mathbf{v} \leftarrow \mathbf{r}_a + \sum_{i=1}^N \mathbf{r}_i$             $\triangleright$  sum
9:      $\mathbf{r}_a \leftarrow \sigma(\mathbf{v} H_L^N)$             $\triangleright$  smooth function
10:     $\mathbf{i} \leftarrow \text{softmax}(\mathbf{r}_a W_L)$             $\triangleright$  sparsify
11:     $\mathbf{f} \leftarrow \mathbf{f} + \mathbf{i}$             $\triangleright$  add to fingerprint
12: Return: real-valued vector  $\mathbf{f}$ 

```



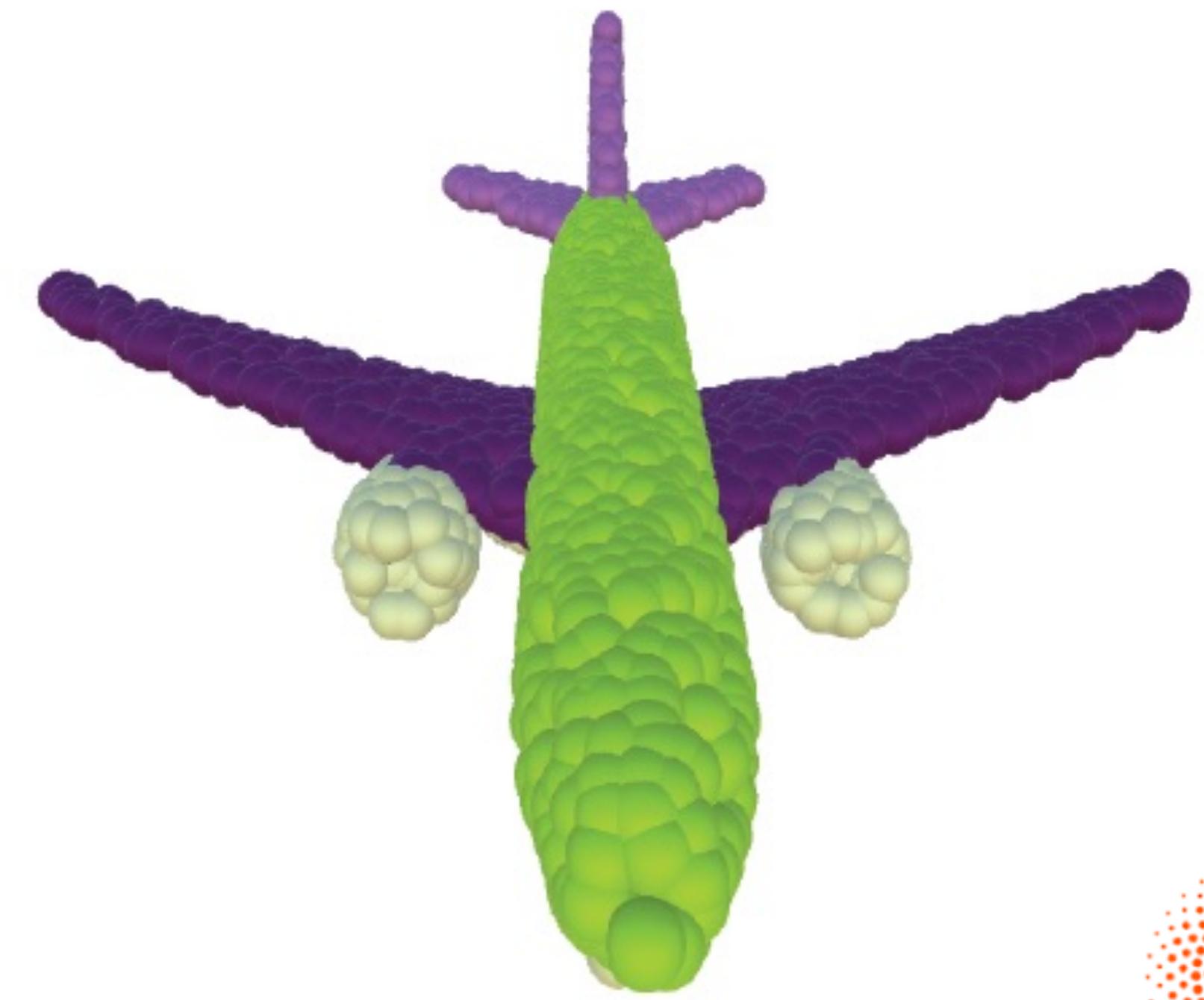
Further Reading & Coding

- A few recent reviews that could guide you through the many applications and networks
 - A nice BLOG article on GNNs
 - Another nice BLOG article on GNNs
 - A generic review
 - A particle-physics specific one
- A few GitHub entries
 - JEDI-net Interaction Networks for jet tagging on these data
 - PUPPIML: GGNN for pileup subtraction
- A small GarNet example that fits an FPGA on these data

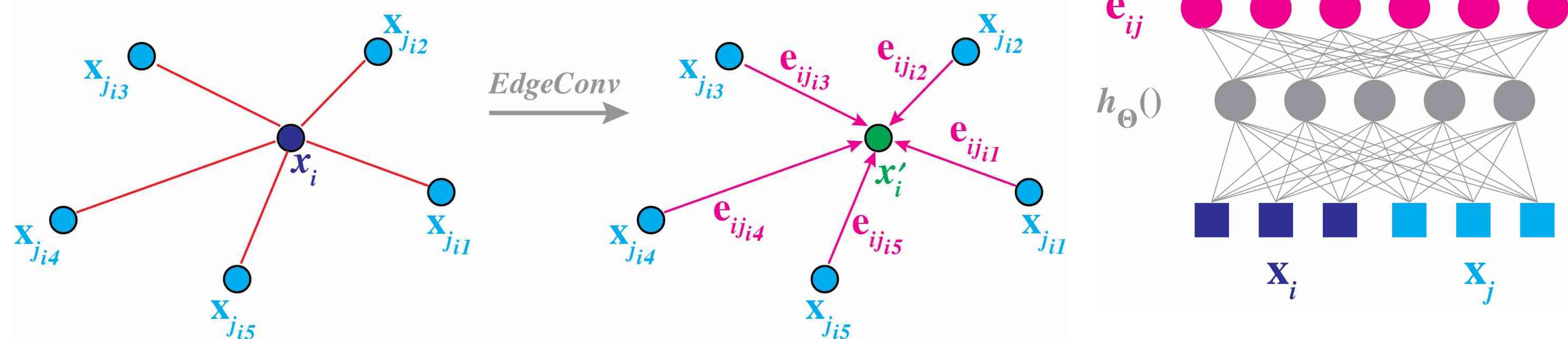


Edge Conv

- *Dynamic Graph CNN (DGCNN) is THE message-passing neural network*
- *It uses EdgeConv layers to perform point-cloud segmentation*
- *Segmentation is the process of clustering pixels in an image into objects*
- *EdgeConv was capable of extending semantic segmentation beyond nearby-pixel clustering*
 - *the two wings of the airplane are associated to the same cluster, since they are found to be similar*

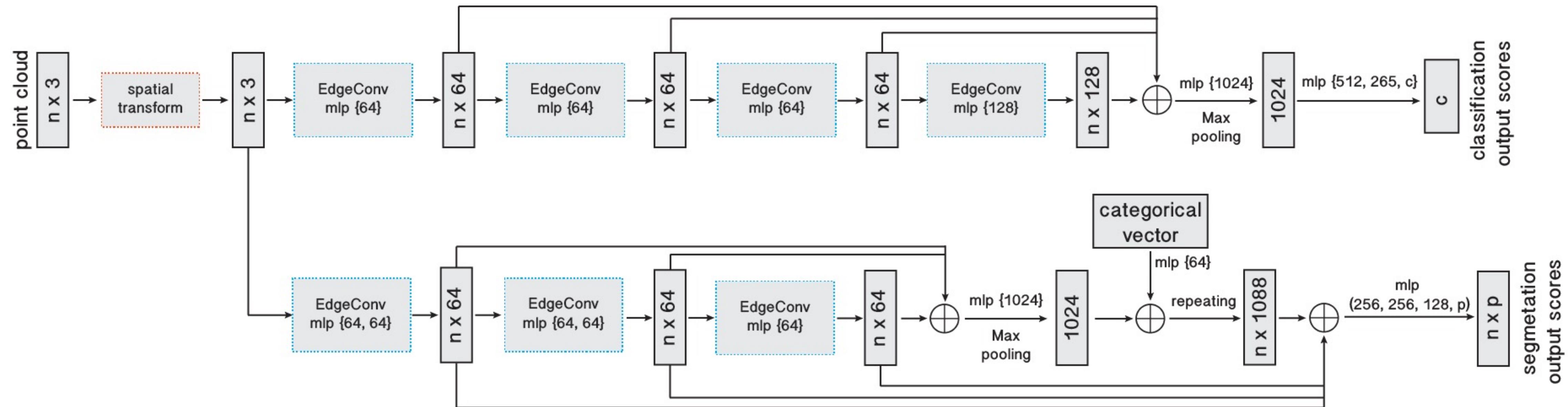


- EdgeConv is a typical message passing architecture, using fully-connected networks to learn edge representation (the h functions)



EdgeConv

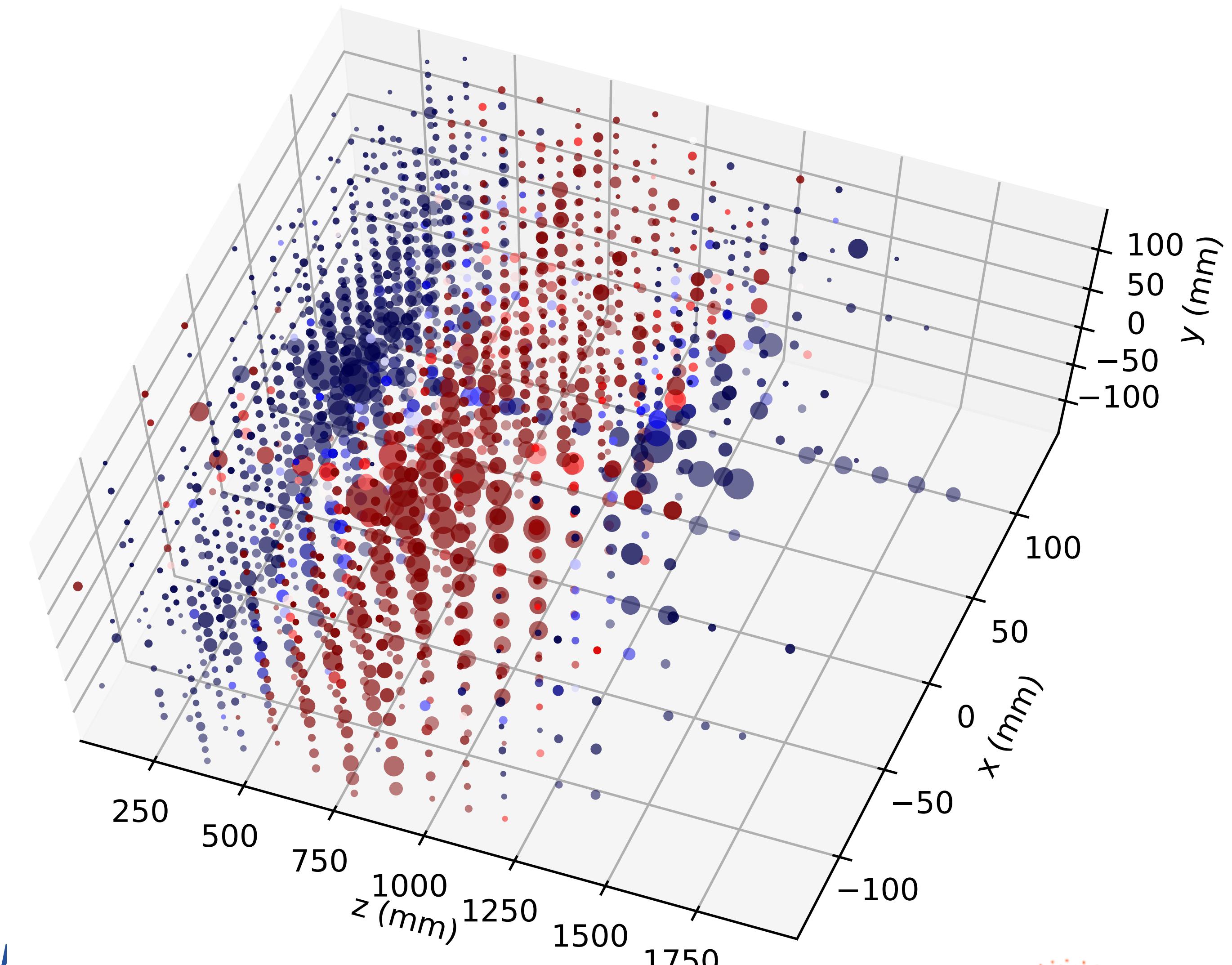
- But the actual model is much more complicated than that



- Each EdgeConv layer runs a message passing and creates an updated representation of the graph of points
- Similar to a CNN, but capable of processing unordered sets of points

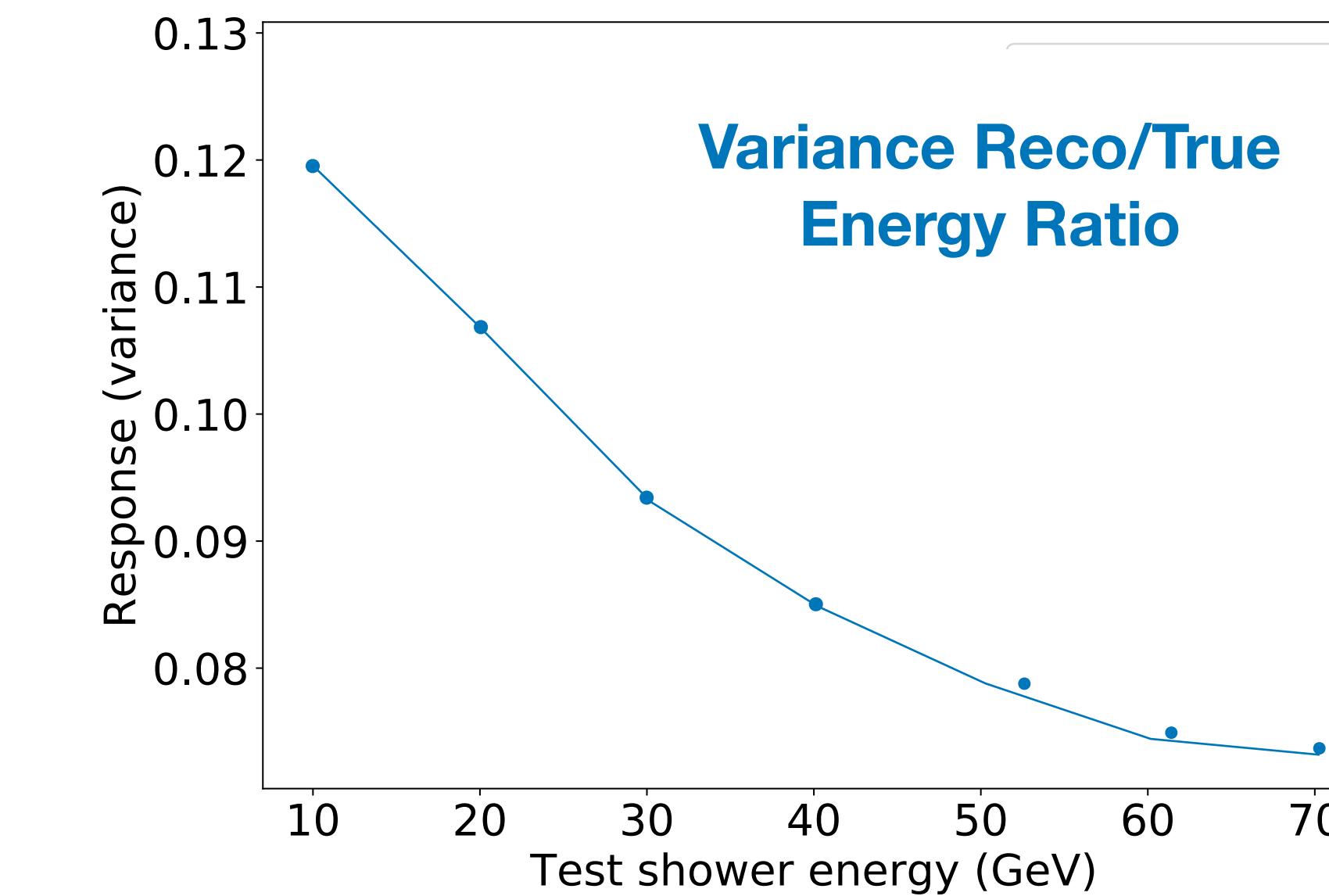
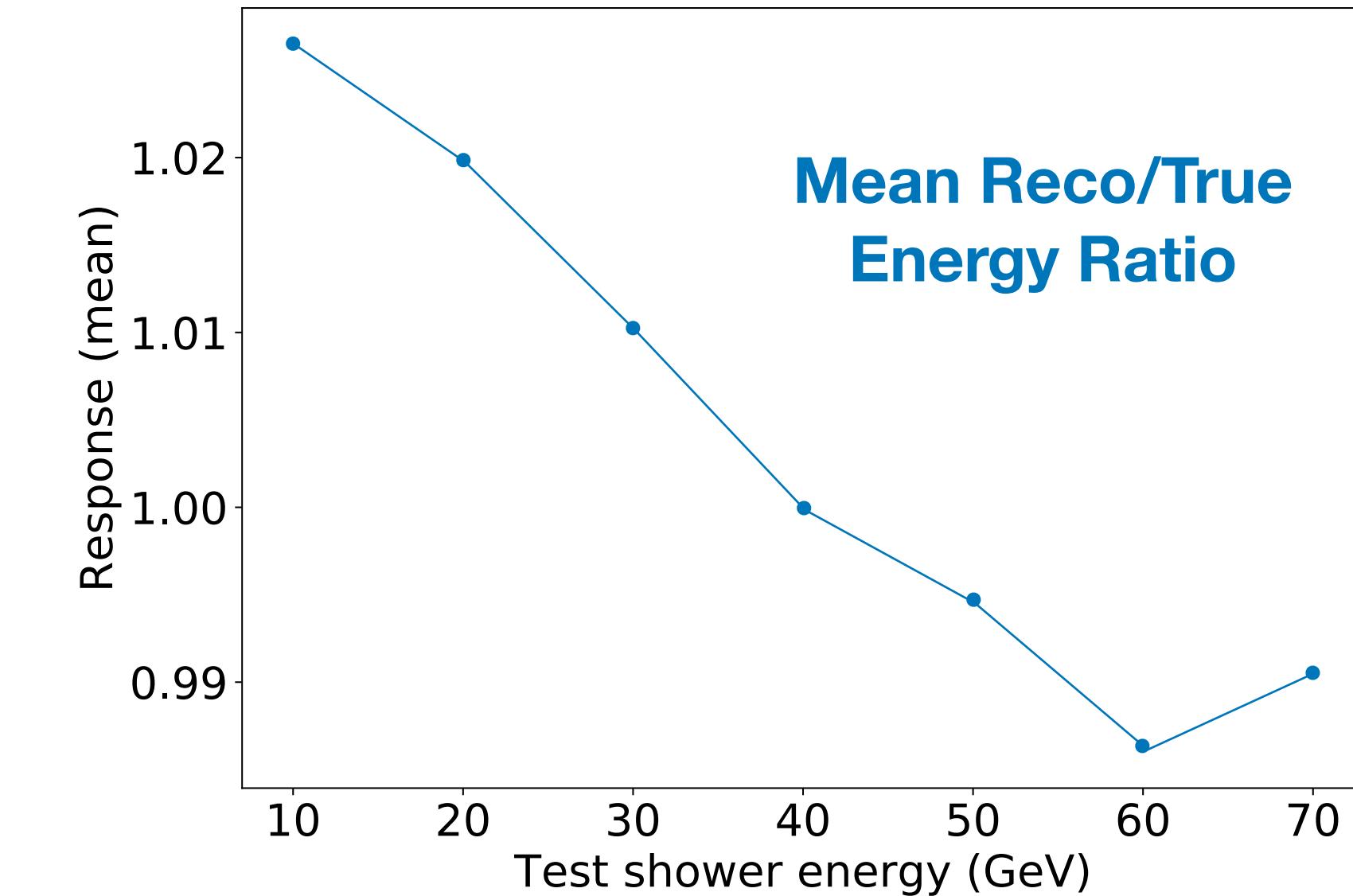
EdgeConv for Particle Physics

- DGCNN fits very well particle reconstruction in High Energy Physics
- Particles seen as energy showers in calorimeters
- DGCNN can be trained to distinguish overlapping showers from different particles
- Success comes at some computational cost:
 - 15 sec/event on a CPU
 - Lowered to 5 sec/event on GI when using a batch of 100

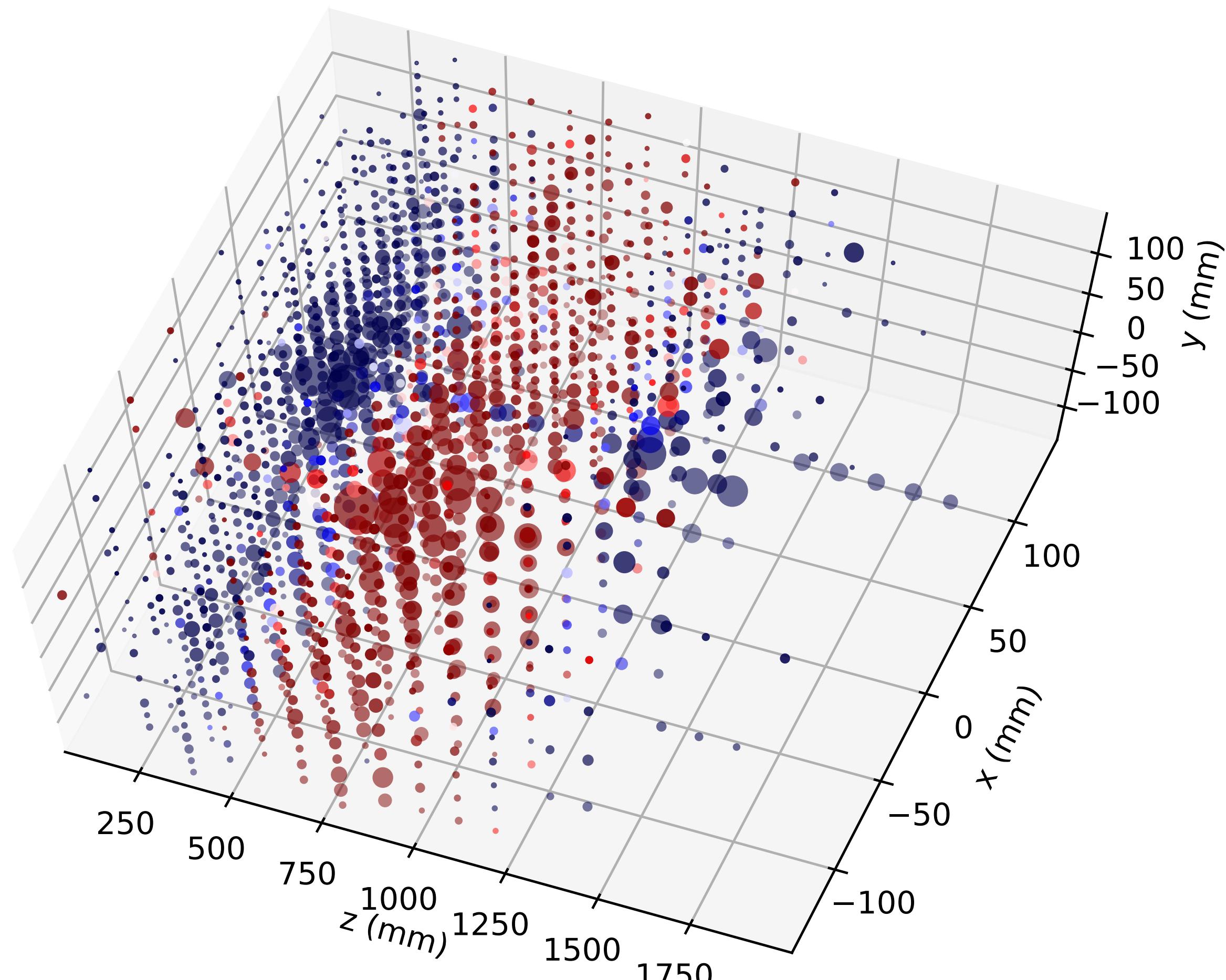


EdgeConv for Particle Physics

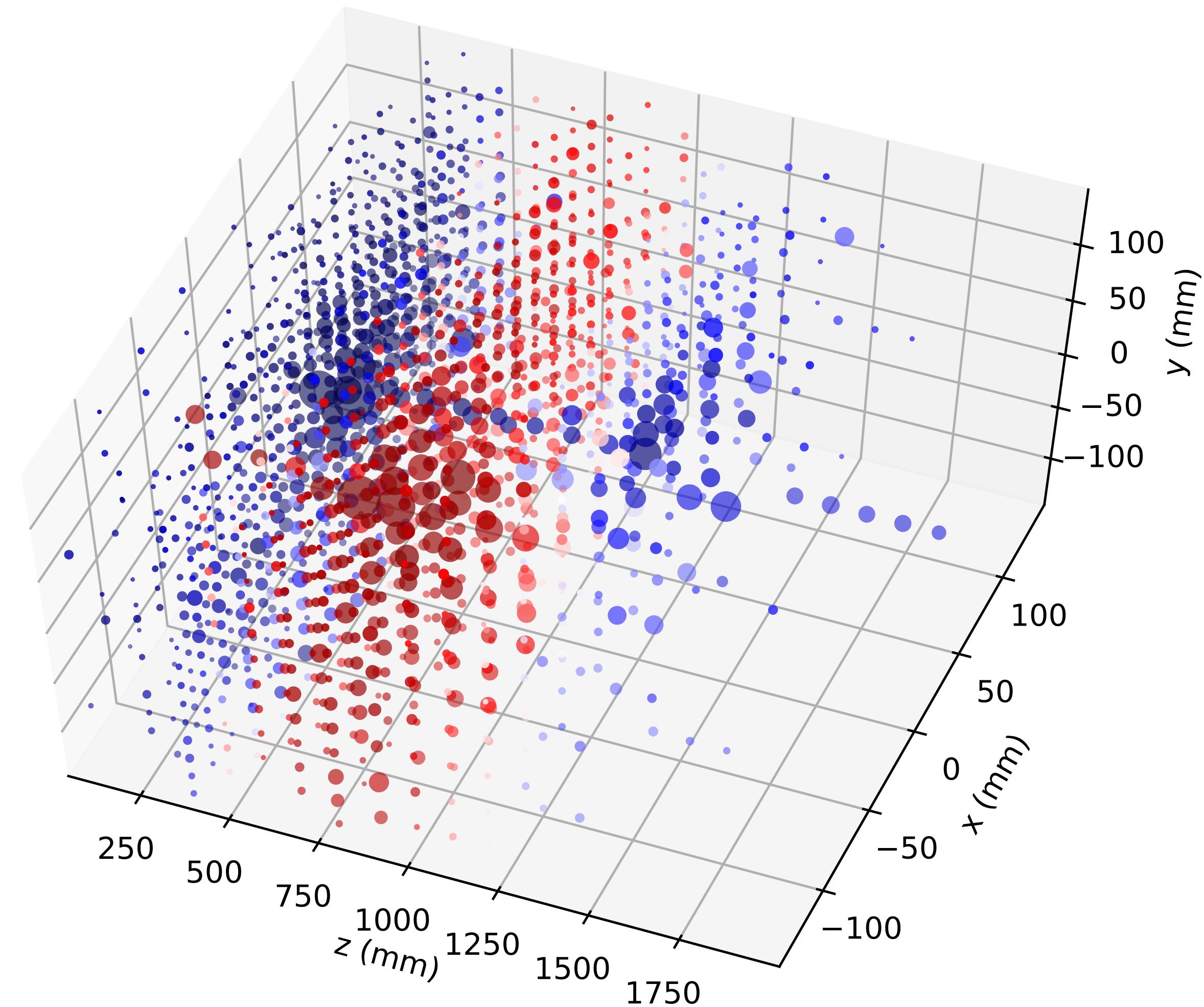
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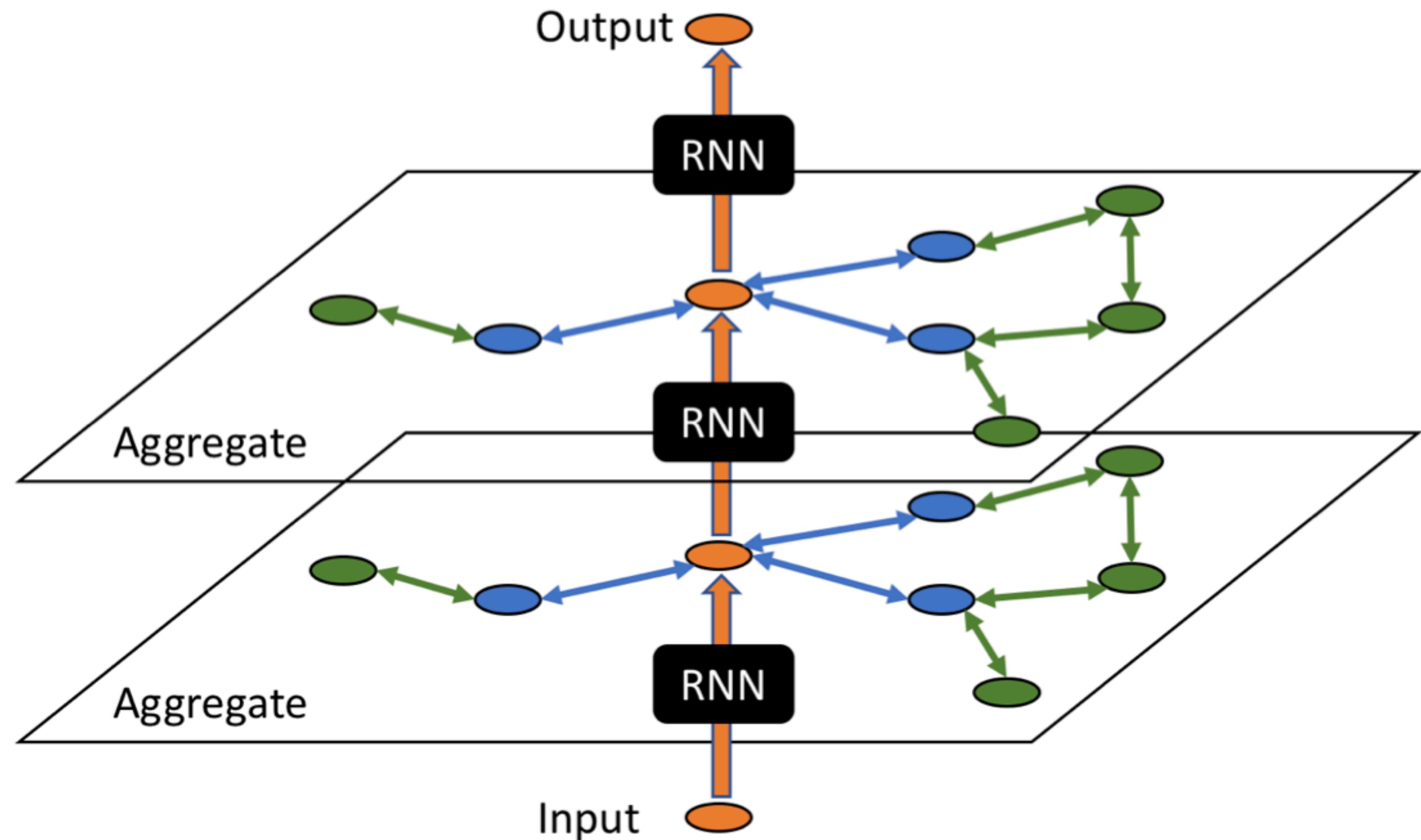
Separating overlapping showers



(a) Truth



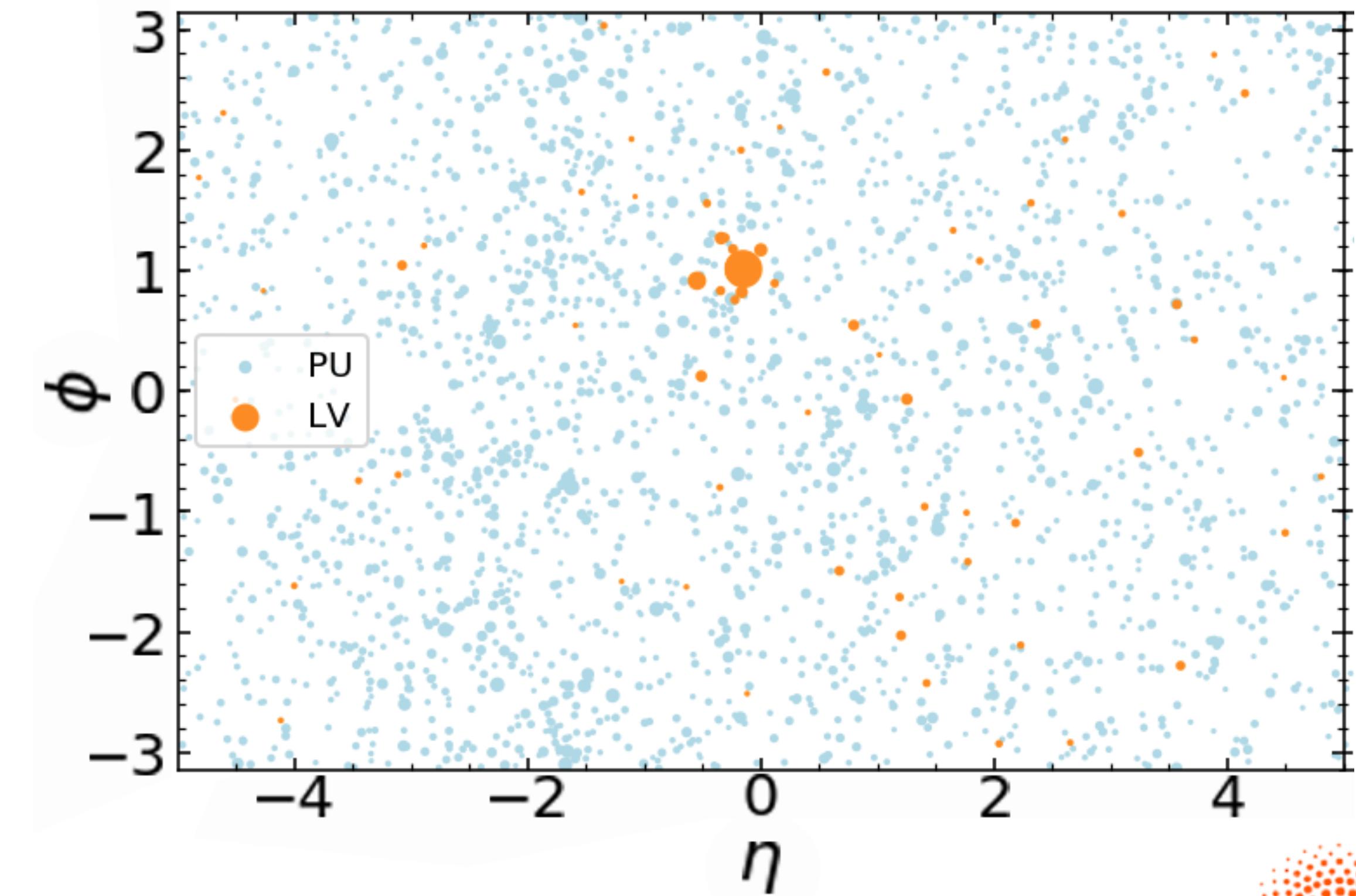
(b) Reconstructed



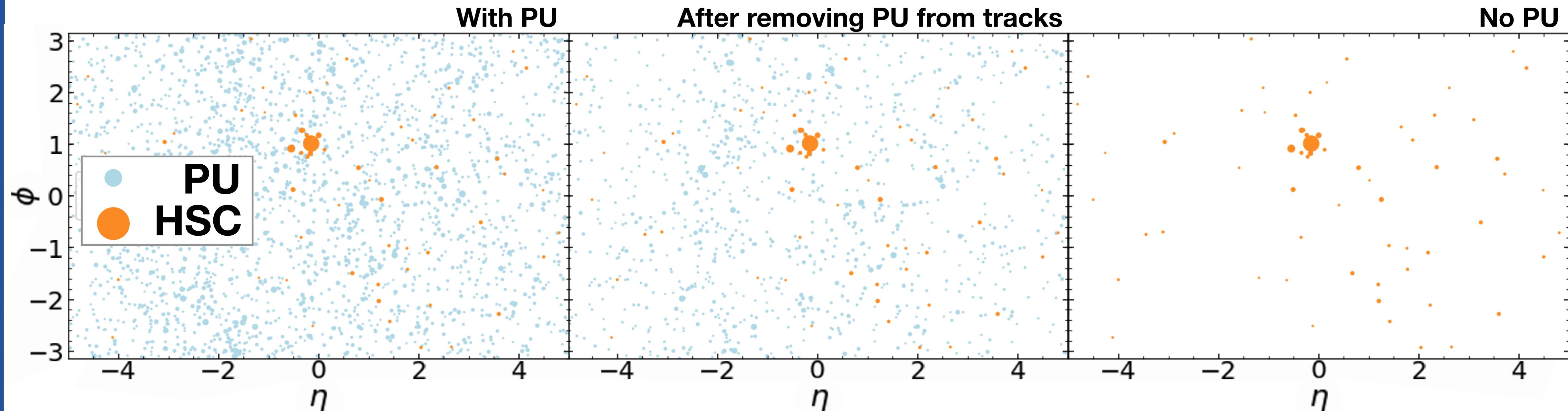
Gated Graph Neural networks

Example: pileup removal

- At the LHC, parasitic collisions (pileup) happen simultaneously to your interesting one (hard-scattering collision)
- They typically happen at ~ same x and y, but at different z
- Charged particles are tracked back to their origin and associated to the interesting collision or to a parasitic one
- Neutrals cannot be tracked back

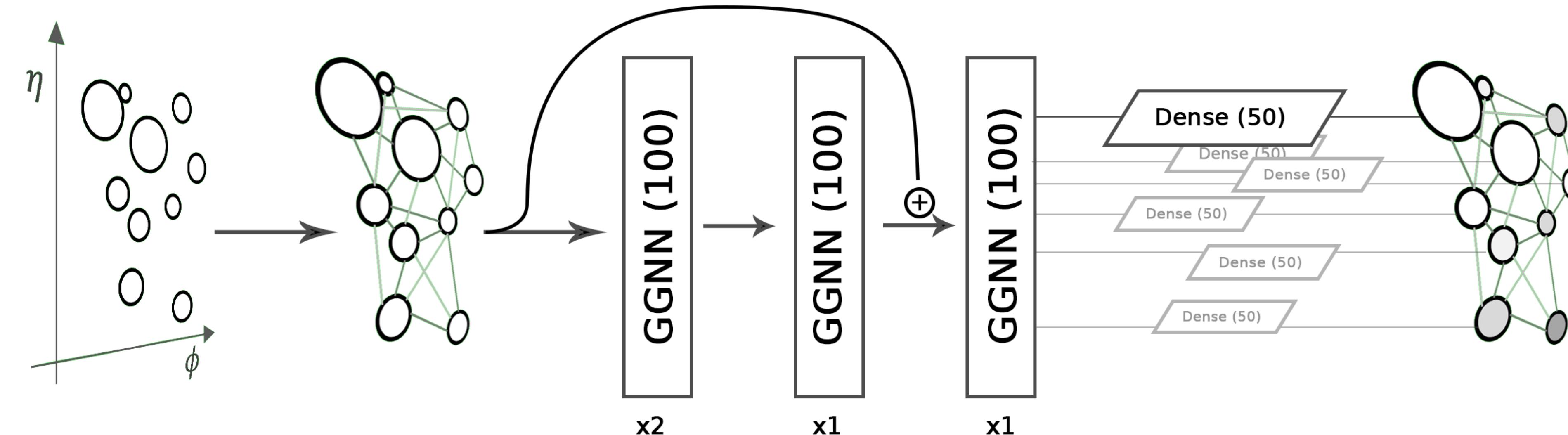


Example: pileup removal



- We want to learn if a given neutral comes from PU or from the hard-scattering collision
- We look at the problem projecting the solid-angle particle distribution in a plane (we unroll the cylindrical detector into a rectangle)
- Each point is a particle (size represents the energy carried by each particle)
- We know the particle charge, plus some extra feature we might want to use (e.g., particle kind [electron, muon, etc.])
- We have labels for charged particles, but not neutrals

Graph Networks for PU removal



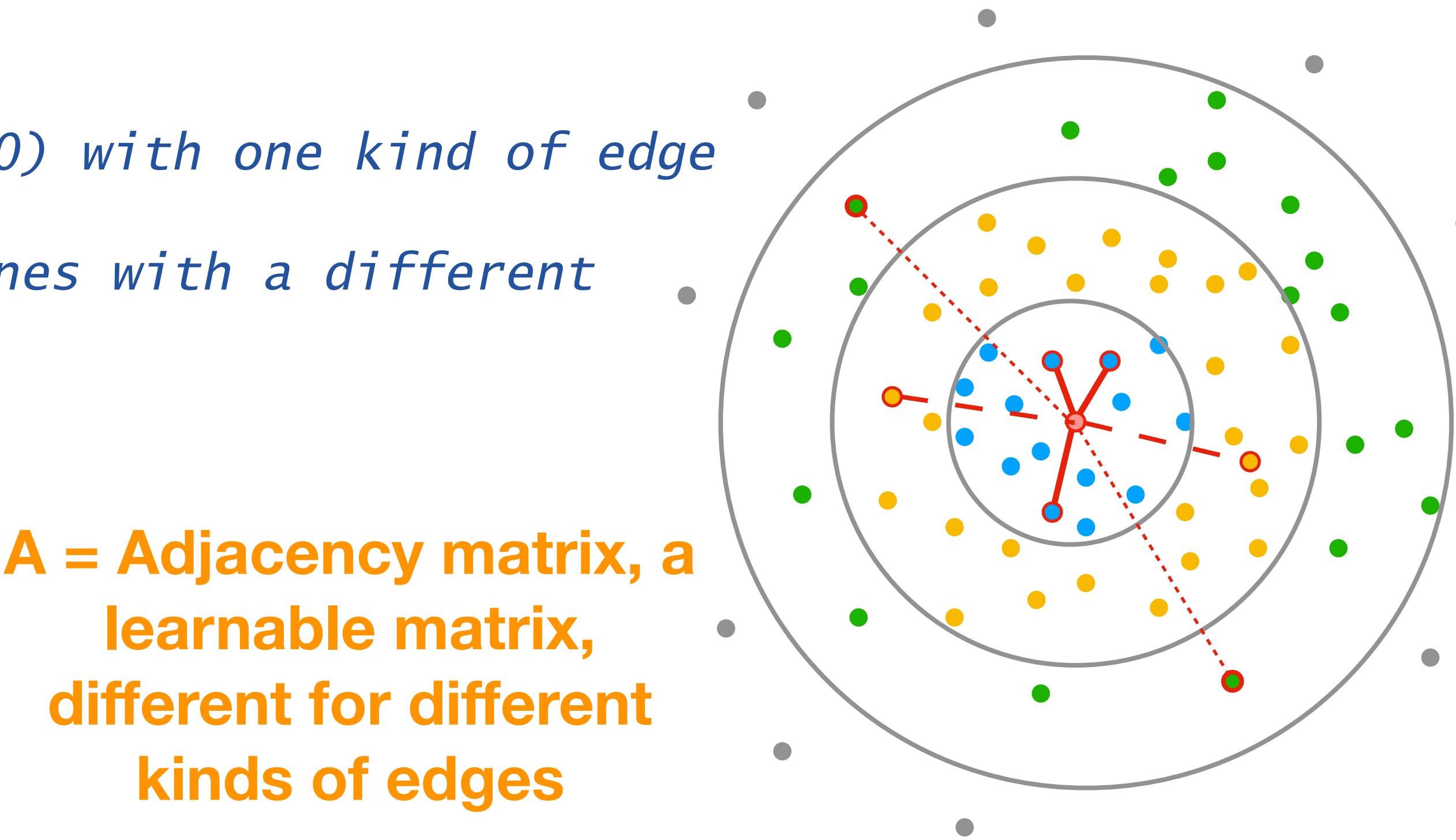
- We use Gated Graph Neural Network (GGNN), a special kind of message-passing architecture
- Start from a set of particles, each represented as a set of features h
- Build the graph
- Use a recurrent network (GRU) to “pass” messages in sequential steps and evolve the particle representation
- At each iteration, we connect to different neighbours (start with close-by, then go further)

Building the graph

- Start with one particle (the red one)
- Connect it to the closest ones ($R < R_0$) with one kind of edge
- Connect it to the next-to-closest ones with a different kind of edge
- ...
- Each edge comes with a message

$$m_j = \frac{1}{N} \sum_j^N m_{v,v_j}$$

Gathered message
Messages
A
f_j

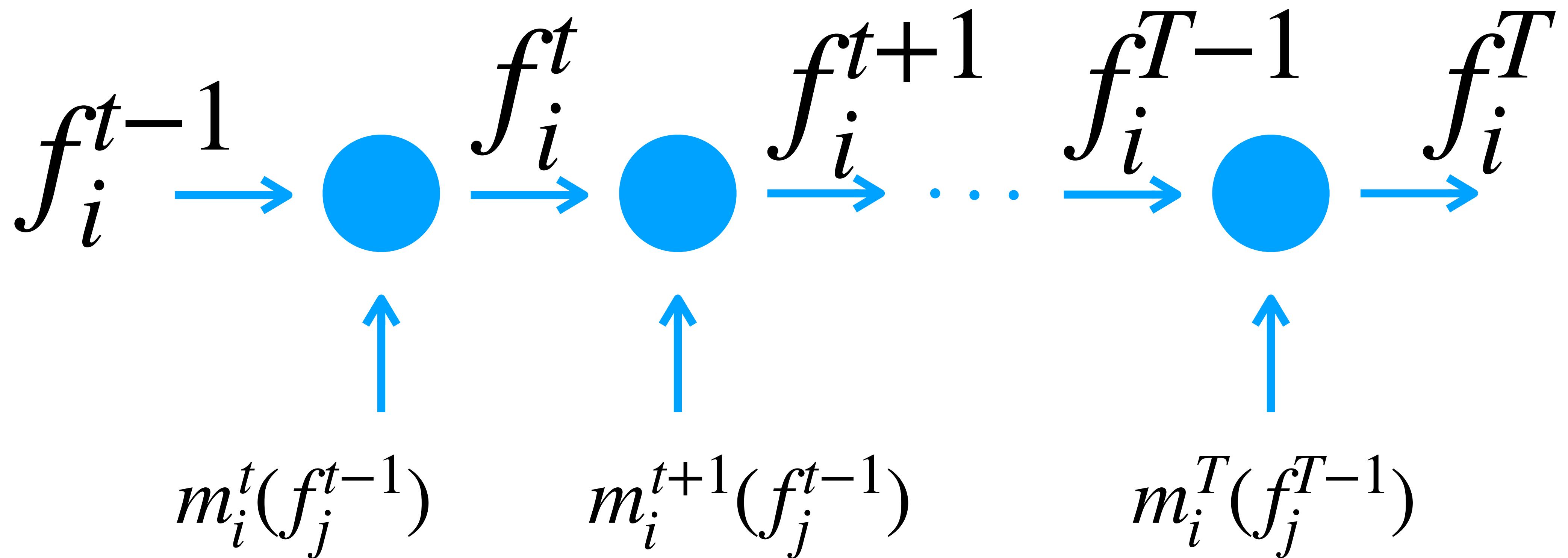


A = Adjacency matrix, a learnable matrix, different for different kinds of edges

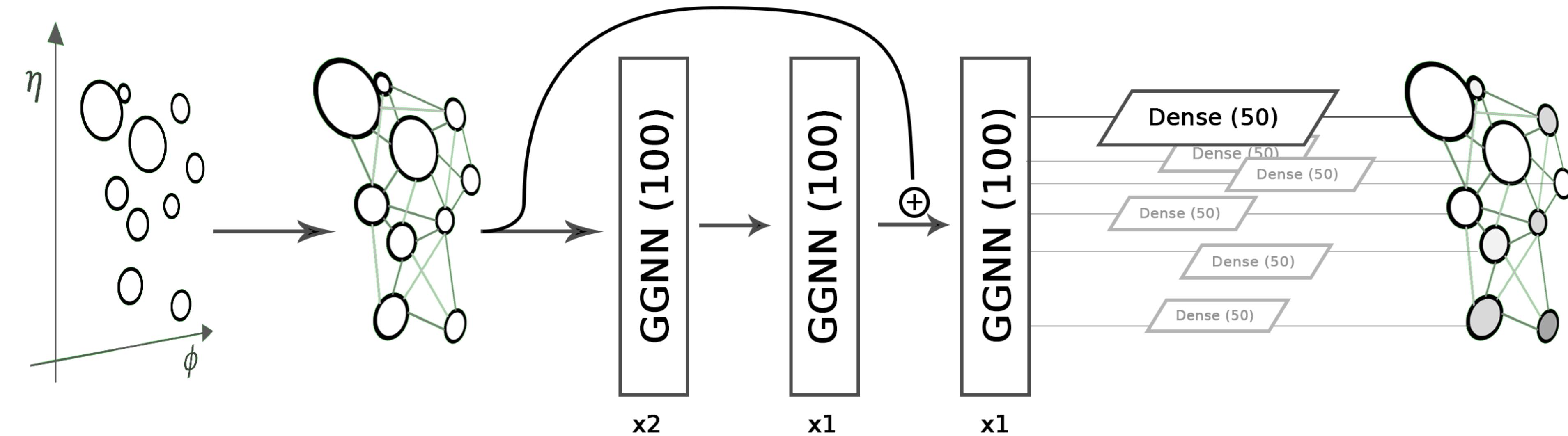
features of the j-th vertex

multiple message passing

- The procedure is repeated T times using a GRU with n steps



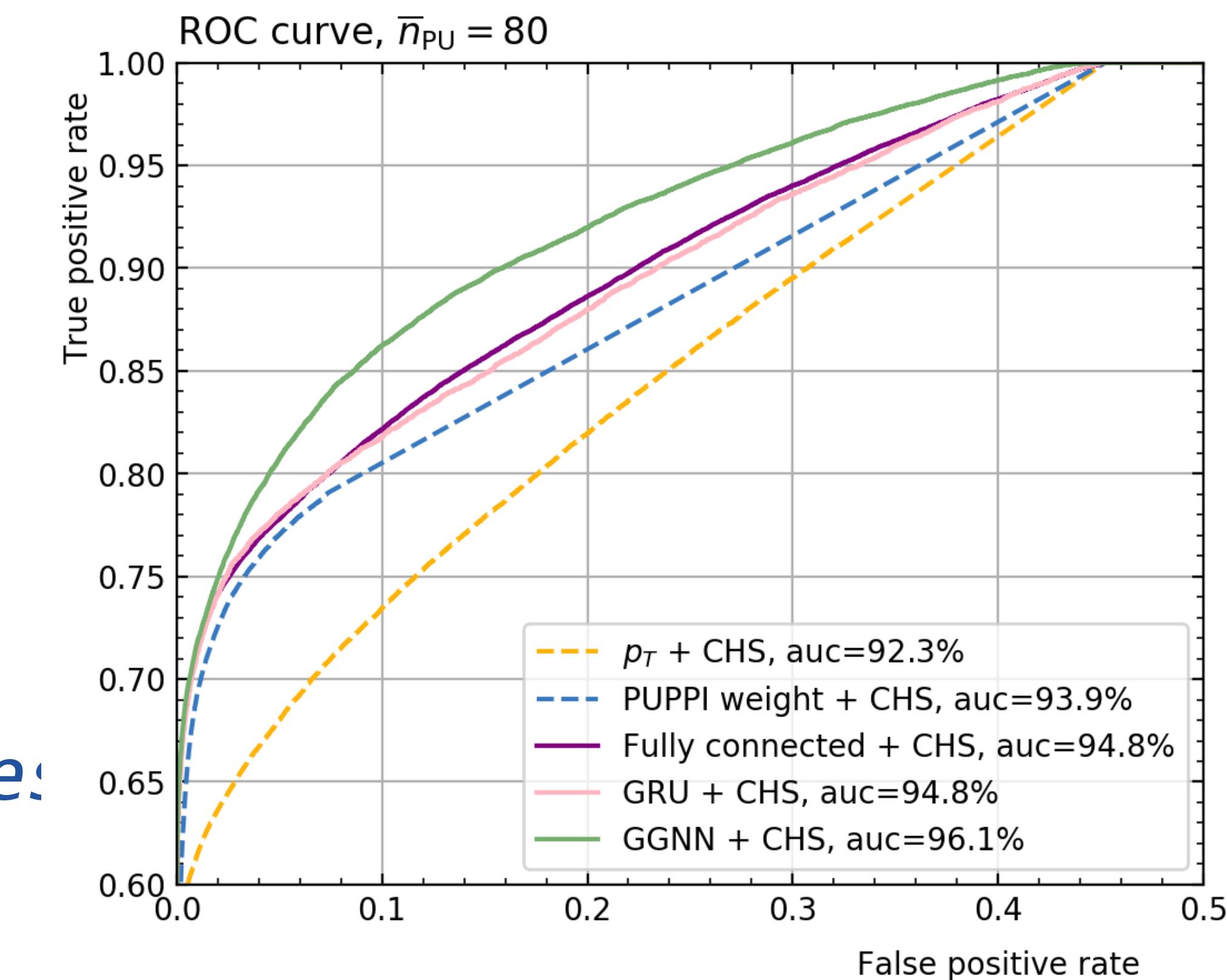
Done 3 times (for 3 GRU layers)



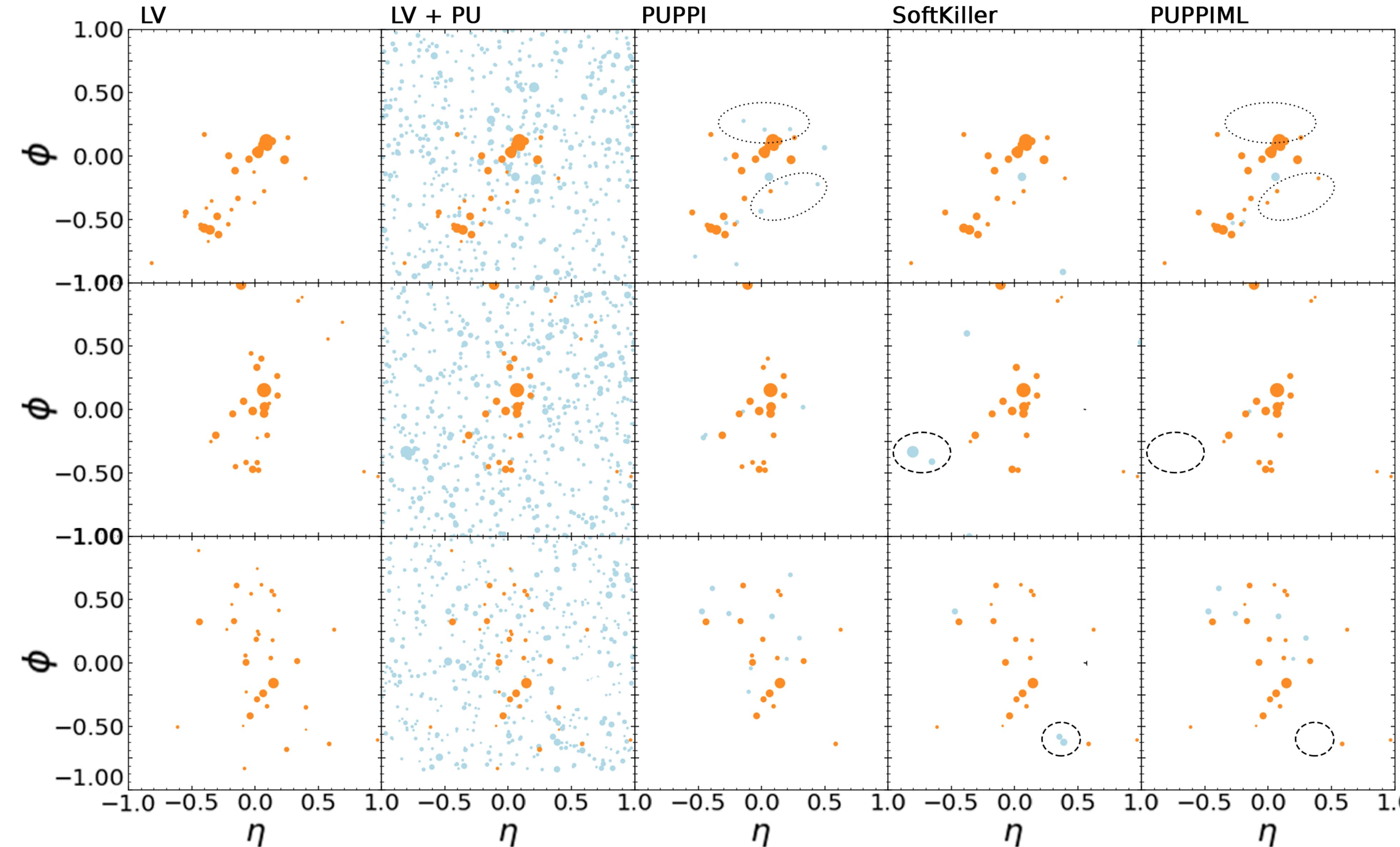
- The representation created by each layer is passed to the next
- A ResNet-like skip connection is implemented (input \rightarrow last layer)
- The per-particle outcome set of features (function of the features of the connected particles) is used to train a dense classifier: PU vs interesting particle?

- Improve state-of-the-art algorithms substantially
- Little dependence of algorithm tuning on pileup conditions
- Small/No performance loss with average number of PU collisions
- Outperforms alternative particle-based architectures: (DNNN, simple GRU)

| \bar{n}_{PU} | 20 (CHS) | 80 (CHS) | 140 (CHS) | 80 (No CHS) |
|-----------------------|----------|----------|-----------|-------------|
| p_T | 92.3% | 92.3% | 92.5% | 64.9% |
| PUPPI weight | 94.1% | 93.9% | 94.4% | 65.1% |
| Fully-connected | 95.0% | 94.8% | 94.8% | 68.5% |
| GRU | 94.8% | 94.8% | 94.7% | 68.8% |
| GGNN | 96.1% | 96.1% | 96.0% | 70.1% |



<https://arxiv.org/pdf/1810.07988.pdf>





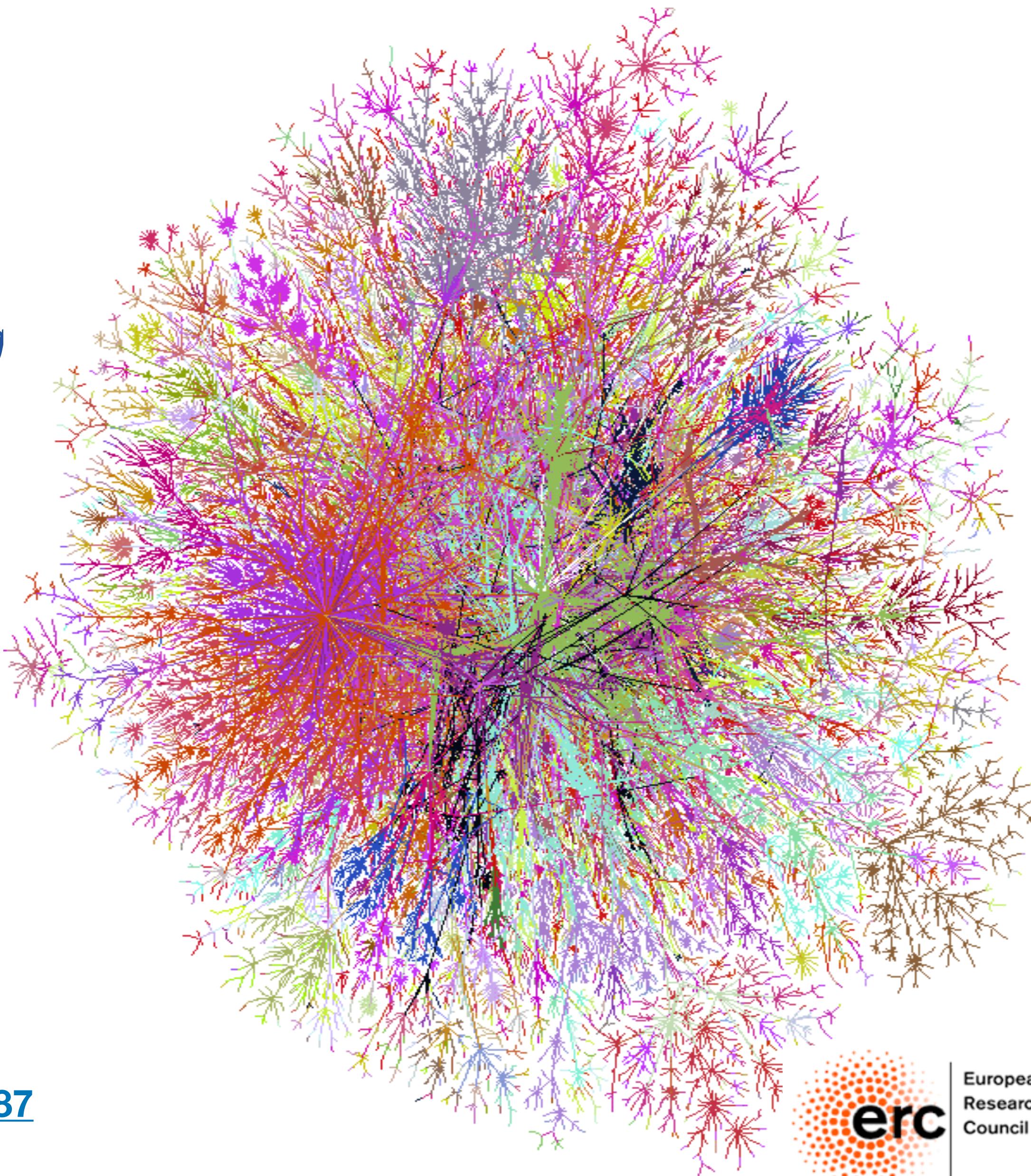
Distance-Weighted Graph Networks

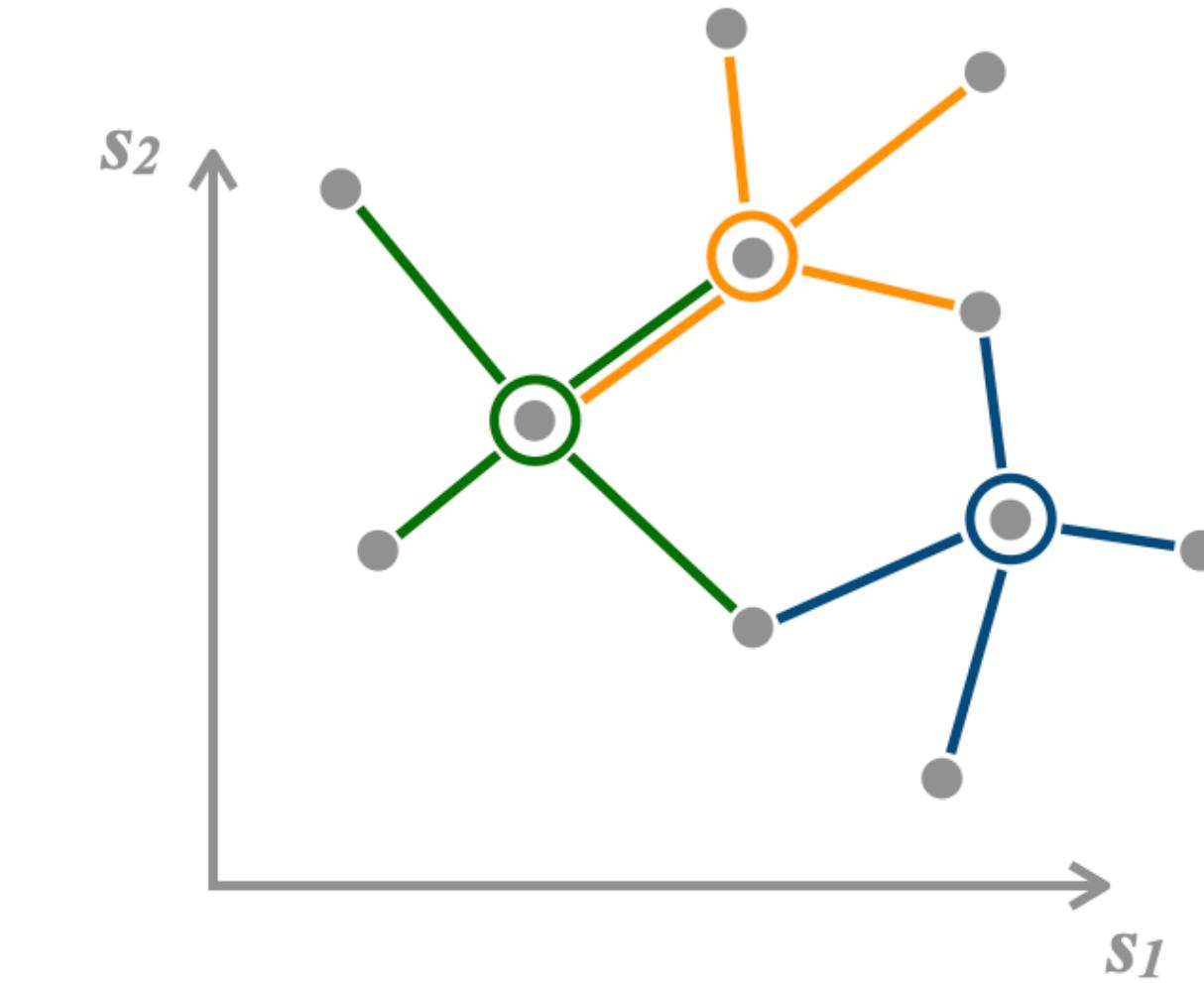
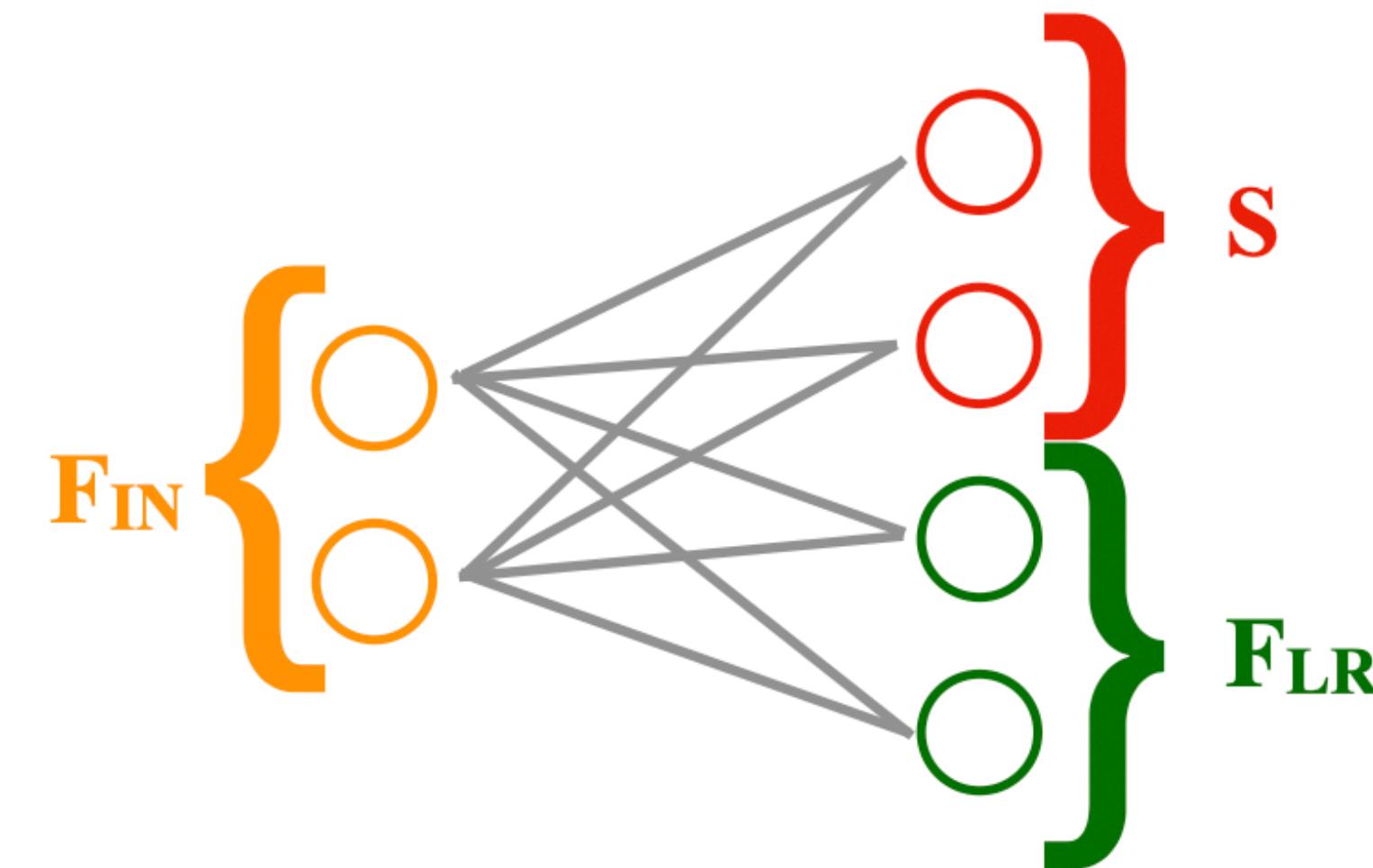
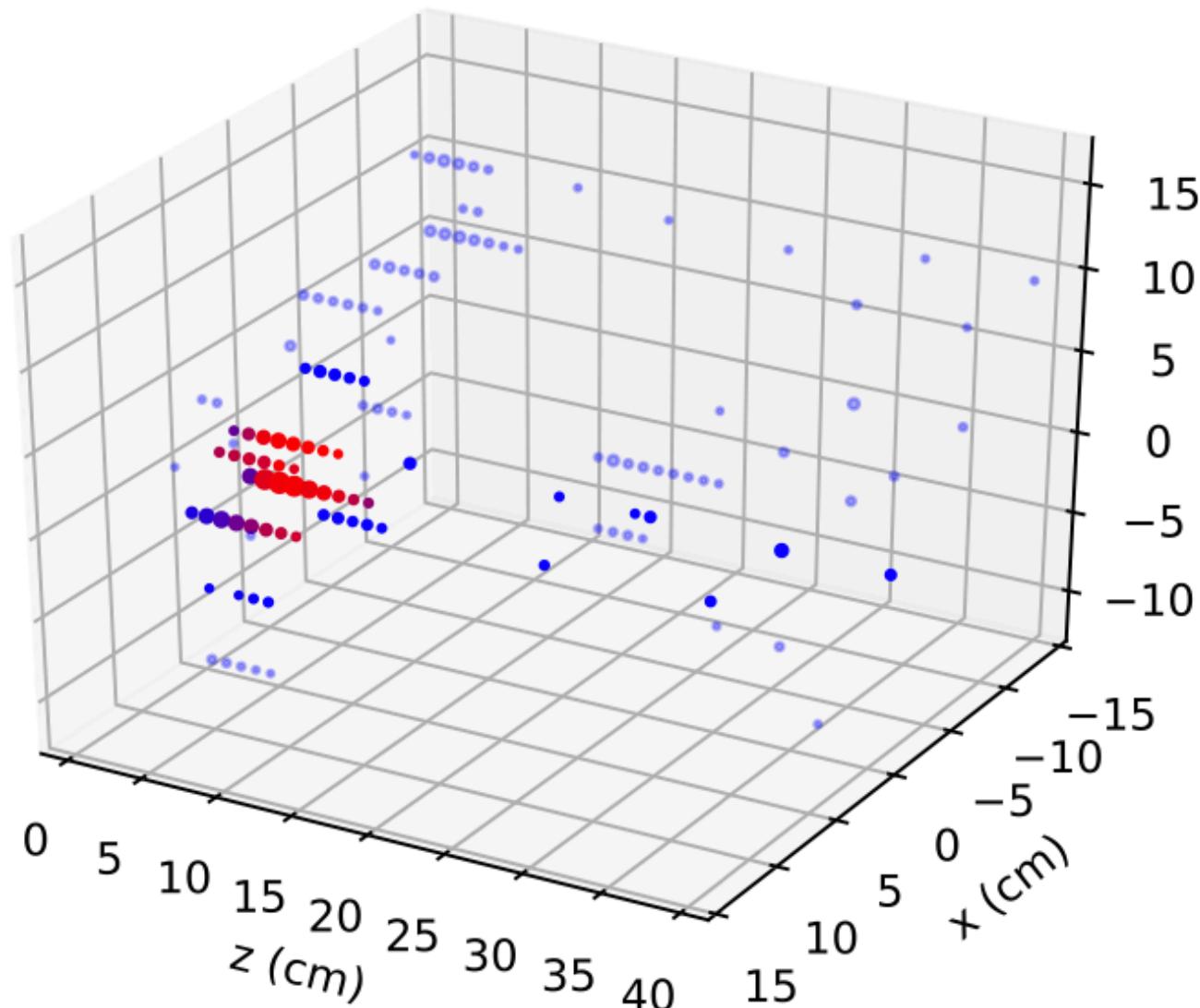


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Reducing memory consumption

- When building a graph of N vertices, number of edges (and number of computing operations) scale with N^2
- This might clash with computing resource limitations (both for training and inference)
- Certainly, this is the case at the LHC
 - real-time event selection runs in short time
 - most of the selection runs as electronic circuit on electronic board
- Gravnet & Garnet: resource friendly graph architectures <https://arxiv.org/abs/1902.07987>

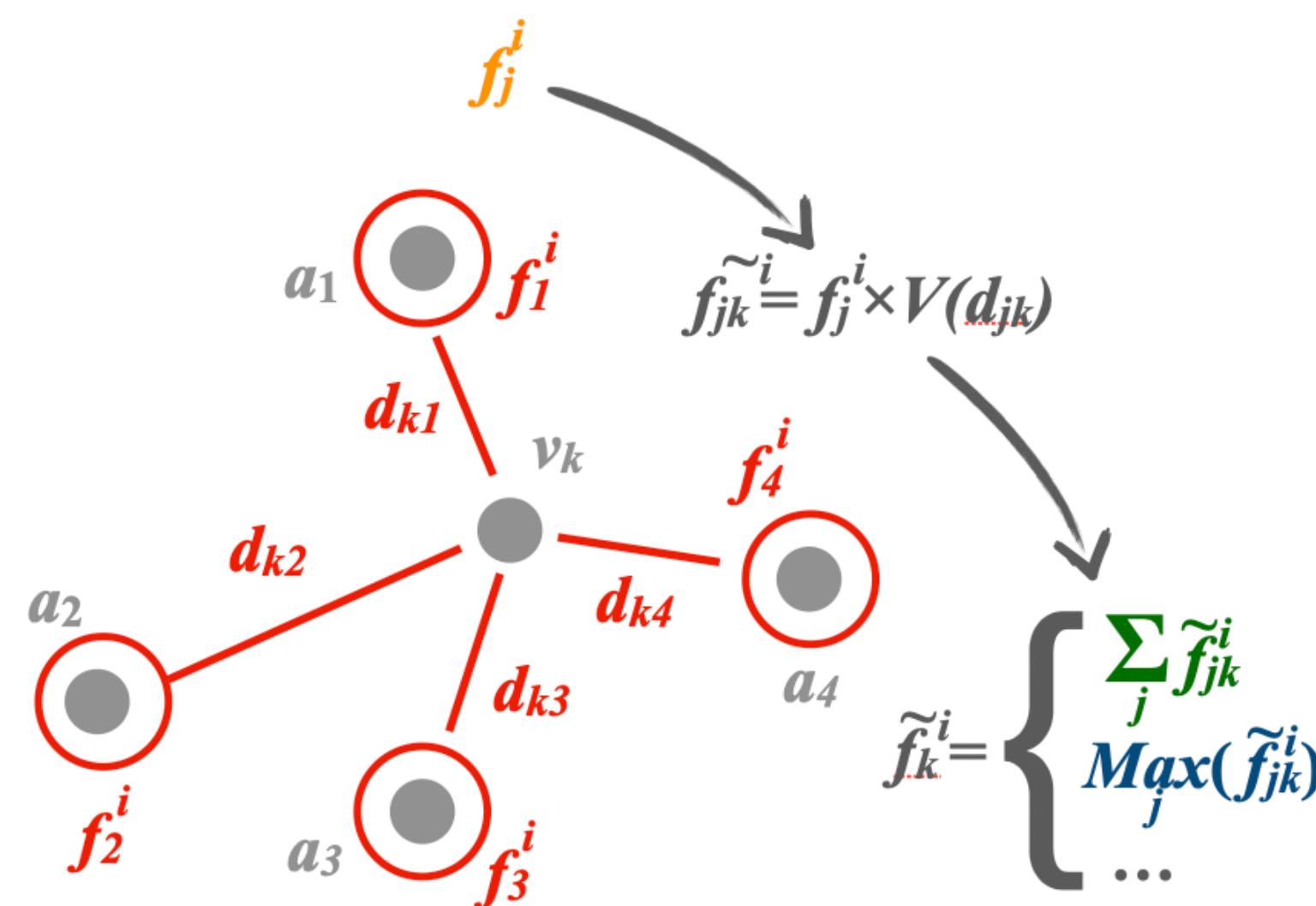
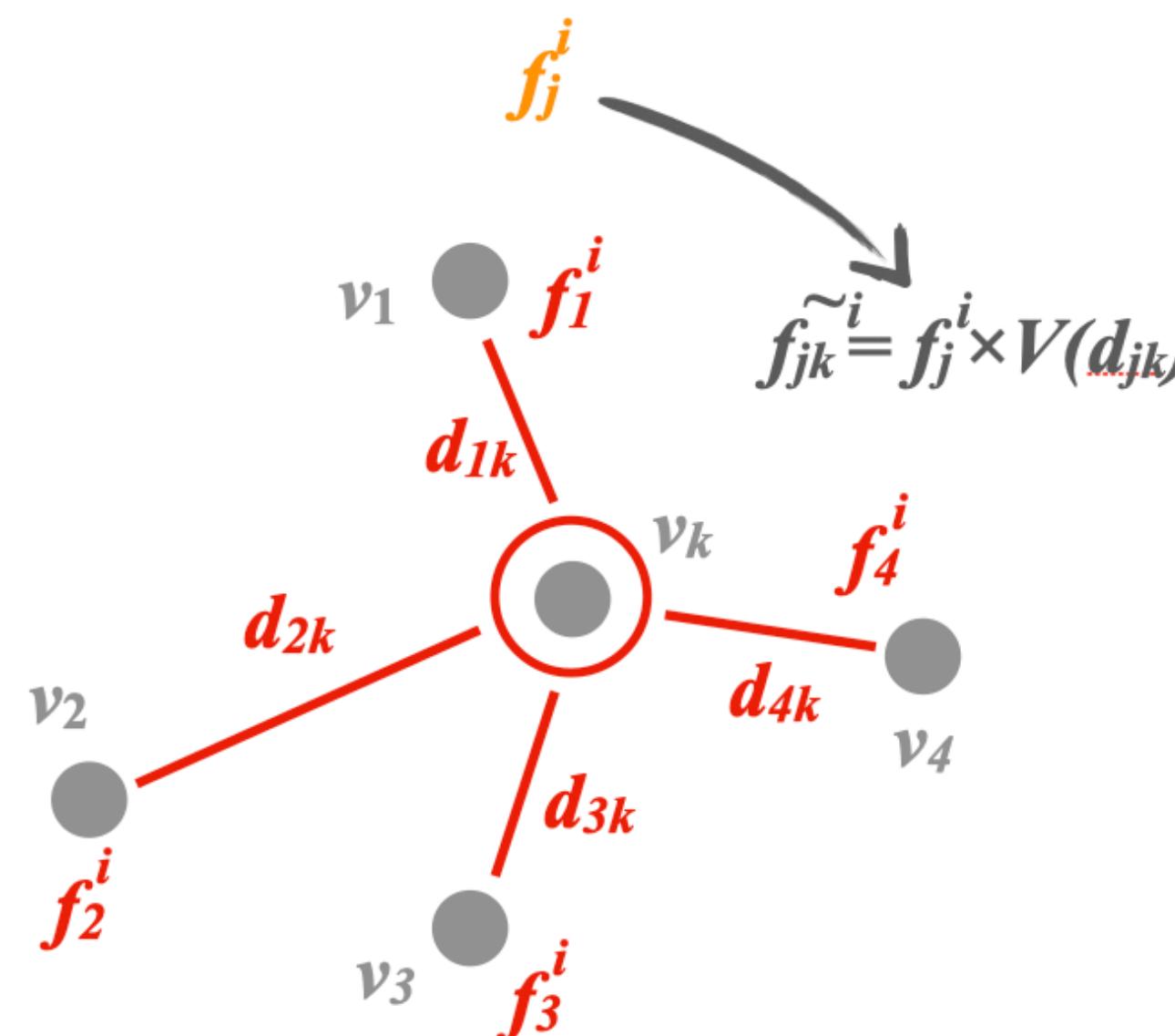




1) Start with a graph in geometric space. Each vertex feature vector F_{IN} is characterized by coordinates and features

2) Each F_{IN} is processed by a linear network, returning two outputs: a coordinate vector s & a learned representation F_{LR}

3) With s and F_{LR} we build the new graph in the learned space

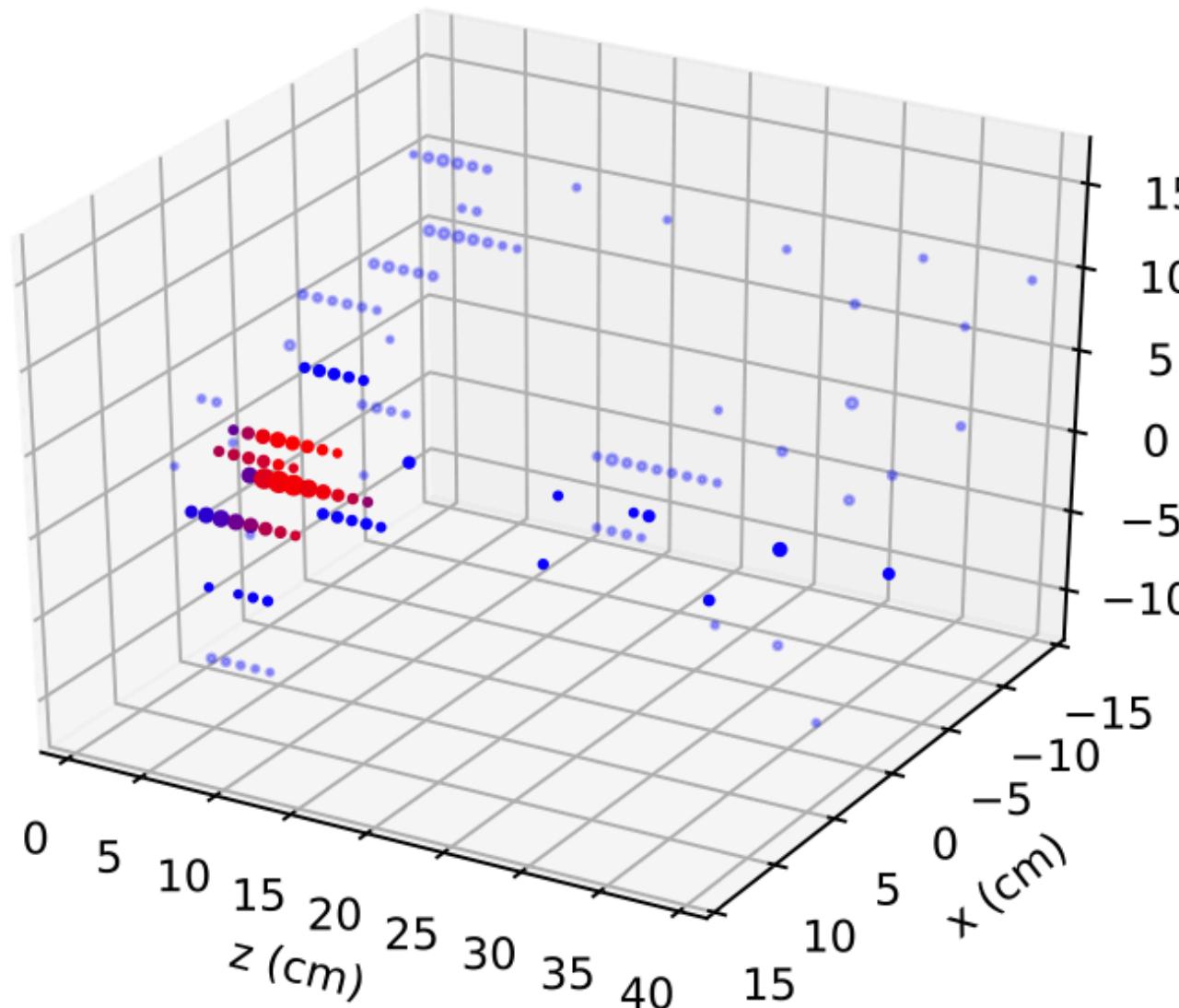


4) Unlike DGCNN,
the message
function is a
potential function
(we use e^{-d^2} where
 d is the Euclidean
distance in
learned space)

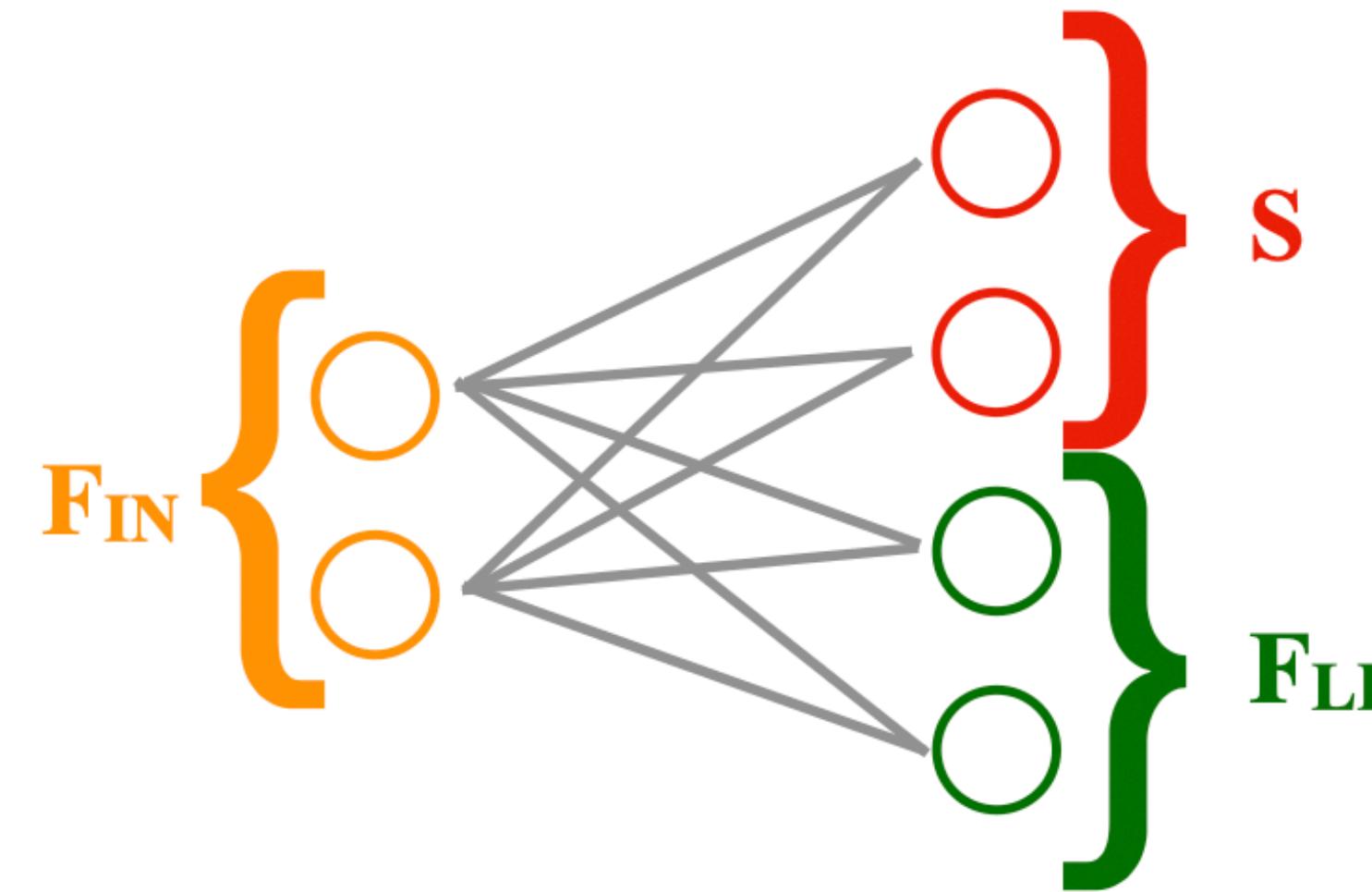
5) Message
aggregated with
different
functions (Max,
Average,...)

6) Final
representation
is learned from
the engineered
features and
the original
ones

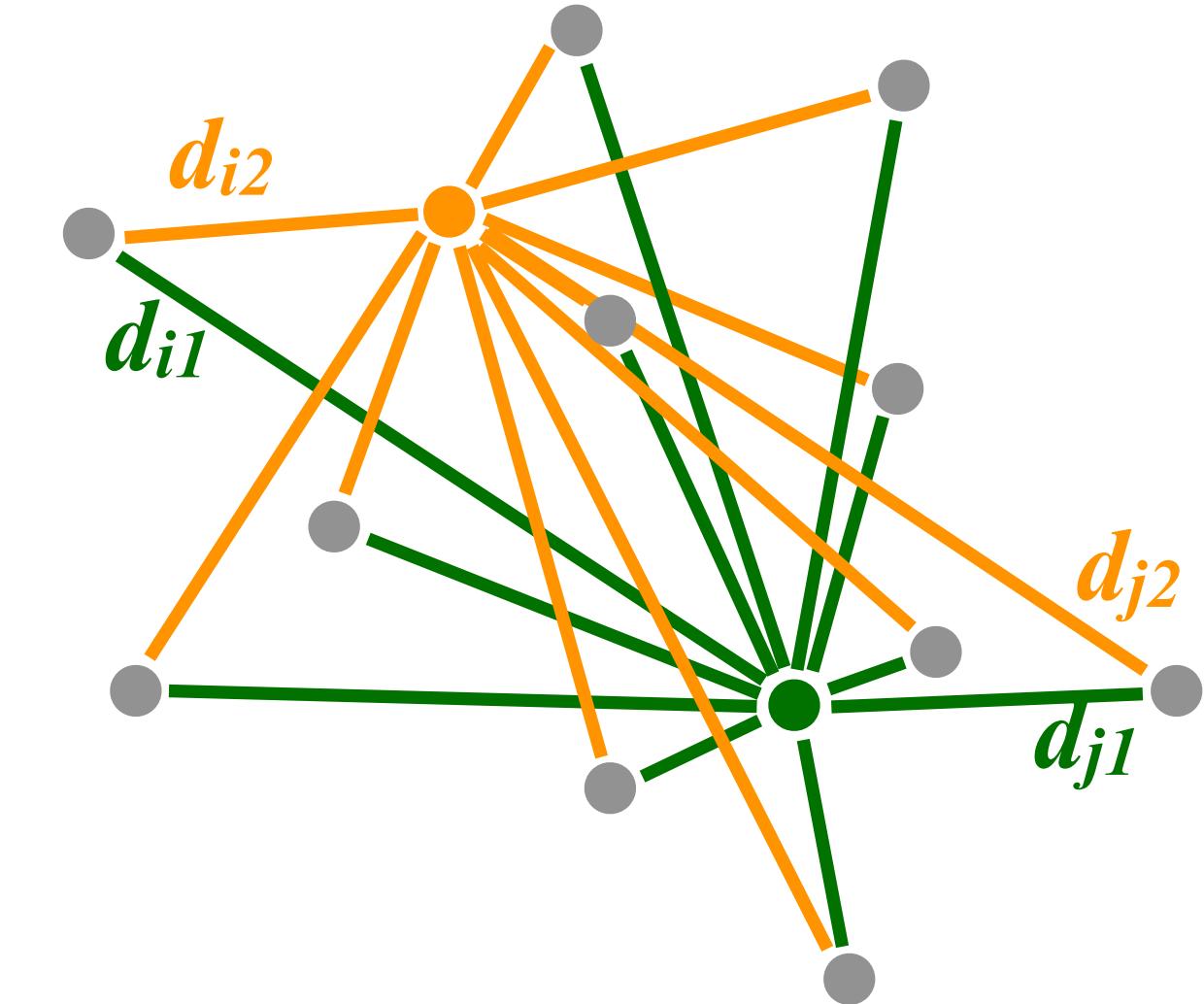
(simplified) Garnet



1) Start with a graph in geometric space. Each vertex feature vector F_{IN} is characterized by coordinates and features



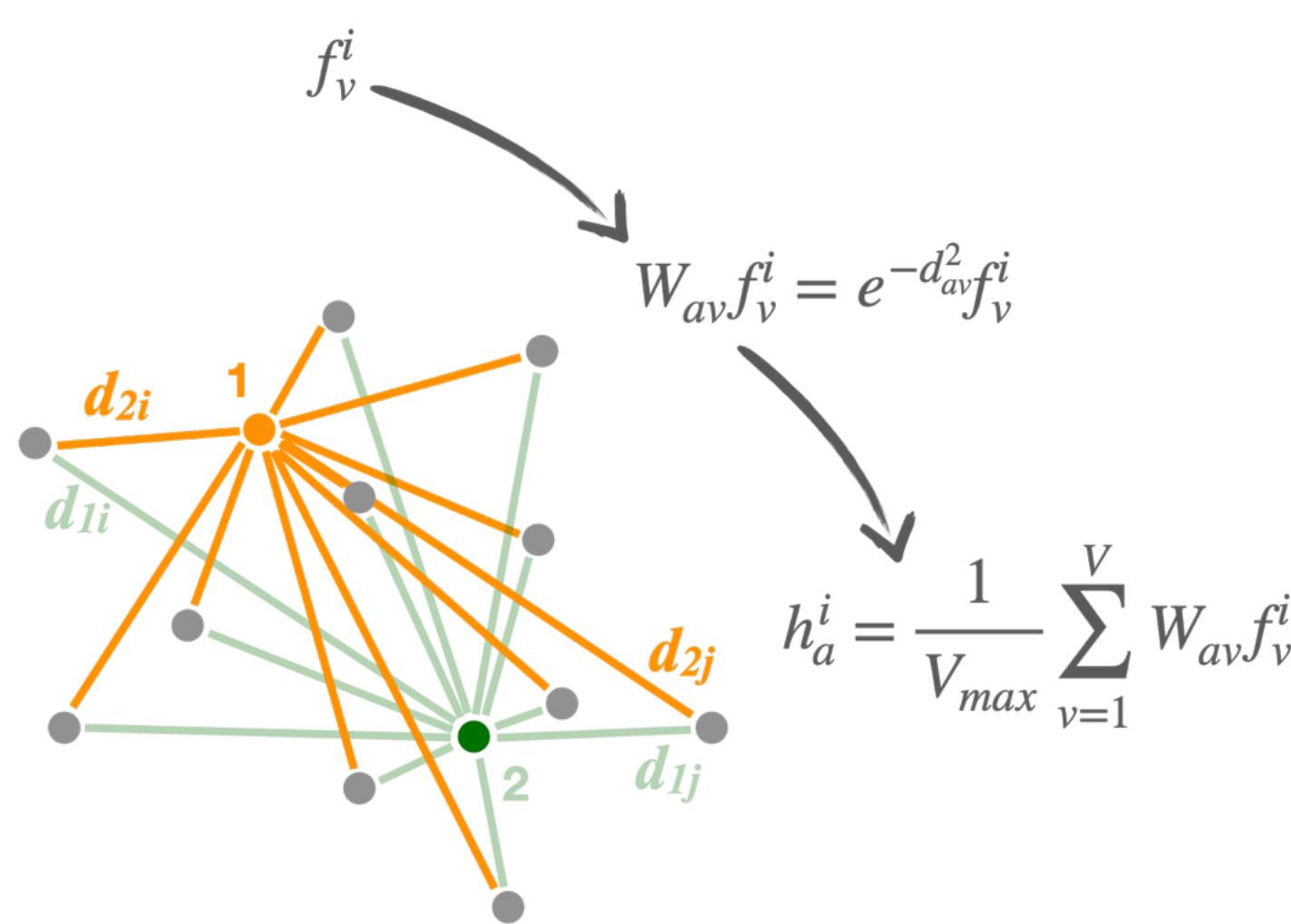
2) Each F_{IN} is processed by a linear network, returning two outputs: a vector of distances s & a learned representation F_{LR}



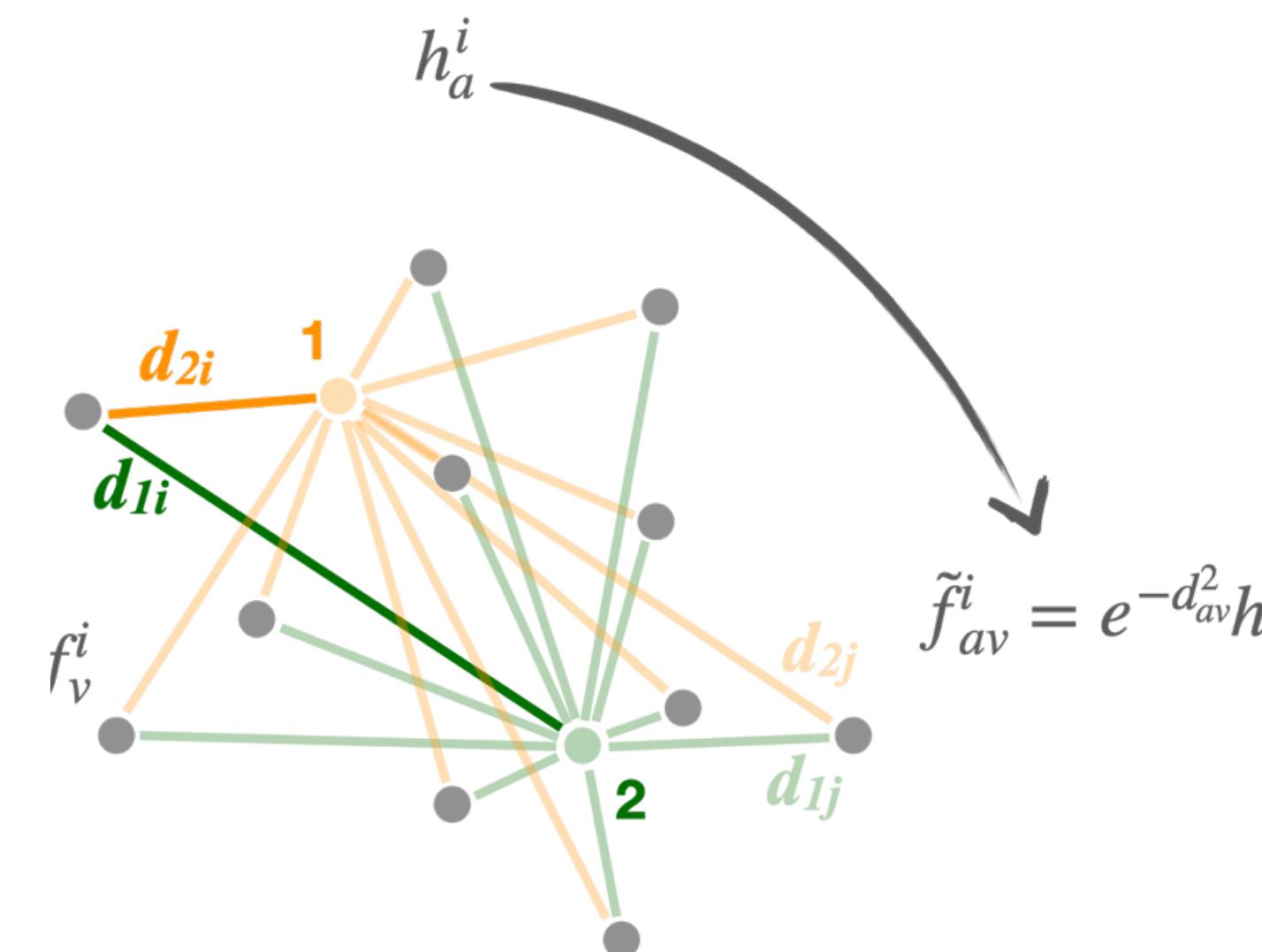
3) s are the distances from N_s aggregators

<https://arxiv.org/abs/1902.07987>

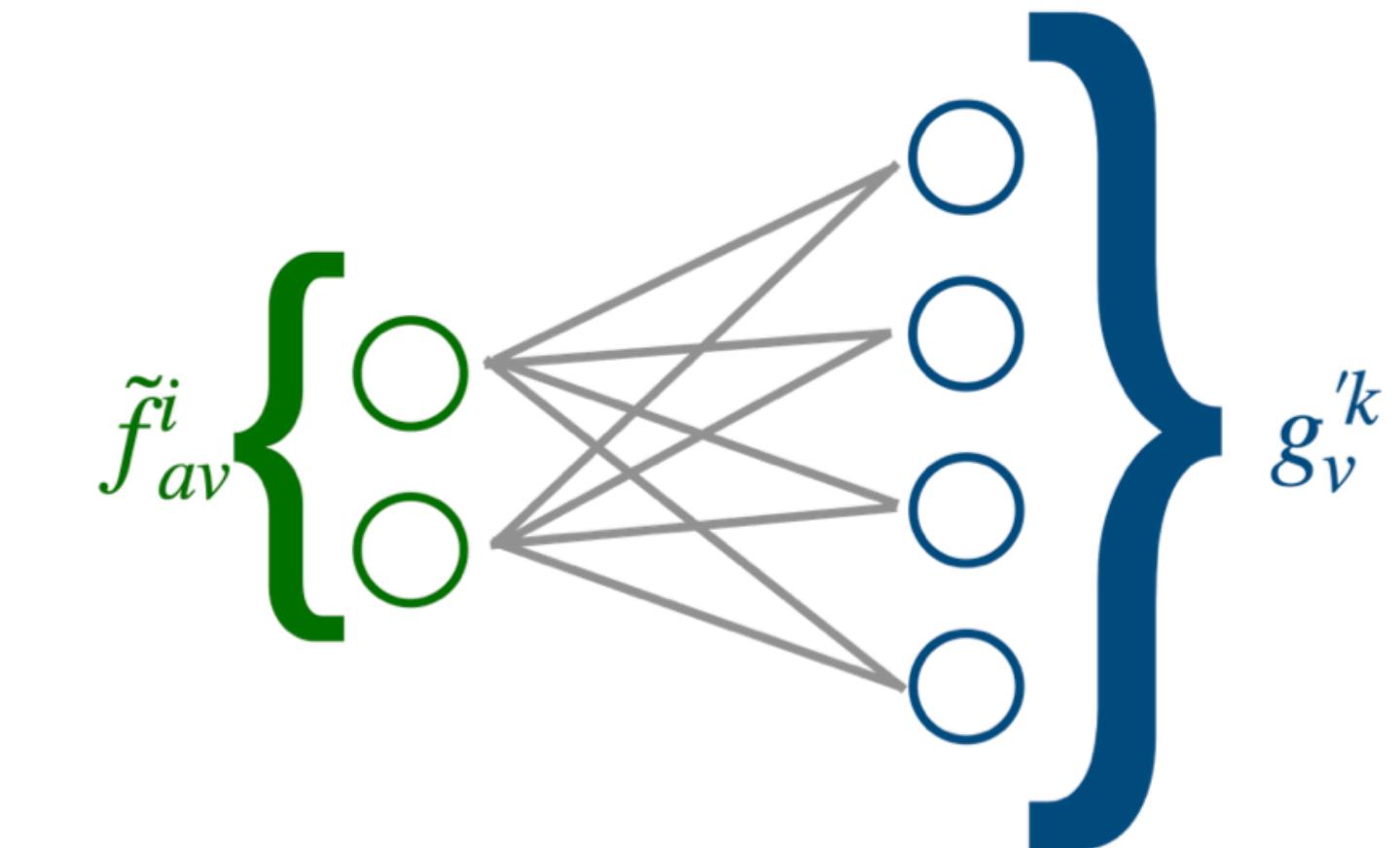
(simplified) Garnet



4) Fwd distance-weighted messages from vertices are gathered at aggregators (weight $W_{ab} = e^{-d_{ab}}$ where d is Euclidean distance in learned space)



5) Bkw distance-weighted messages from aggregators are gathered at vertices (weight $W_{ab} = e^{-d_{ab}}$)

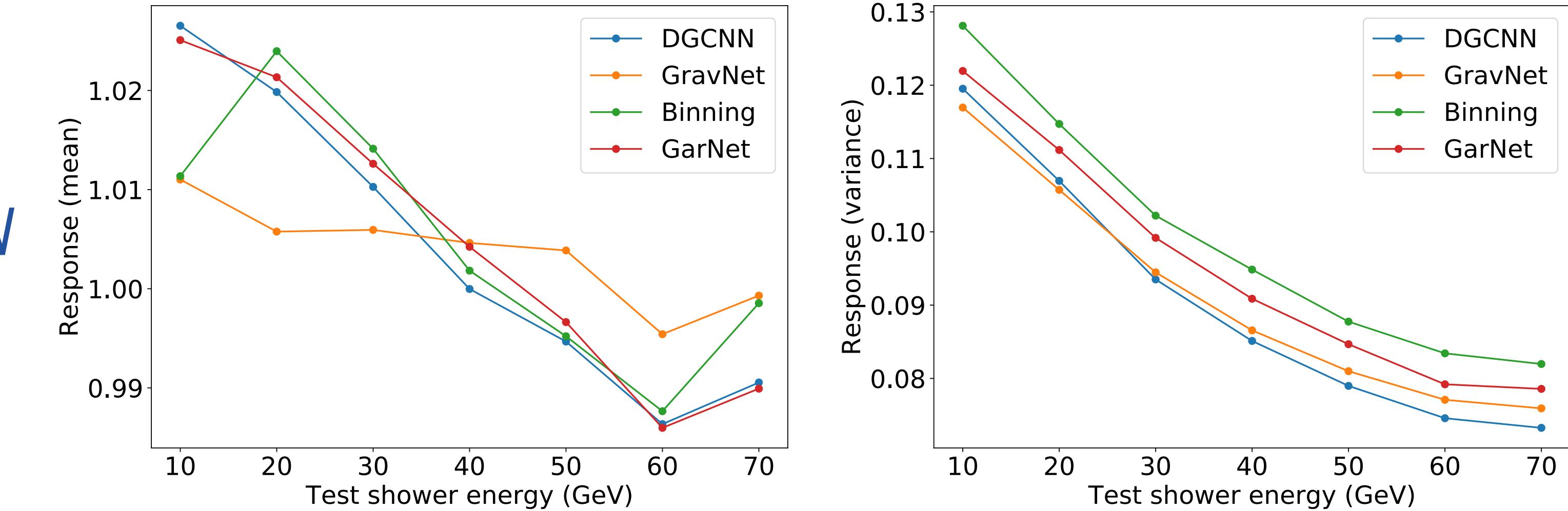


6) Final representation is learned from the engineered features and the original ones

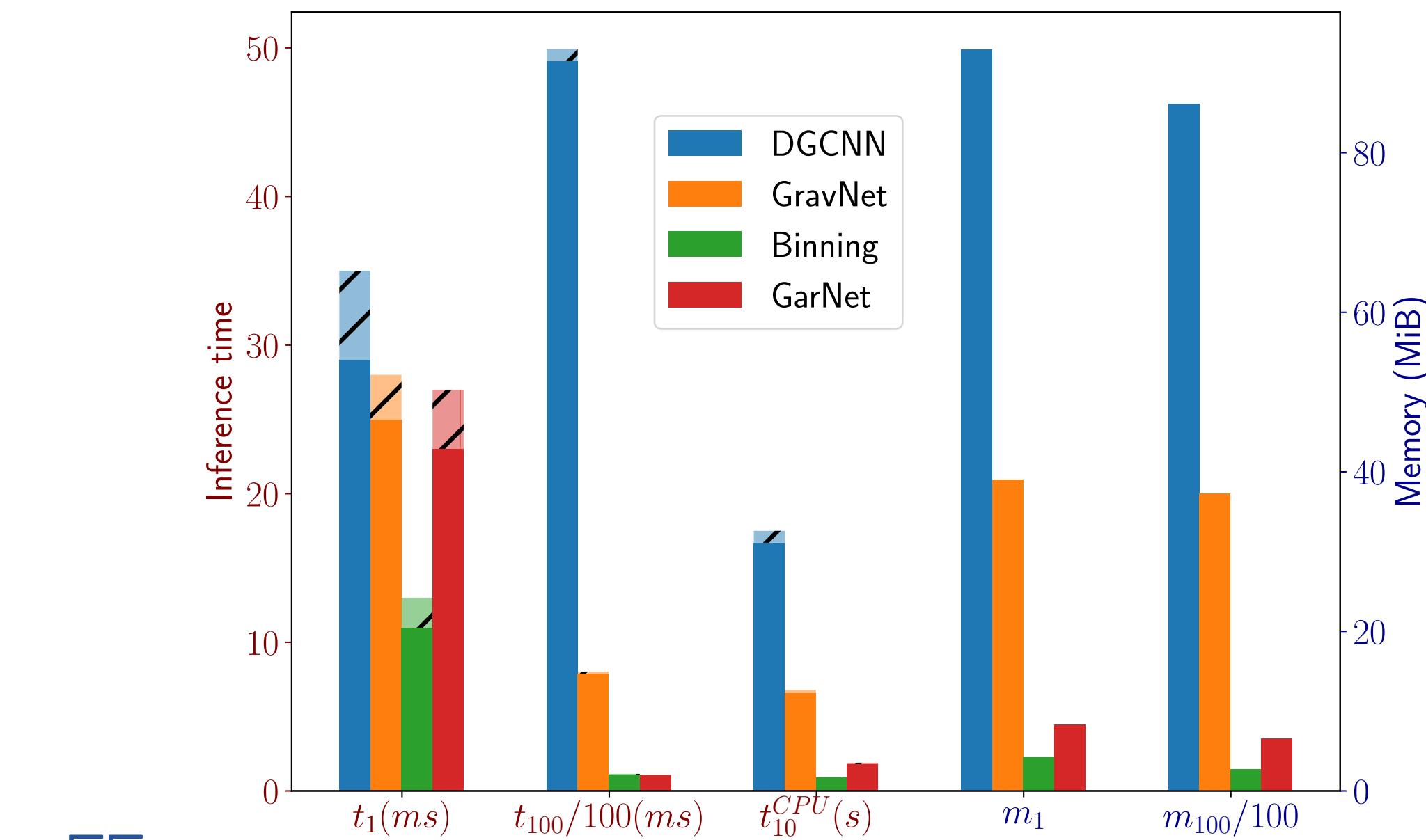
<https://arxiv.org/abs/1902.07987>

Garnet & GravNet for Calorimetry

- Good performance achieved, comparable to DGCNN and traditional approaches



- Using a potential ($V(d)$) to weight up the near neighbours allows to keep memory footprint under control (with respect to other graph approaches)

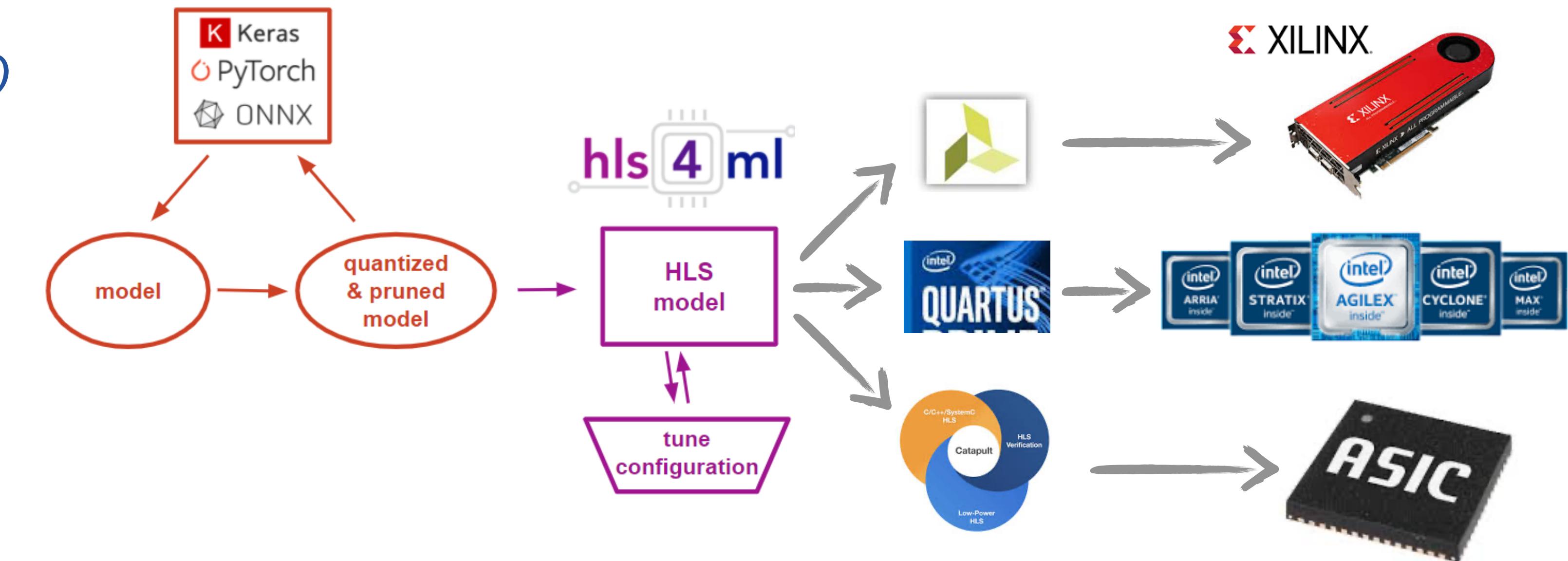


GravNet on FPGA

- GarNet is so light that it can be turned into a logic circuit
- Each (simplified) GarNet layer sums up to simple math, that fits very well what an FPGA can do
- We have a tool ([hls4ml](#)) to automatically turn such a network (and other networks) into a circuit, that can be emulated on FPGA
- Inference goes as fast as 1 μ s

$$g'_v^k = \sum_{a=1}^S W_{av} \left(\sum_{j=1}^{F_{\text{in}}} \tilde{w}_{ja}^k G_a^j + \tilde{b}_a^k L_a \right) + c^k,$$

$$\tilde{w}_{ja}^k = \sum_{i=1}^{F_{\text{LR}}} u_{ia}^k w_j^i, \quad \tilde{b}_a^k = \sum_{i=1}^{F_{\text{LR}}} u_{ia}^k b^i, \quad G_a^j = \frac{1}{V_{\max}} \sum_{v=1}^V W_{av} g_v^j, \text{ and } L_a = \frac{1}{V_{\max}} \sum_{v=1}^V W_{av}.$$

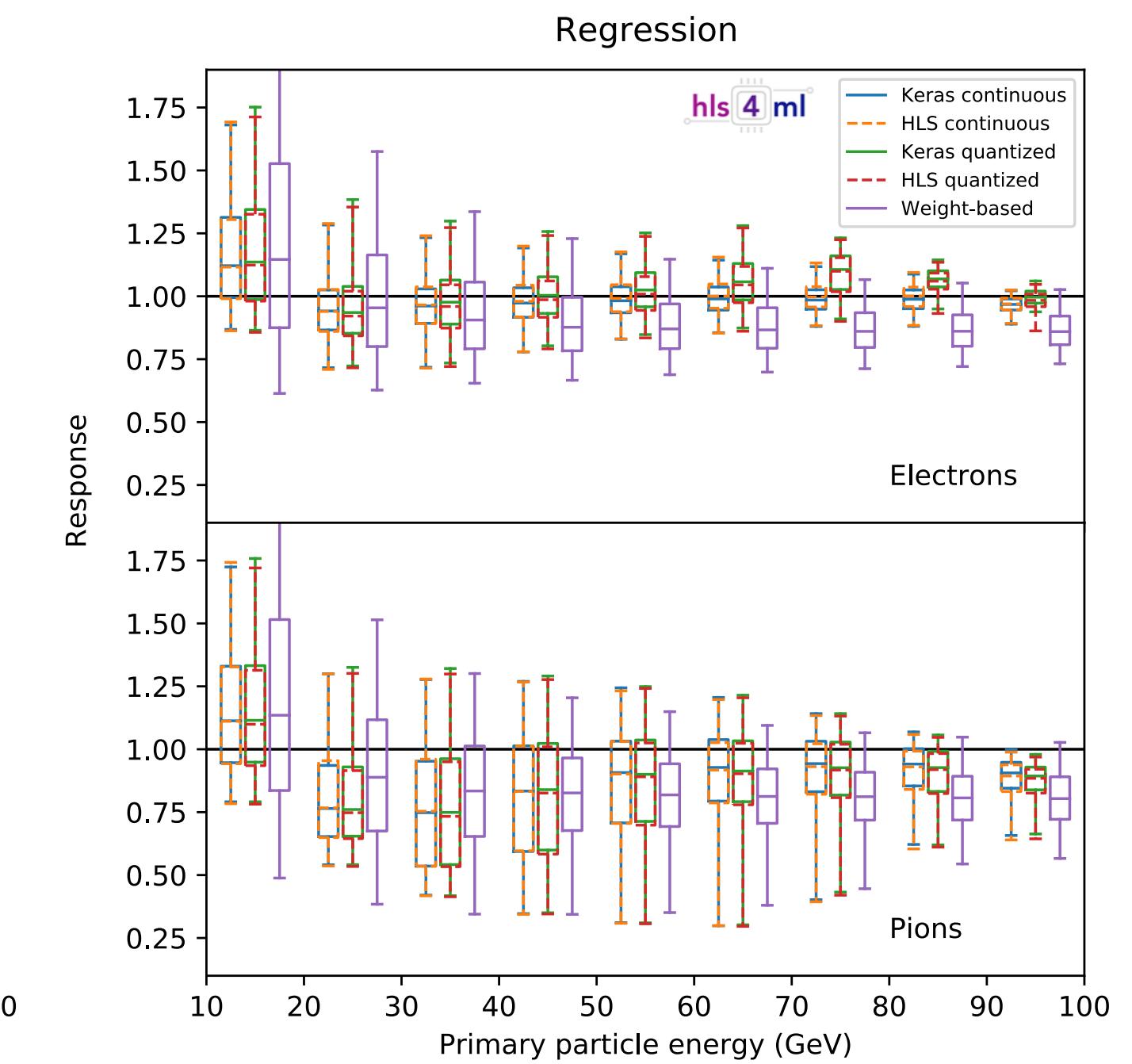
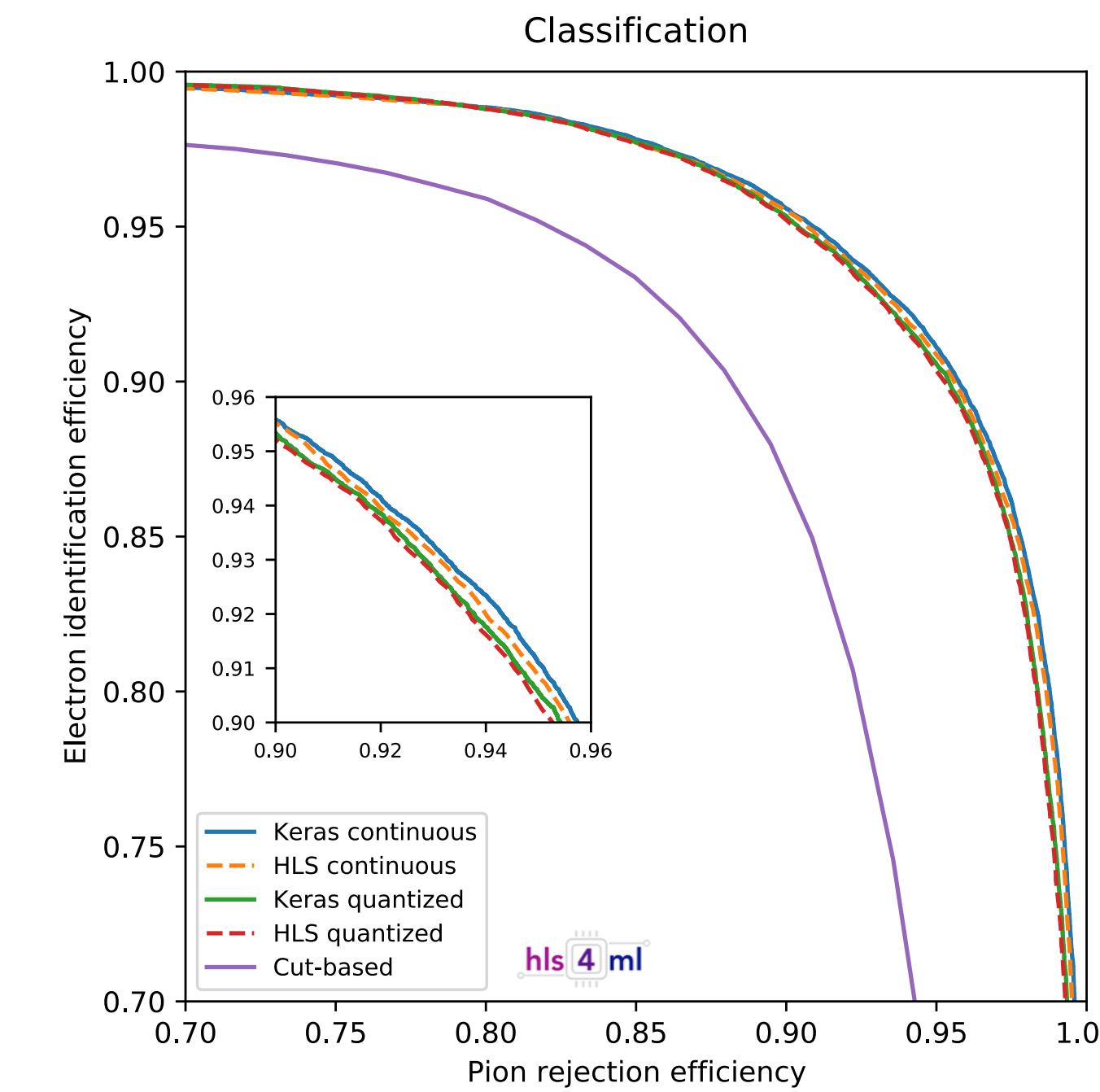


GravNet on FPGA

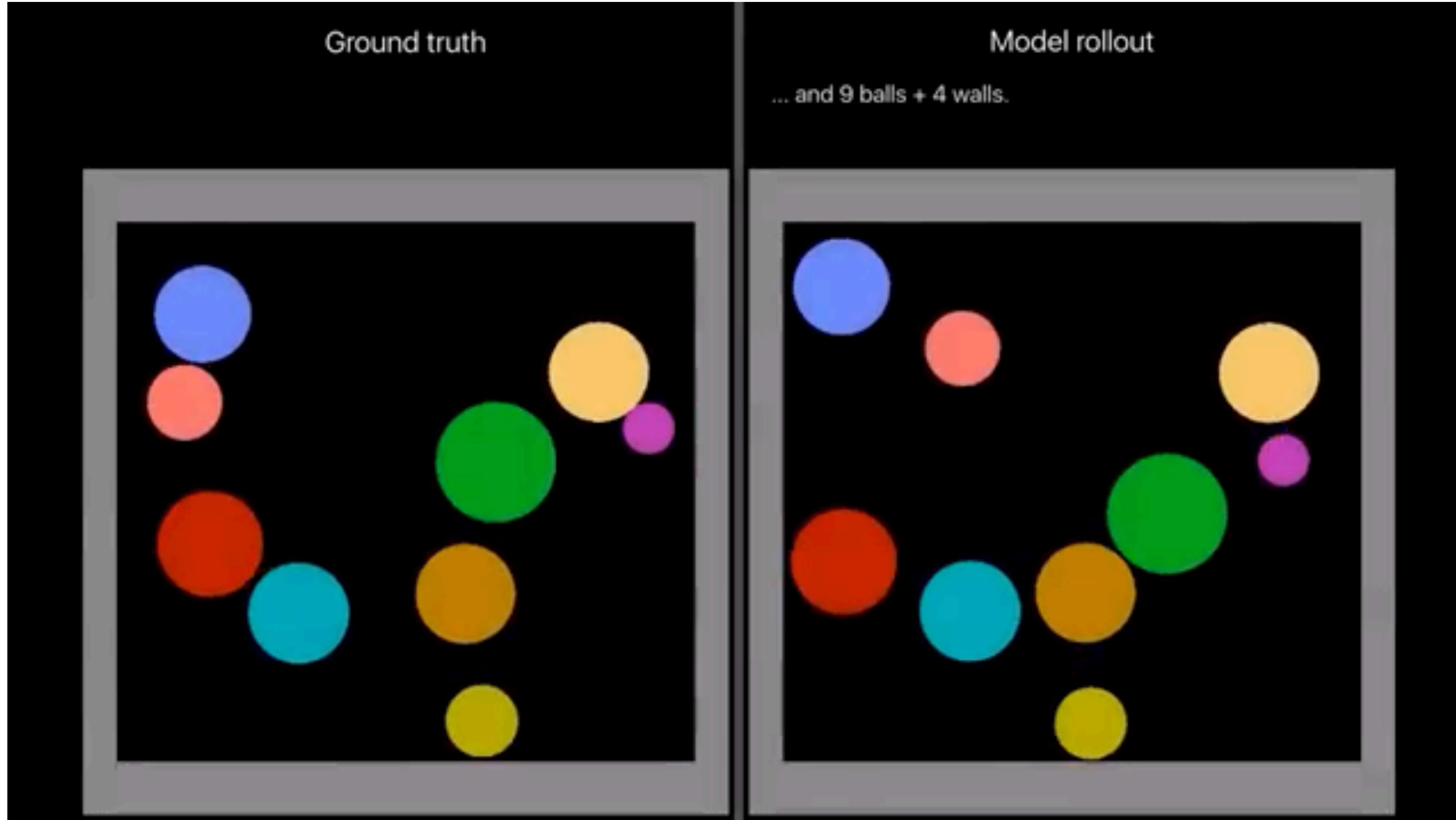
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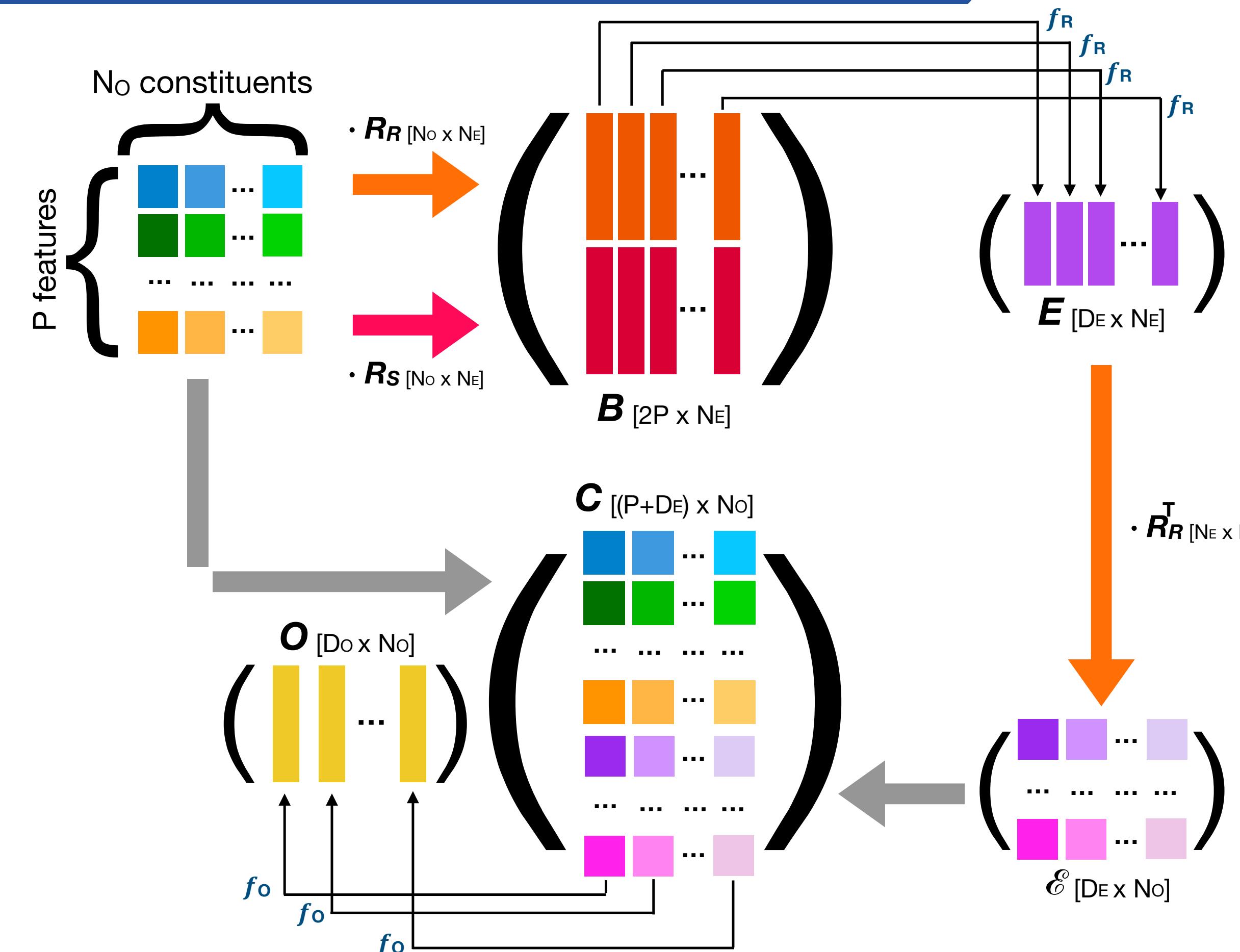
Interaction Networks



<https://arxiv.org/abs/1612.00222>

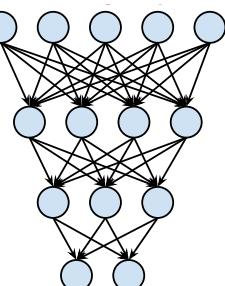
Interaction Networks

- INs process a list of $No \times P$ inputs in pairs, through Receiving and Sending matrices



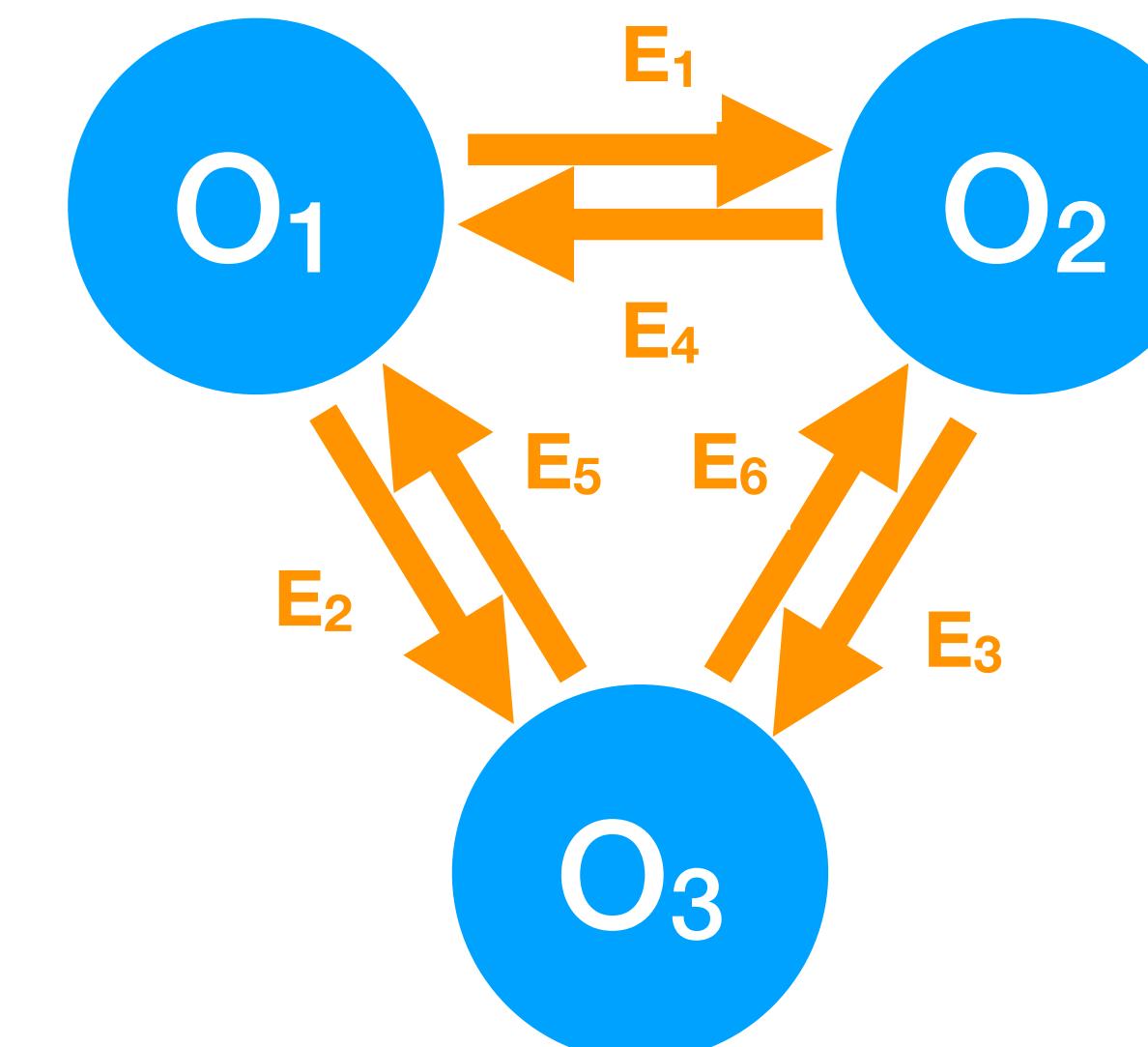
No : # of constituents
 P : # of features
 $N_E = No(No-1)$: # of edges
 D_E : size of internal representations
 D_O : size of post-interaction internal representation

ϕ_C, f_O, f_R
 parameterized as
 neural networks



Interaction Networks

- INs process a list of $No \times P$ inputs in pairs, through Receiving and Sending matrices
- The effect of the interaction is learned by fR and combined with the input to learn (through fo) a post-interaction representation

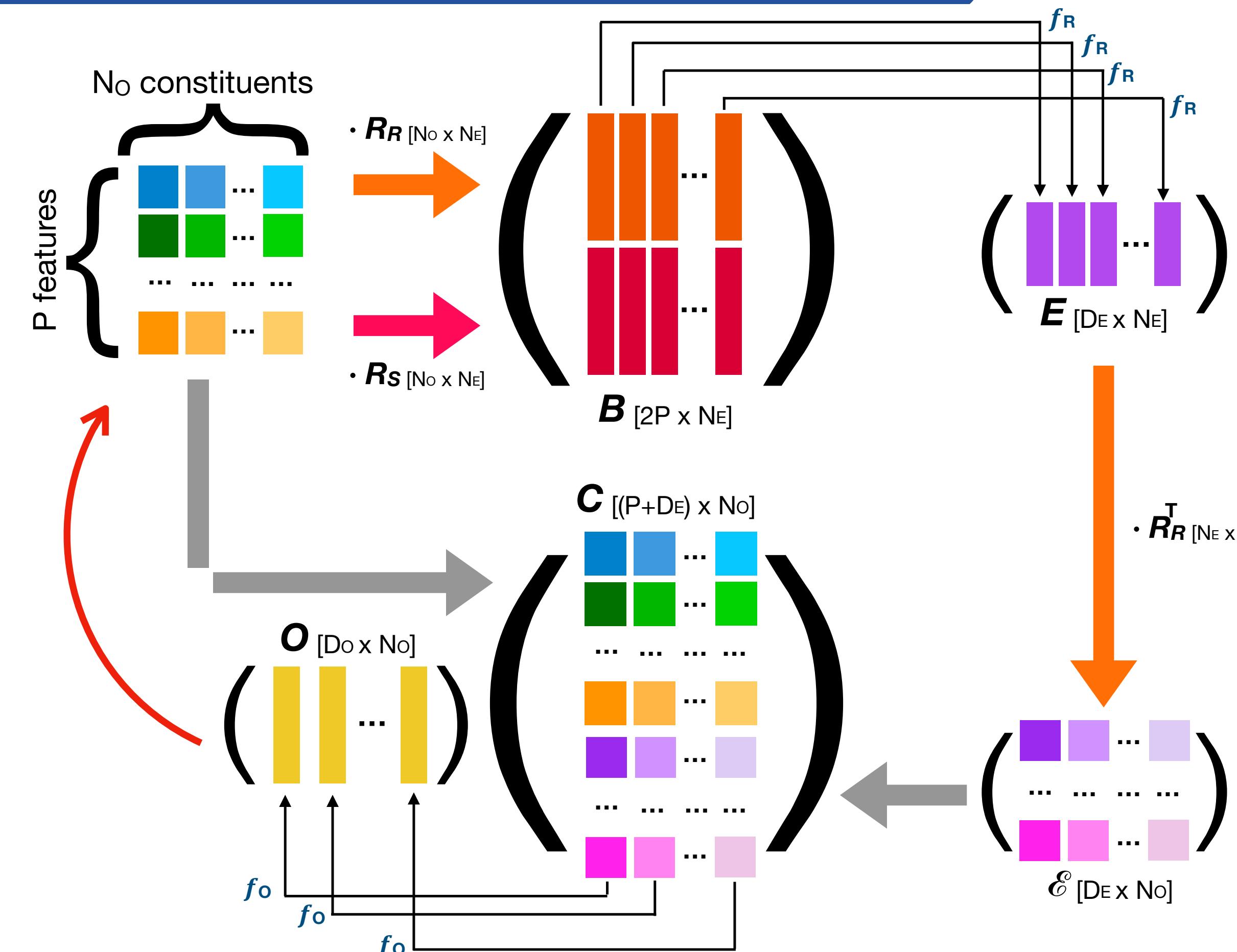


$$R_R = \begin{matrix} & E_1 & E_2 & E_3 & E_4 & E_5 & E_6 \\ O_1 & 0 & 0 & 0 & 1 & 1 & 0 \\ O_2 & 1 & 0 & 0 & 0 & 0 & 1 \\ O_3 & 0 & 1 & 1 & 0 & 0 & 0 \end{matrix}$$

$$R_S = \begin{matrix} & E_1 & E_2 & E_3 & E_4 & E_5 & E_6 \\ O_1 & 1 & 1 & 0 & 0 & 0 & 0 \\ O_2 & 0 & 0 & 1 & 1 & 0 & 0 \\ O_3 & 0 & 0 & 0 & 0 & 1 & 1 \end{matrix}.$$

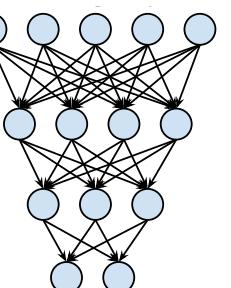
Interaction Networks

- INs process a list of $No \times P$ inputs in pairs, through Receiving and Sending matrices
- The effect of the interaction is learned by f_R and combined with the input to learn (through f_O) a post-interaction representation
- The procedure can then be *iterated* to produce further steps in the interactions



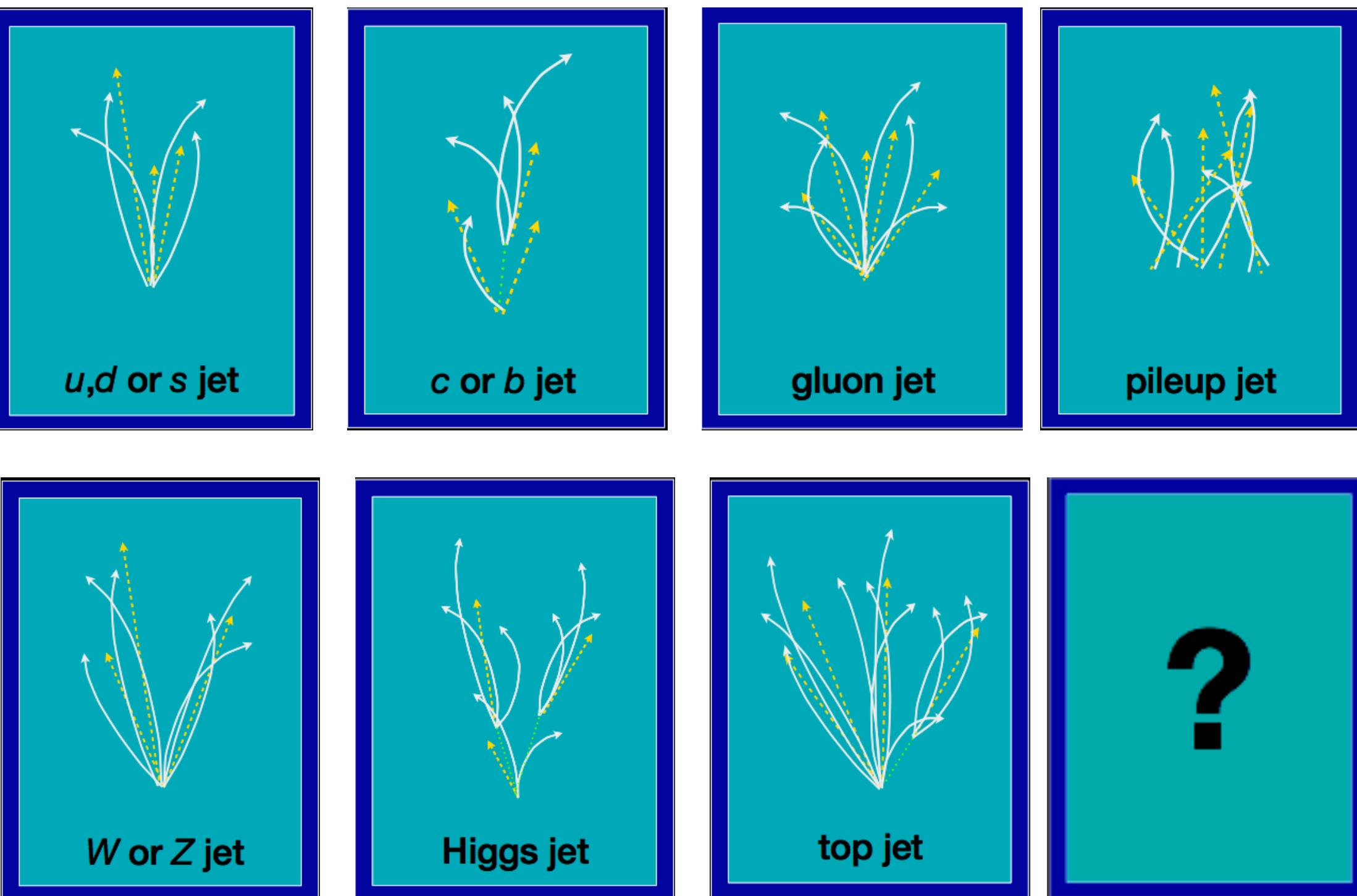
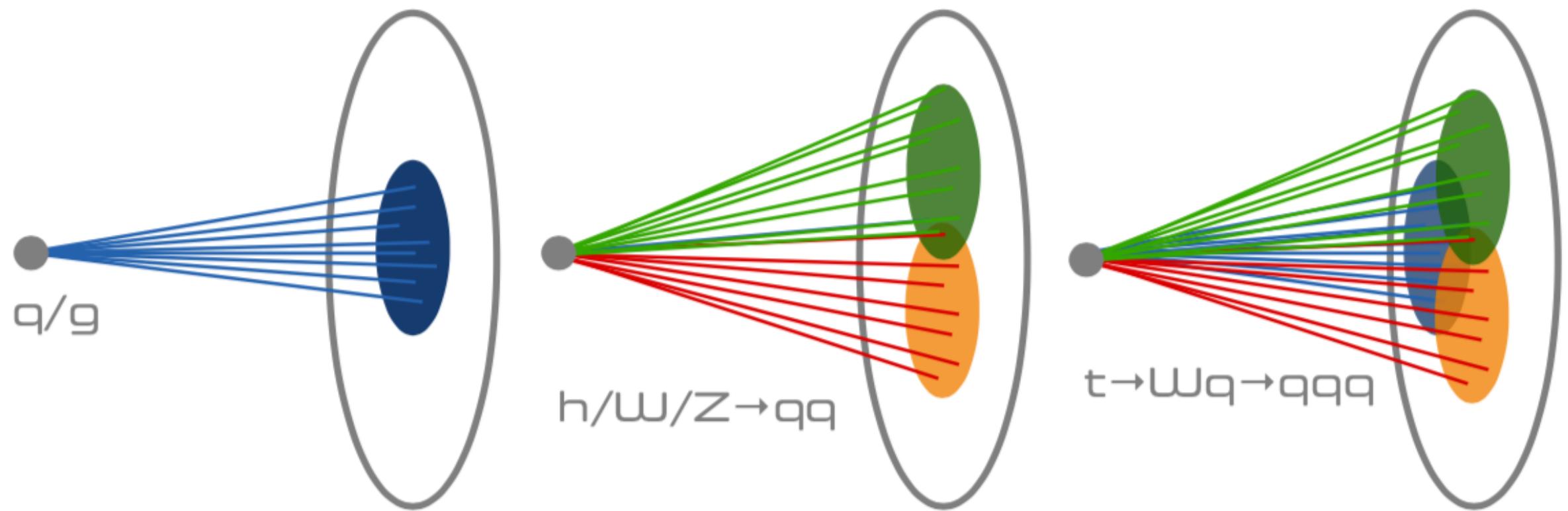
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ϕ_C, f_O, f_R
 parameterized as
 neural networks



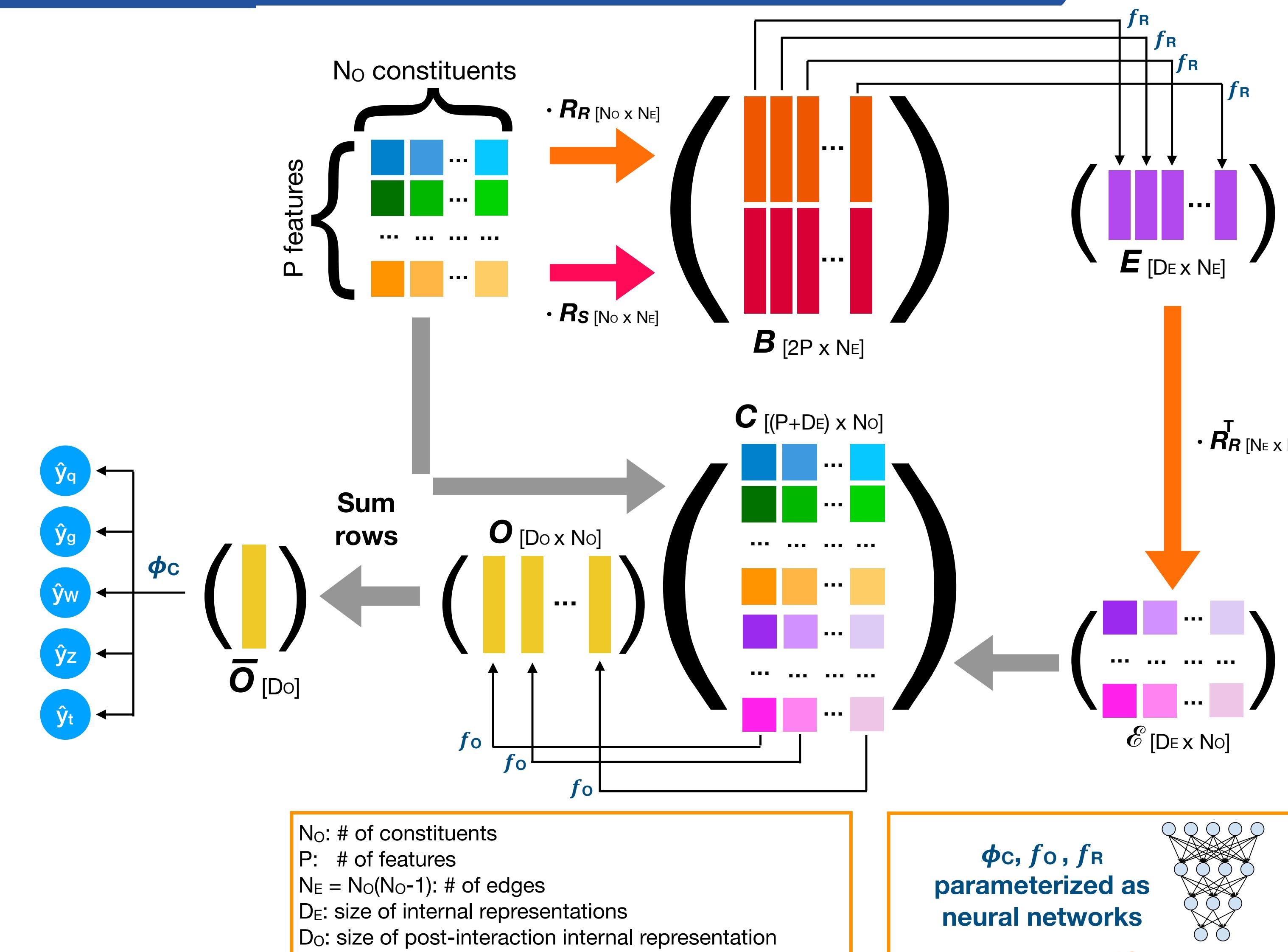
Example: jet tagging

- You have a jet at LHC: spray of hadrons coming from a “shower” initiated by a fundamental particle of some kind (quark, gluon, $W/Z/H$ bosons, top quark)
- You have a set of jet features whose distribution depends on the nature of the initial particle
- You can train a network to start from the values of these quantities and guess the nature of your jet
- To do this you need a sample for which you know the answer

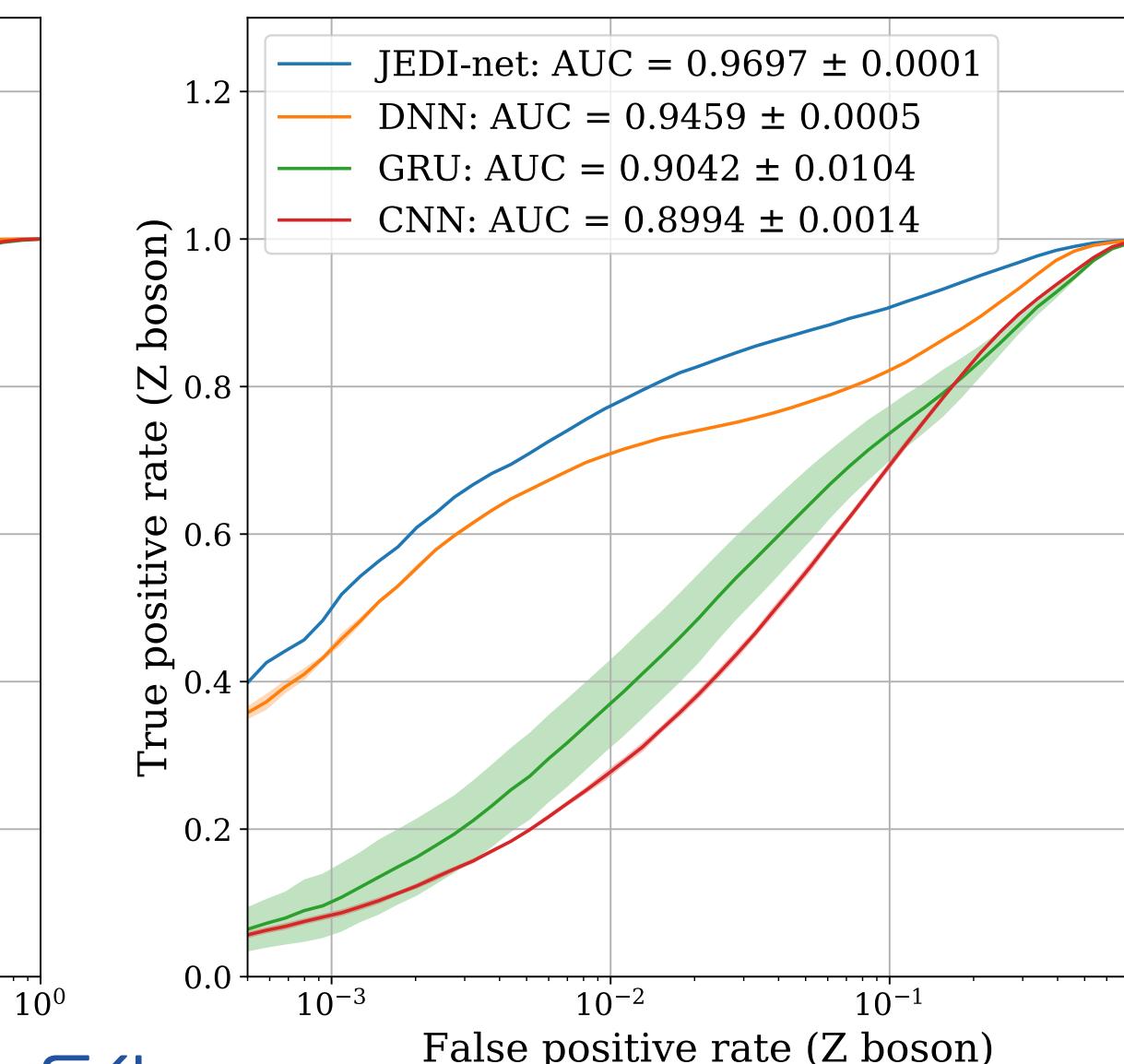
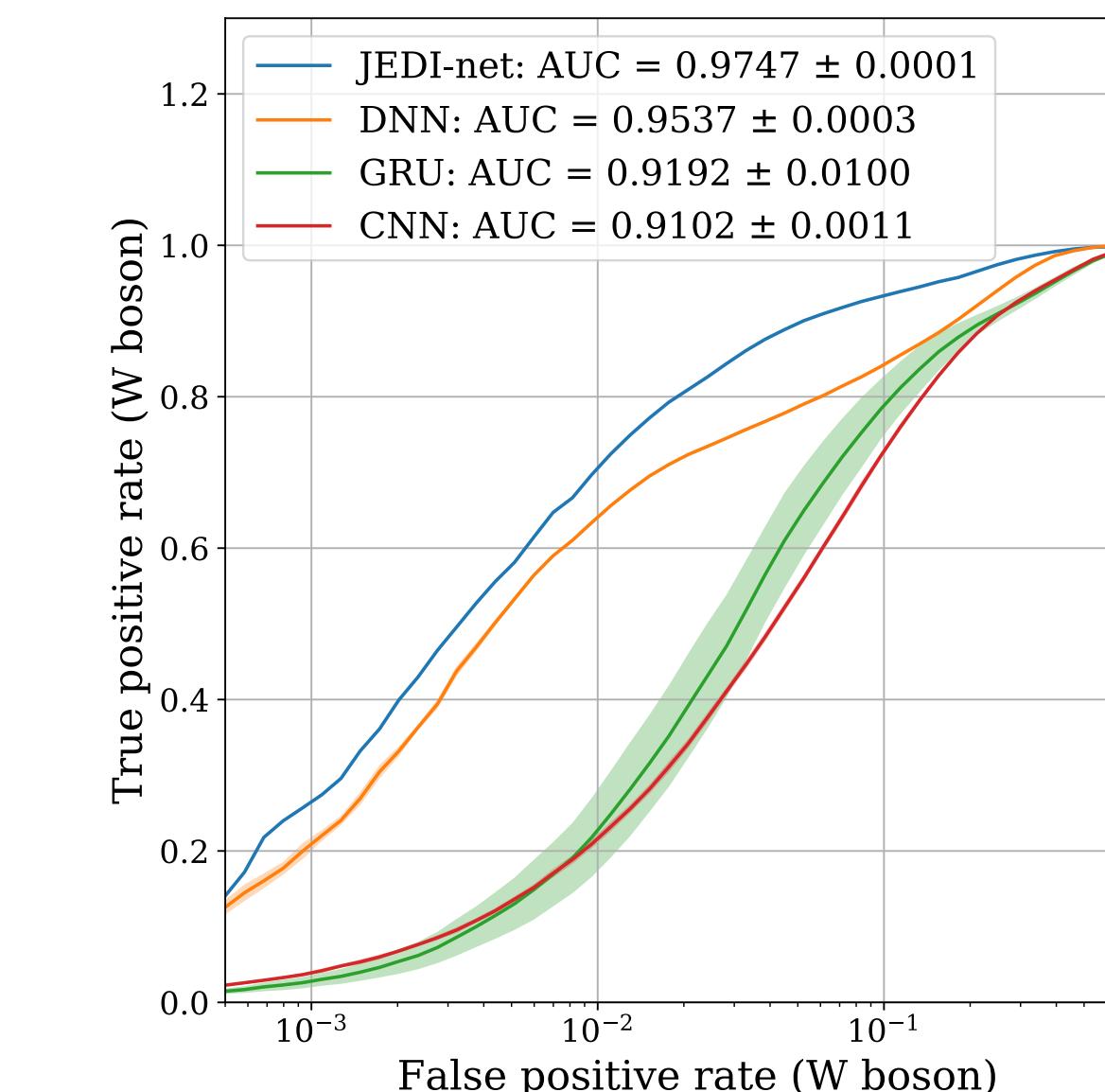
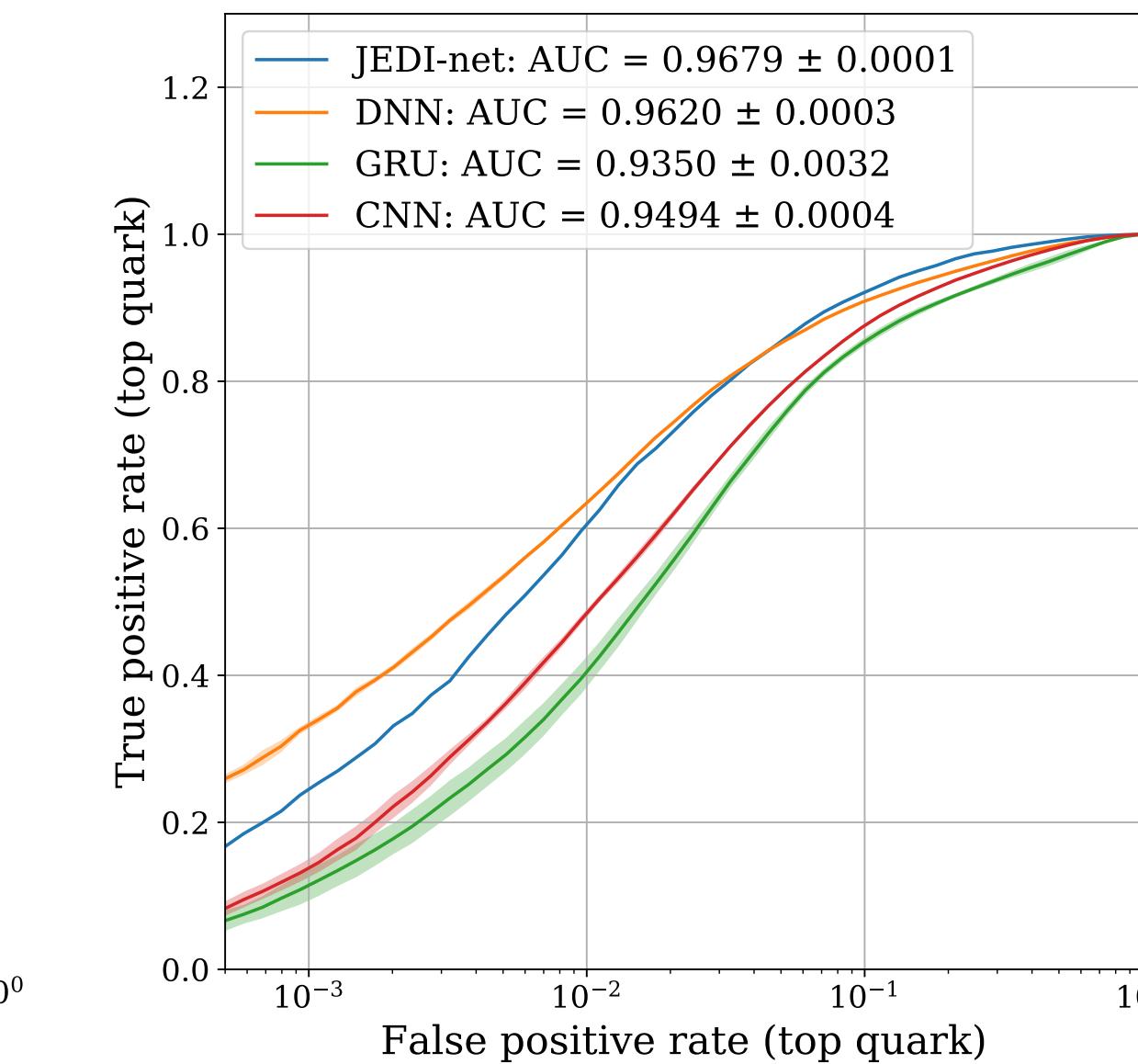
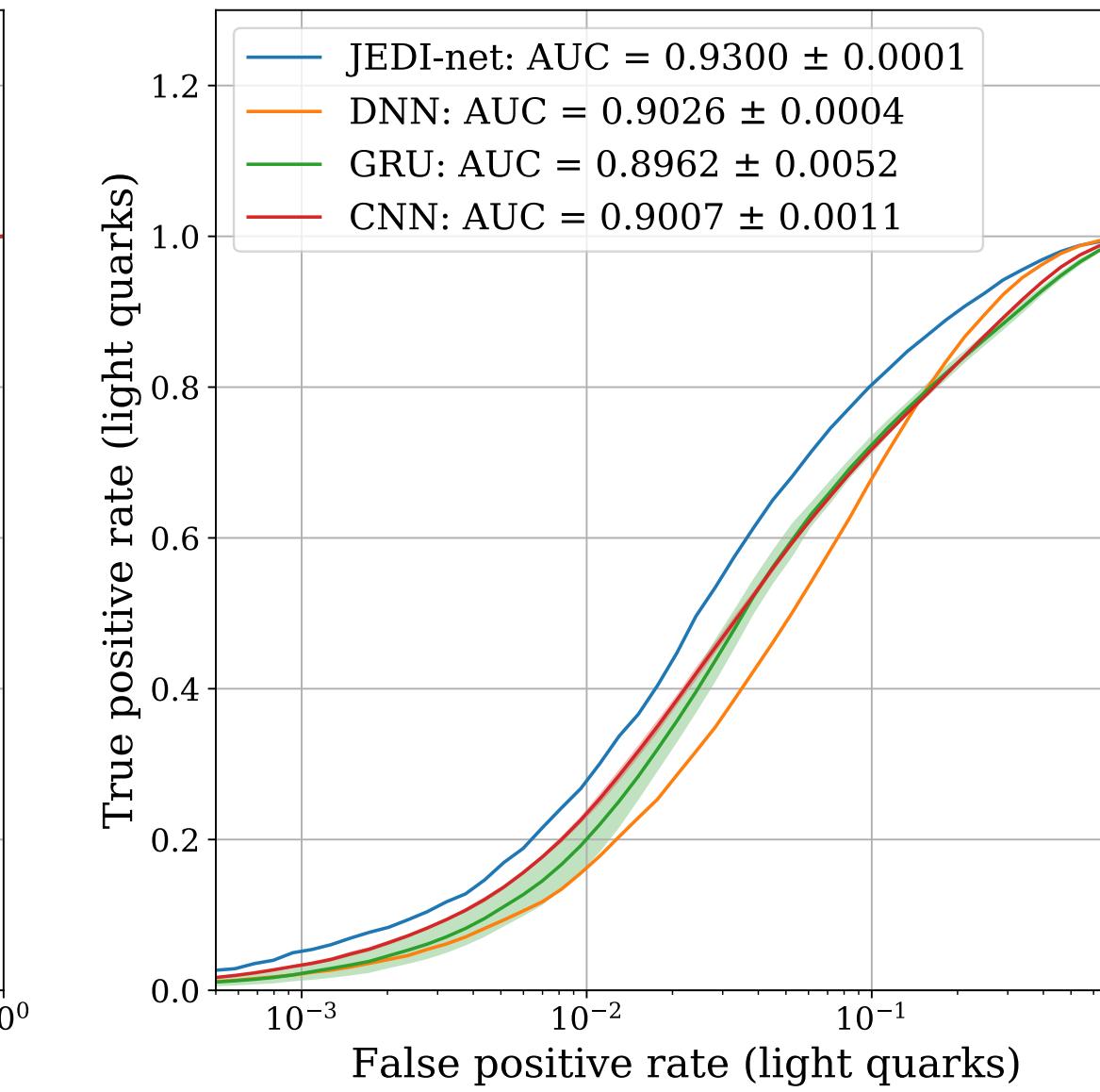
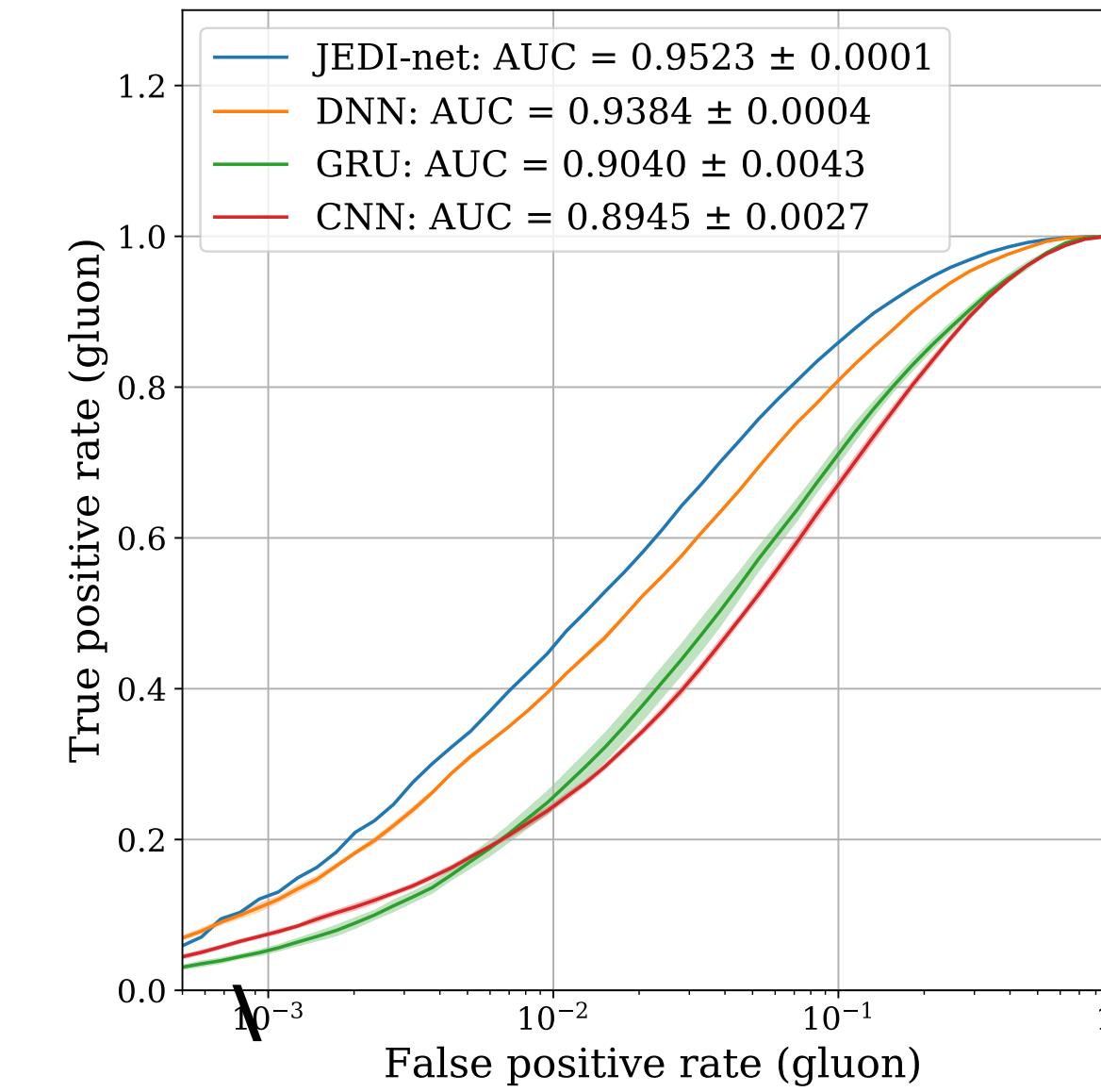


InS for Jet Identification

- In this case, there is no system update needed (i.e., no cycle)
- It is sufficient to use the post-interaction representation as input to a classifier that returns the jet category
- The three networks are simultaneously optimized: the learned representation is chosen to help the classification

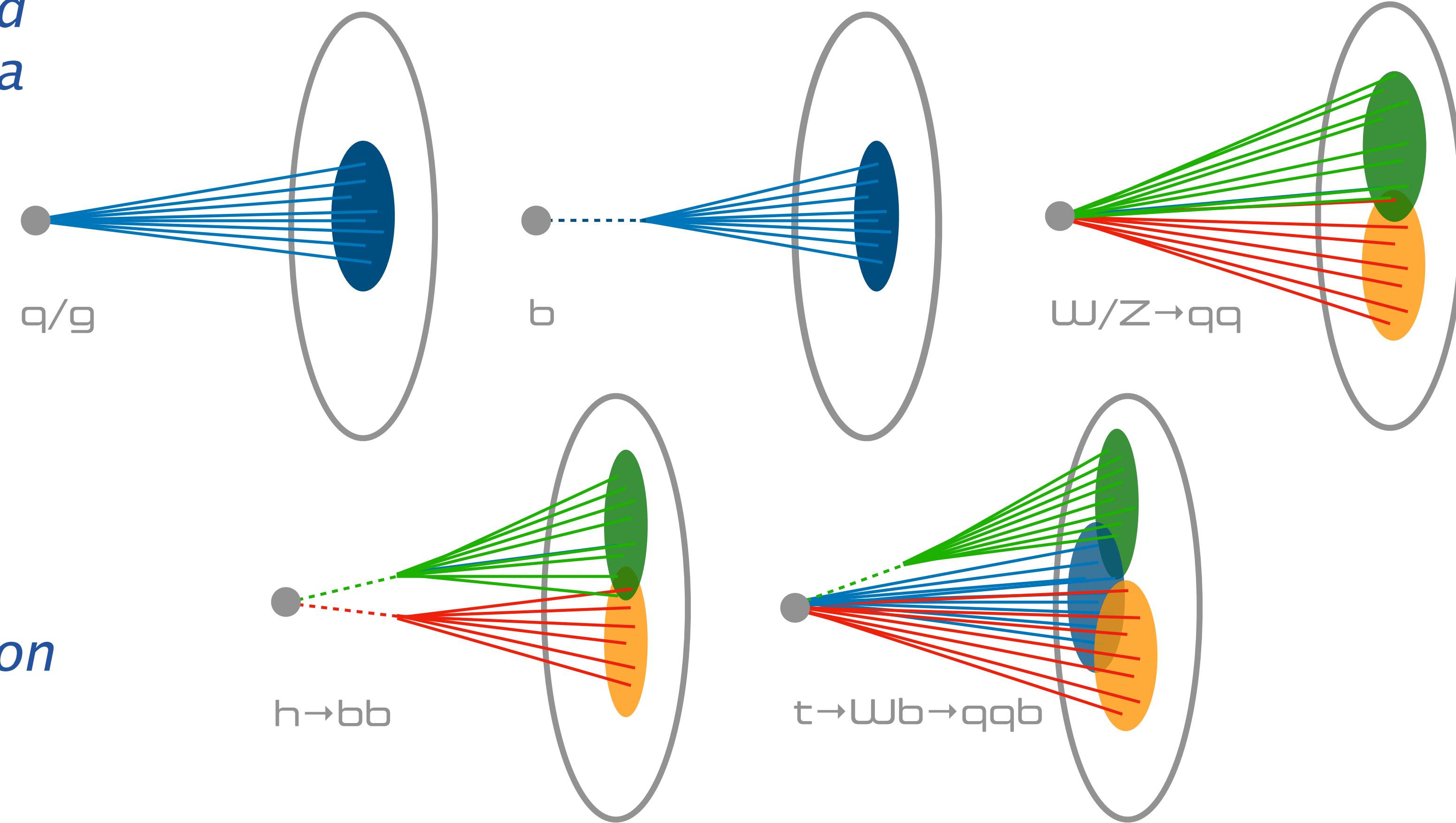


A comparison



Using it for Higgs bosons

- Boosted Higgs bosons are similar to W s and Z s, but have an extra handle
- It decays to b 's, which decay after displacement
- the displaced vertices provide extra discrimination handle
- The flexibility of the grapple setup allows to add this easily

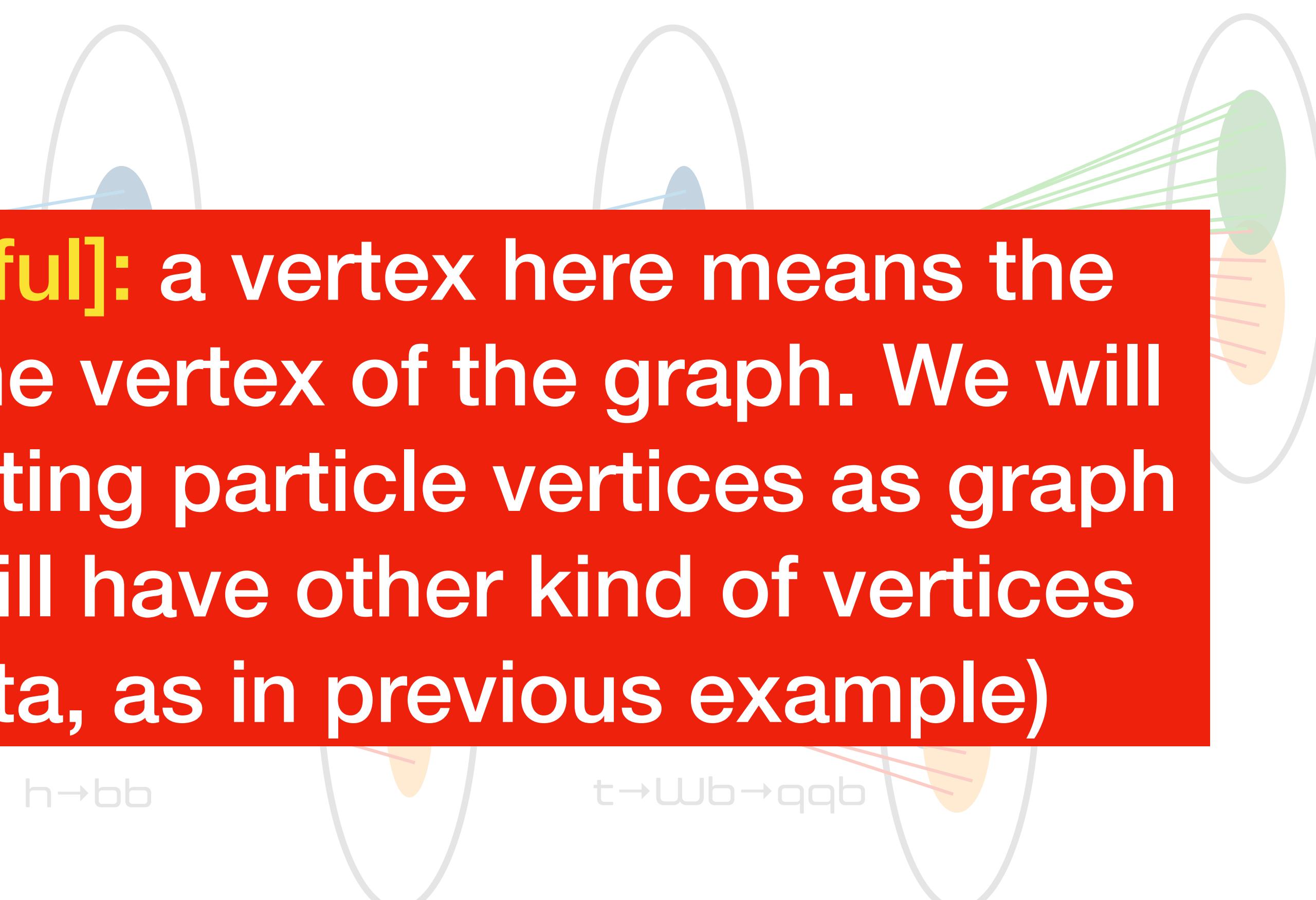


Using it for Higgs bosons

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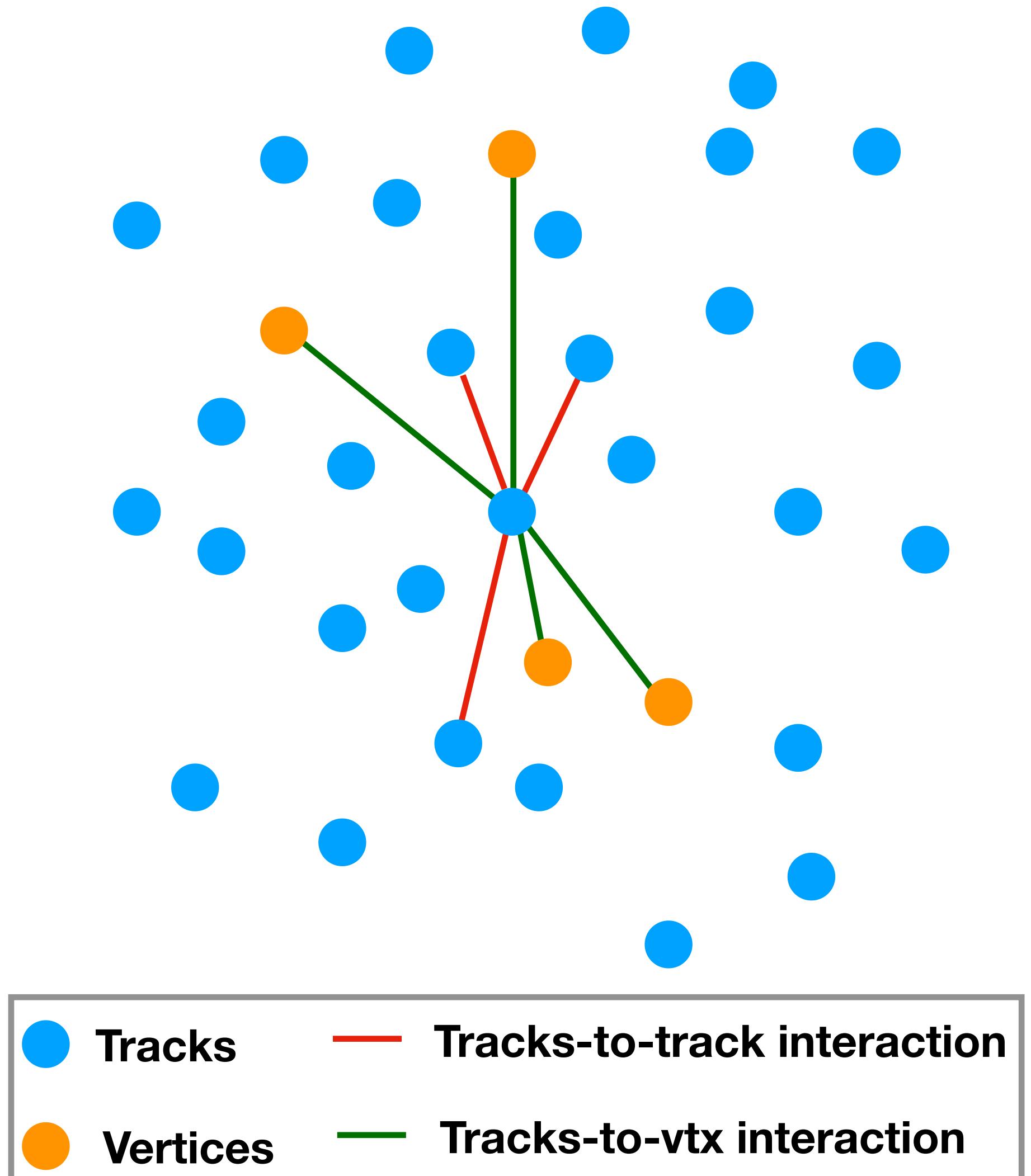
Naming Clash [be careful]: a vertex here means the origin of particles, not the vertex of the graph. We will build the graph representing particle vertices as graph vertex. But the graph will have other kind of vertices (e.g., particle momenta, as in previous example)

- handle
- The flexibility of the grapnel setup allows to add this easily

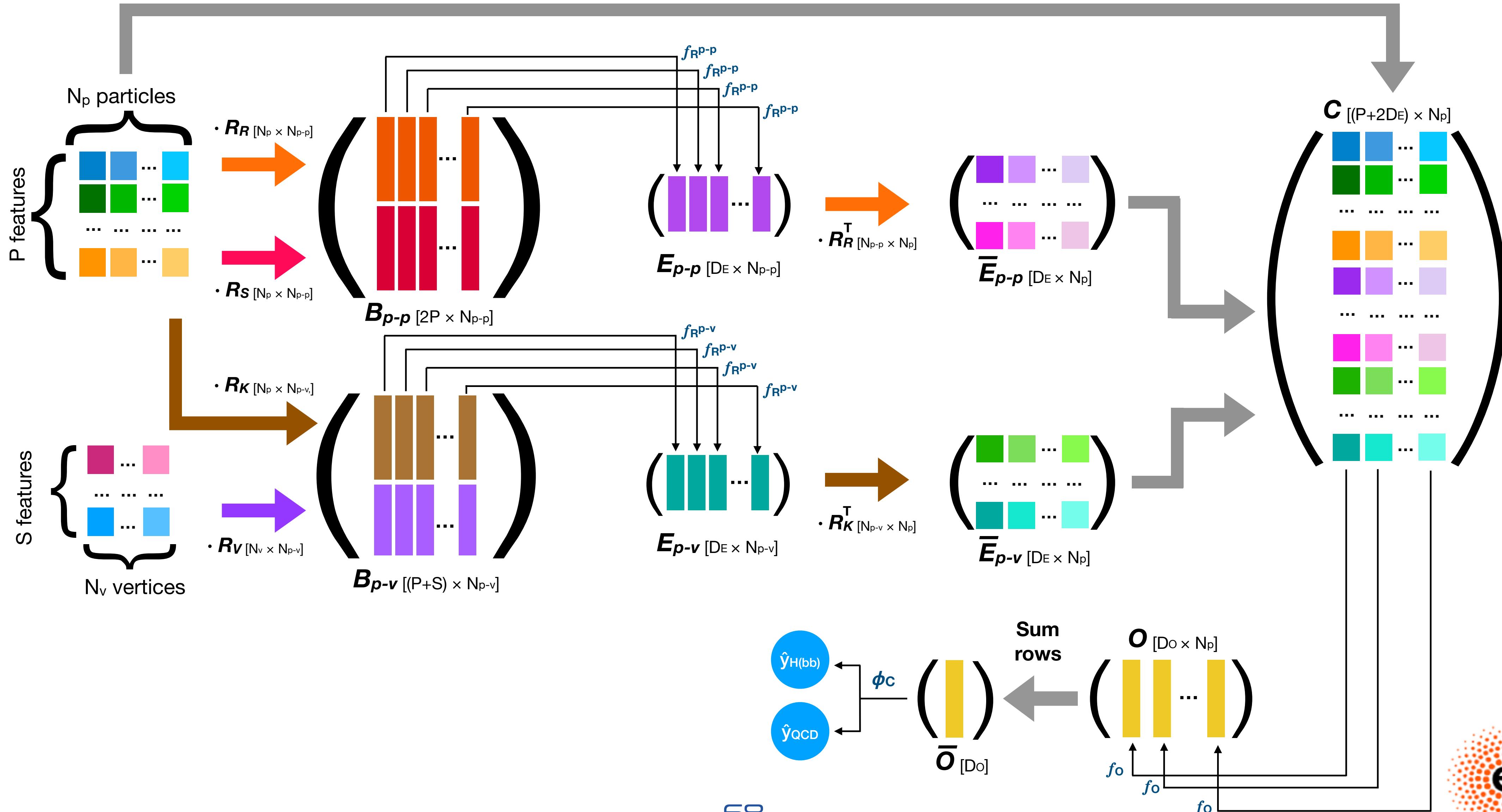


Adding vertices

- Boosted Higgs bosons are similar to W s and Z s, but have an extra handle
- It decays to b 's, which decay after displacement
- the displaced vertices provide extra discrimination handle
- The flexibility of the grapnel setup allows to add this easily

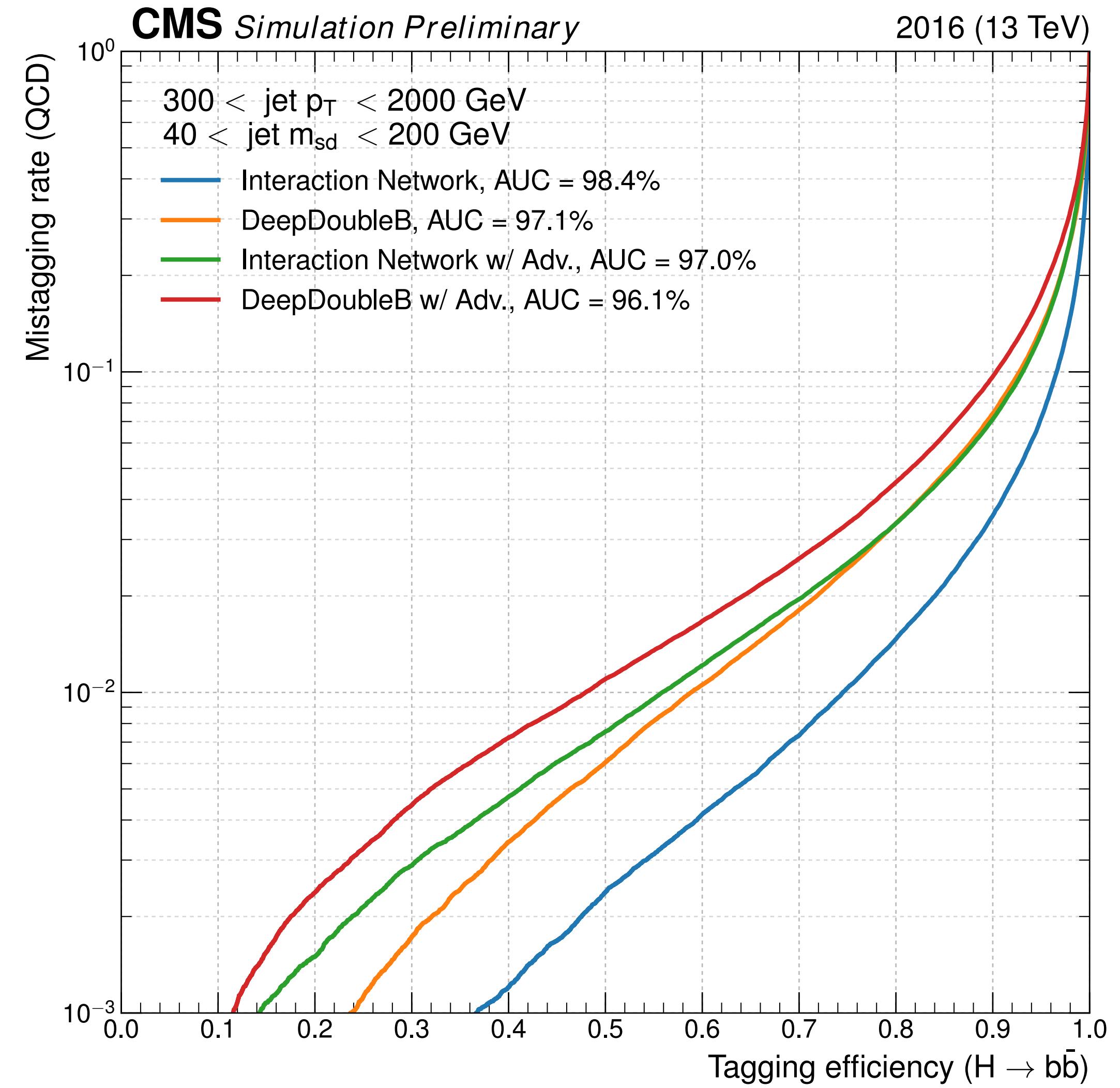


Adding vertices



Higgs boson tagging

- Algorithm trained on CMS simulation from 2016
- Performance compared to the algorithm used in CMS
 - RNN-based tagger exploiting also neutral particles
 - INs outperform the RNN algorithm despite using less information
 - Relying only on tracks make the algorithm even more robust (less dependence on pileup)
- Just one example of how GraphNets could become relevant for next runs



Summary

- *Graph Networks are a powerful tool to learn from sparse data sets*
- *extend CNN concept beyond the case of geometrical proximity -> learned representation*
- *allow to abstract from irregular geometry (molecules, particle-physics detectors, stars in a galaxy, ...)*
- *allow to inject domain knowledge in the game (e.g., enforcing physics rules for message-passing functions [Newton's law in N-body simulation])*
- *But can also be used to learn (how to simulate) physics*