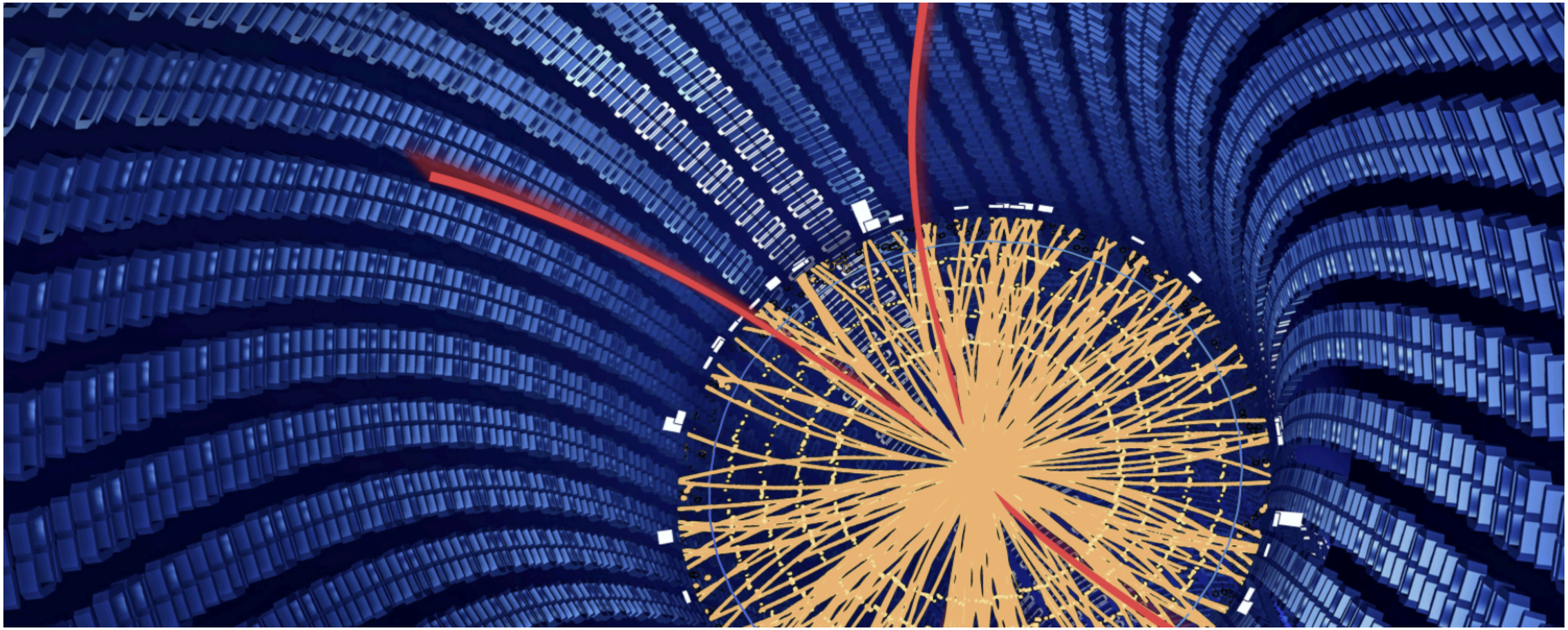
Graph Neural Networks

Maurizio Pierini

Outline

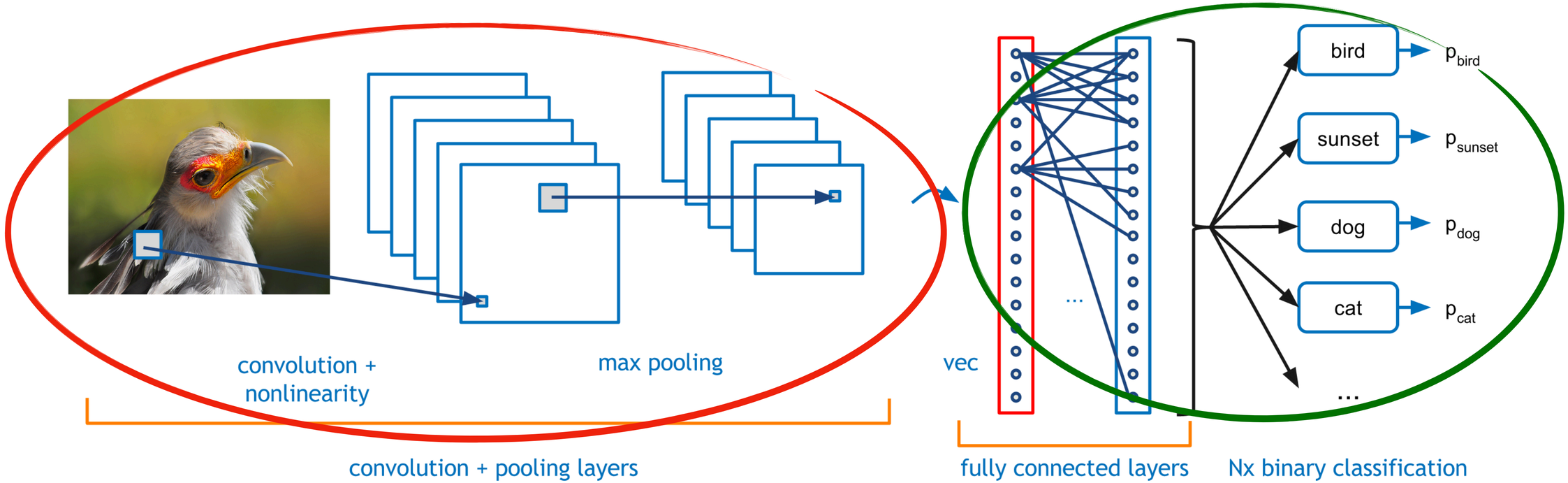
- *Deep Learning, Data representation and Graphs*
- *Message passing*
- *A few examples:*
  - *Edge Conv*
  - *Gated Graph Neural Networks*
  - *Interaction Networks*
  - *Distance-weighted NNs*
- *The GNN exercise (see **dedicated slides**)*



Data Representation

Deep Neural Network in a nutshell

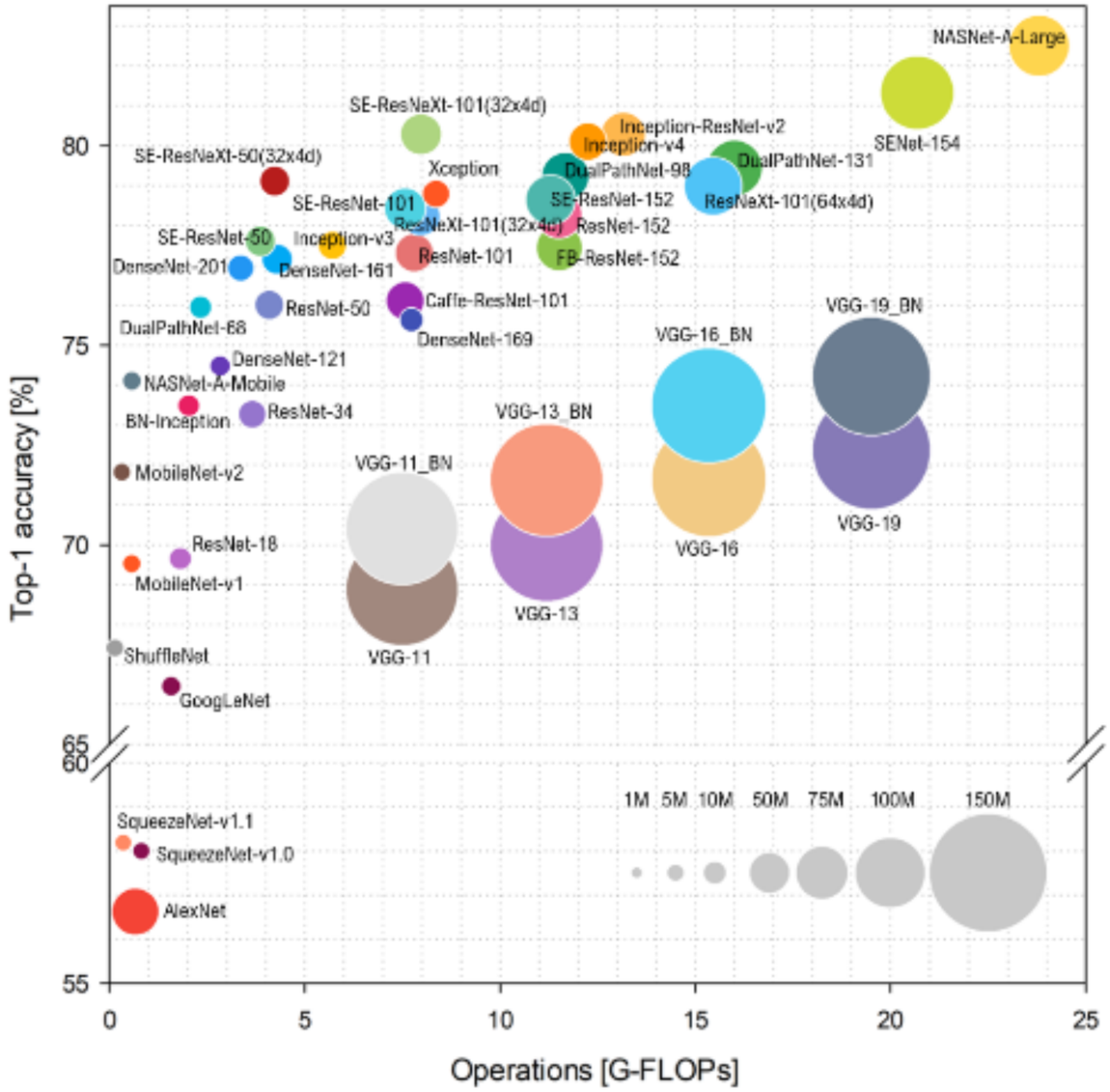
- *DNNs typically rely on two phases:*
  - ***Feature engineering*** *from Raw Data. This is where new & exotic architectures (depending on data type) take the best out of your data*



  - ***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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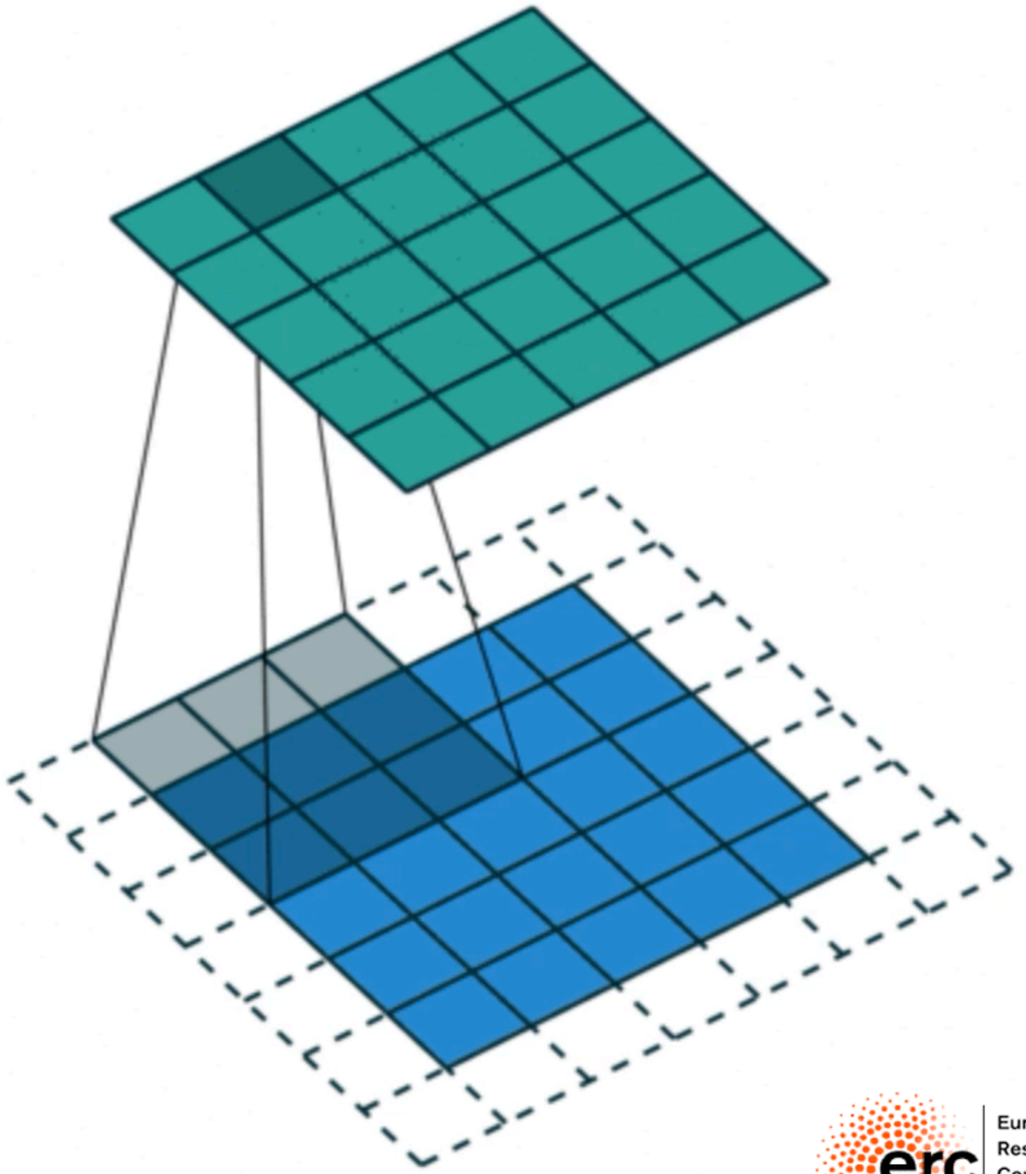

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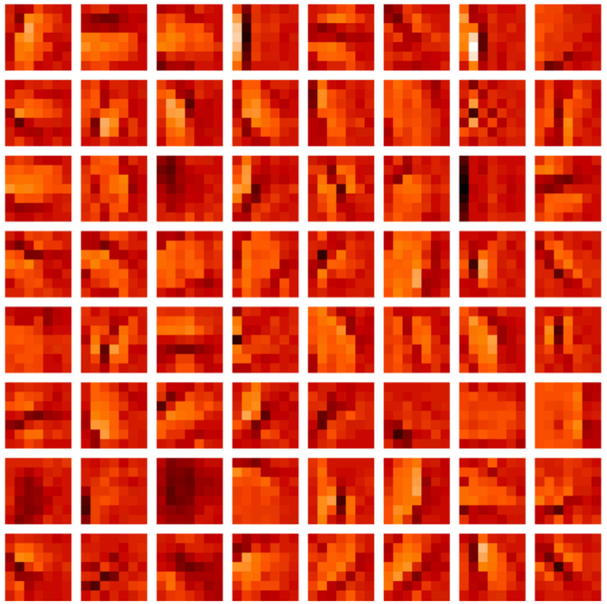
CNN in Science

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



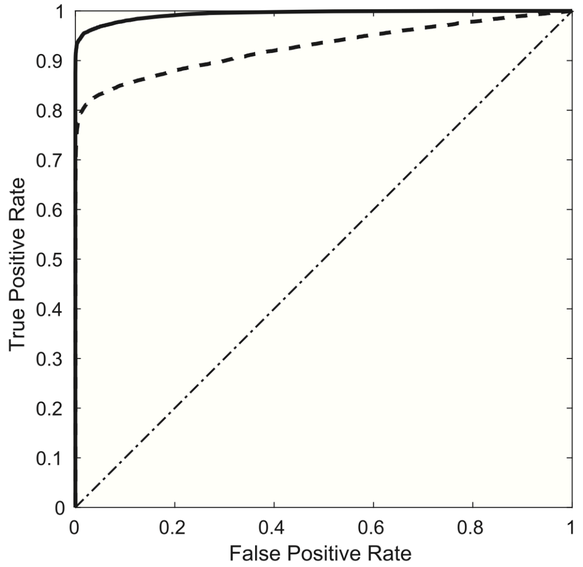
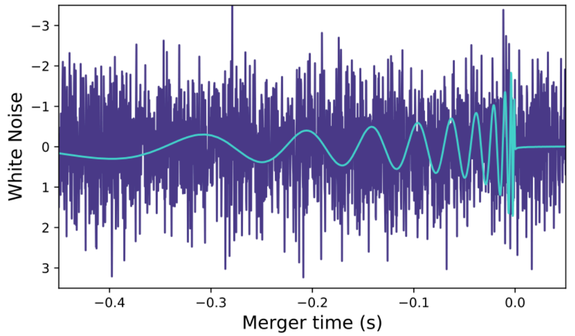
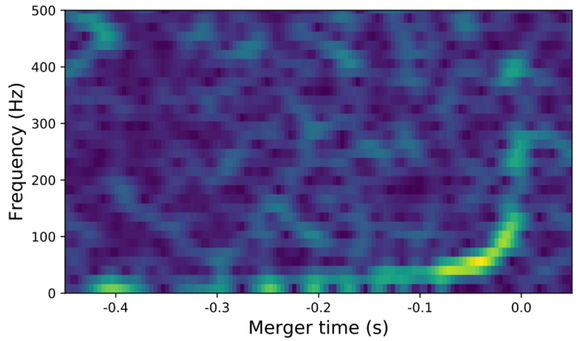


Figure 2. Receiver Operating Characteristic (ROC) curve for the neural network and the data set presented in this work. The dashed line represents the performance of the BLS preceded by a high-pass filter. The dotted–dashed line is the so-called "no-discrimination" line, corresponding to random guess.





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Deep Learning & Natural Language

- *Natural language processing is another big success of Deep Learning*
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  - *data ordered (time sequence, words in sentence, etc.)*
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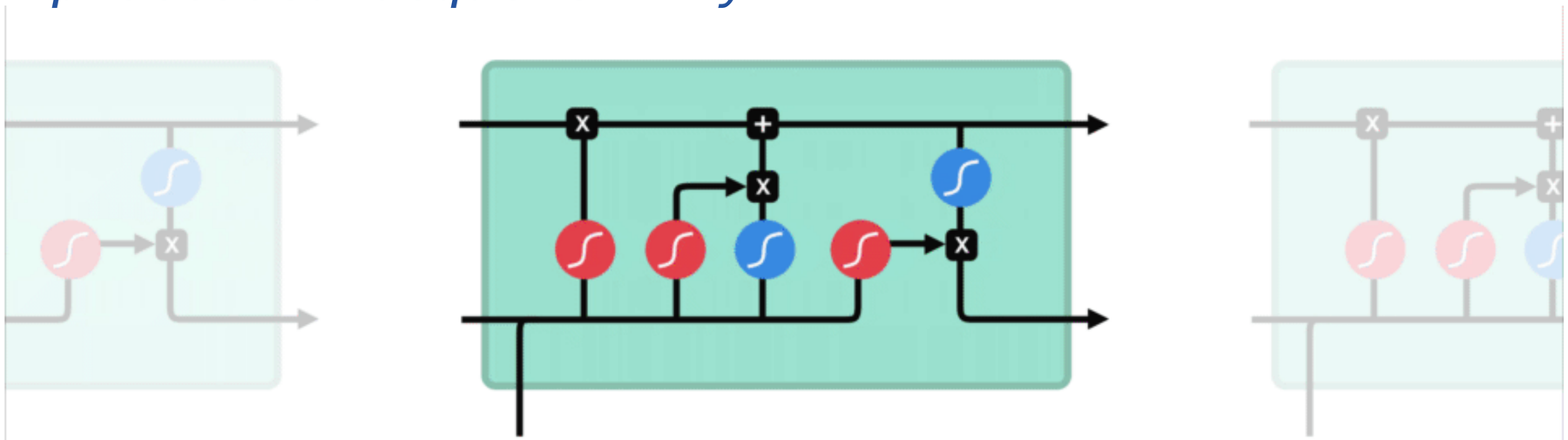
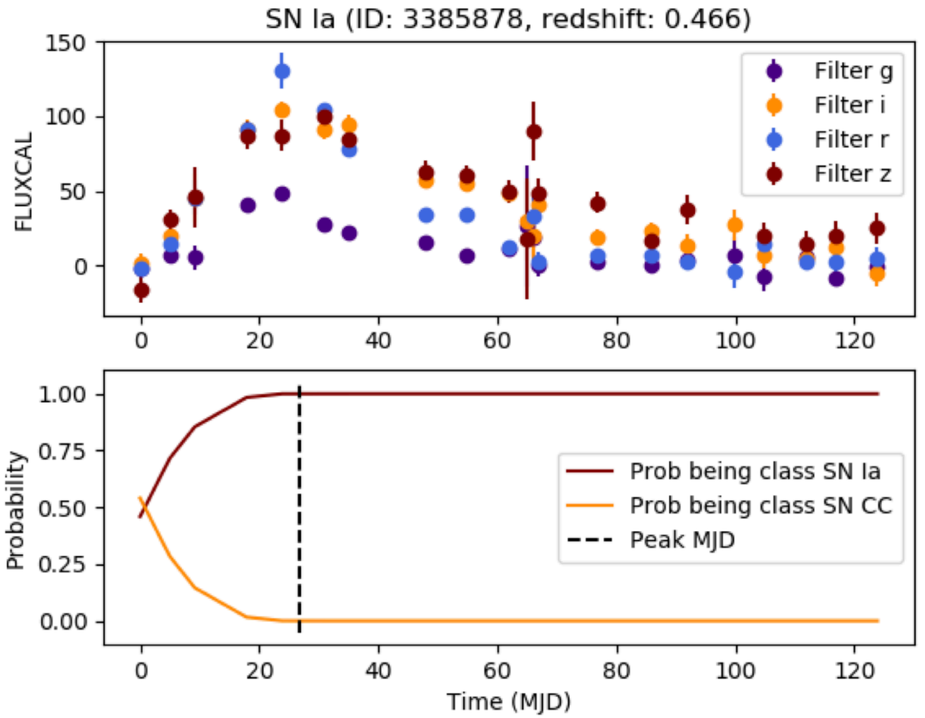
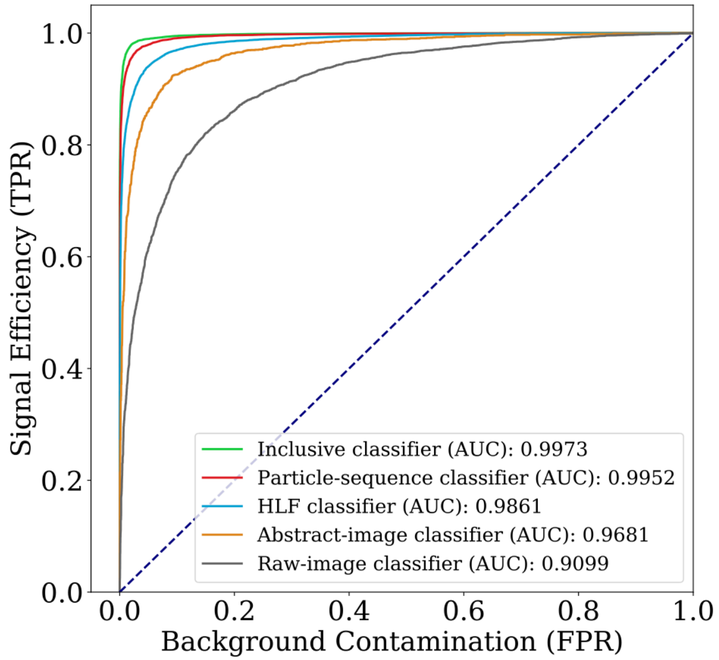
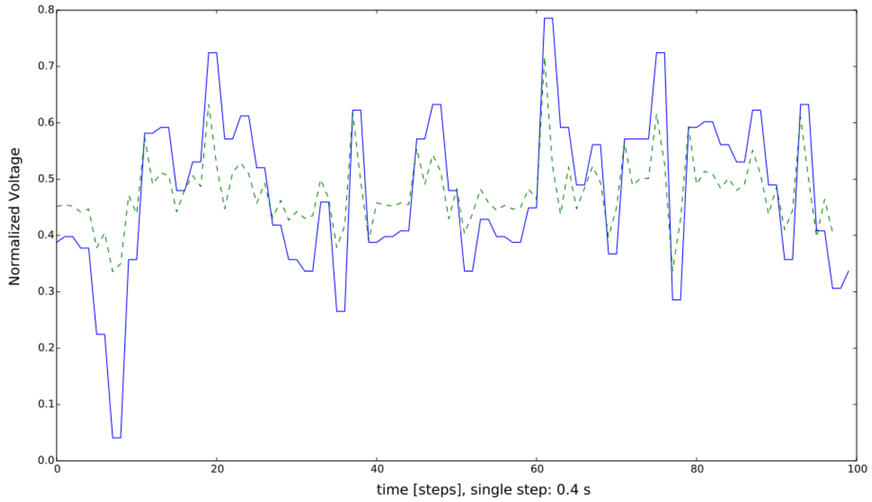


RNN in Science

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







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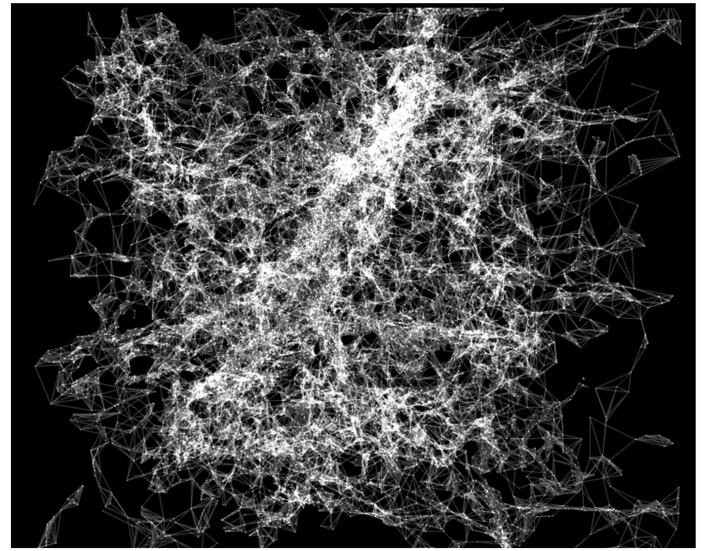
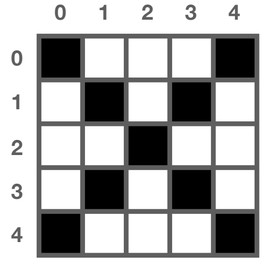
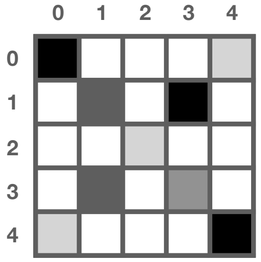
What about irregular data?

- *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*

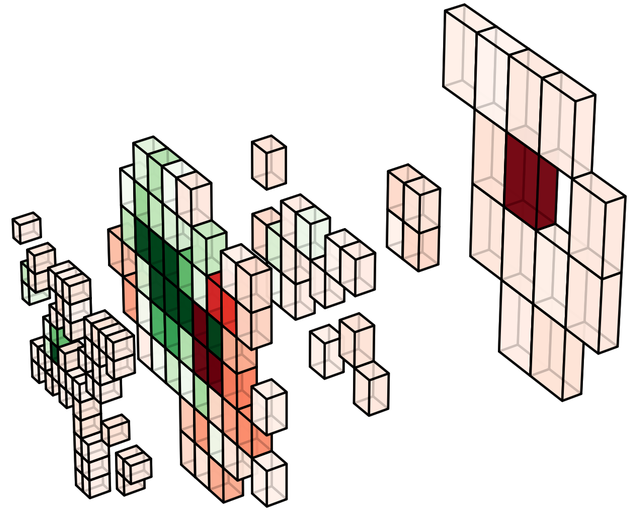




0	0	1	1	2	3	3	4	4
0	4	1	3	2	1	3	0	4



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



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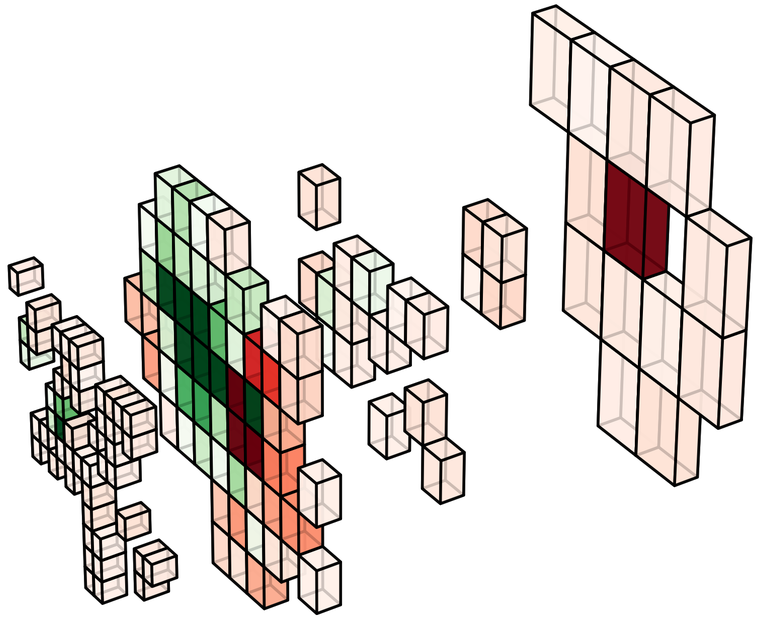
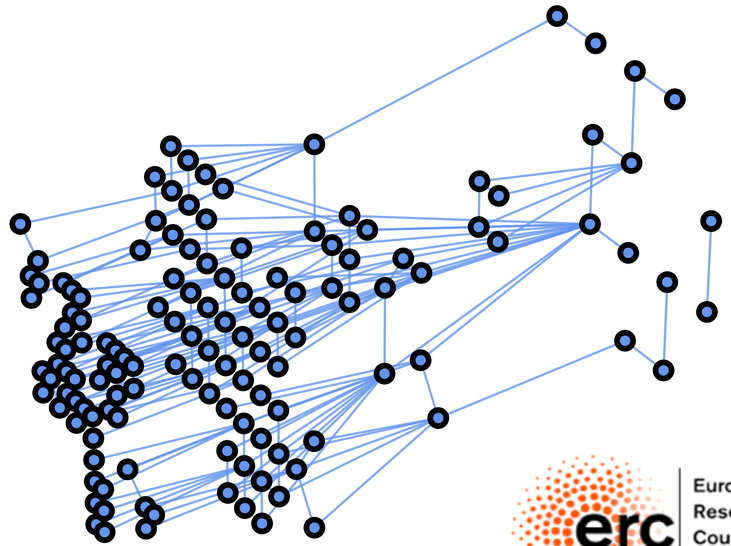
From Sets to Graphs

- *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*





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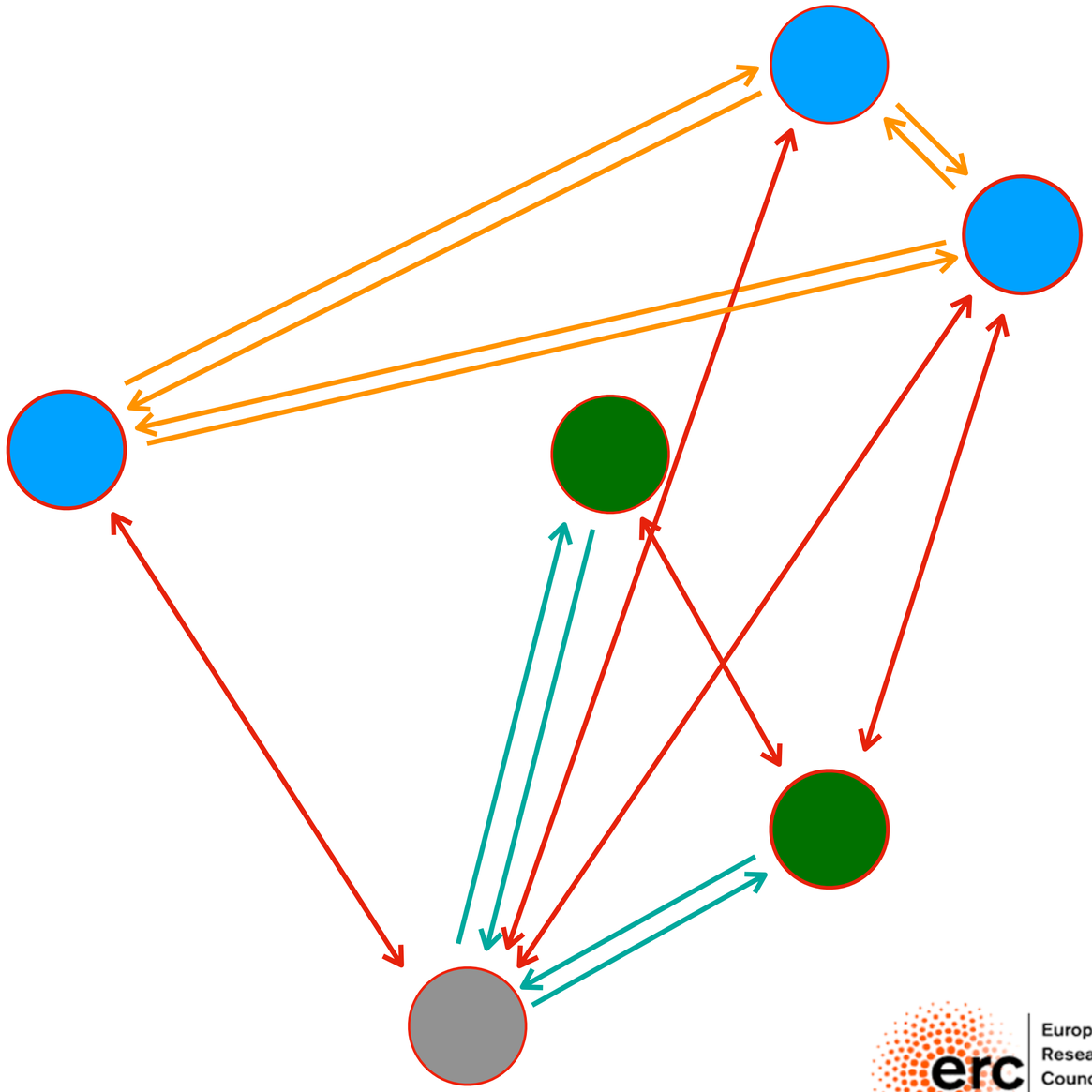
Building the Graph

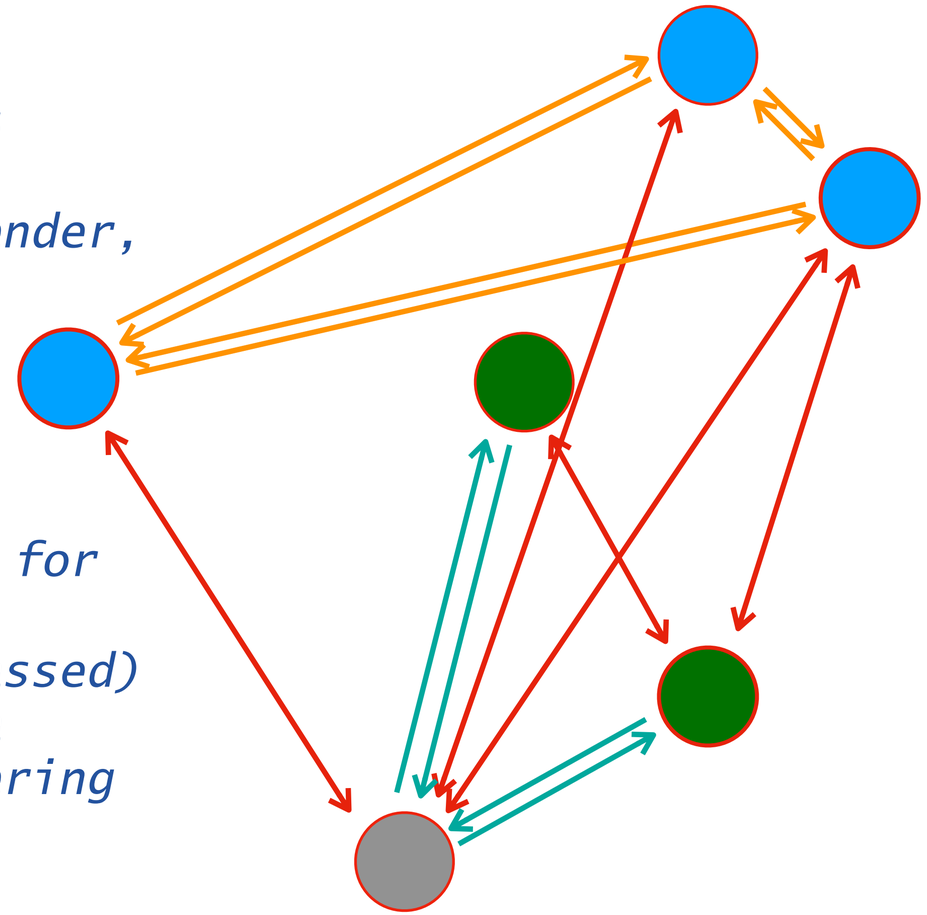
- *Each element of your set is a vertex V*
- *Edges E connect them*
  - *Edges can be made directional*
  - *Graphs can be fully connected (N^2)*
  - *Or you could use some criterion (e.g., nearest k neighbours in some space) to reduce number of connections*
  - *if more than one kind of vertex, you could connect only Vs 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.)*



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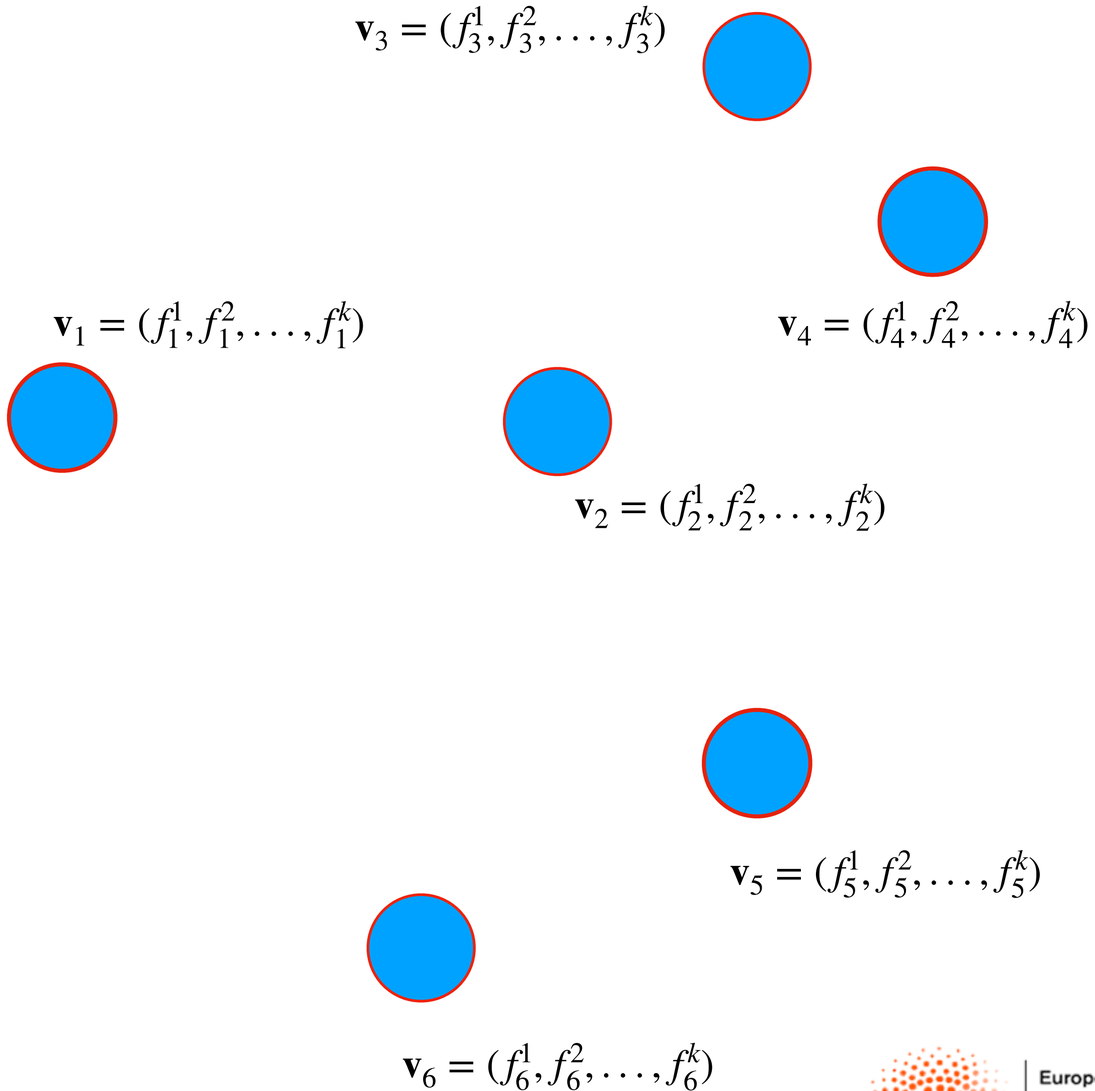
DON'T DO IT!!!!!!

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***



https://arxiv.org/pdf/1704.01212.pdf

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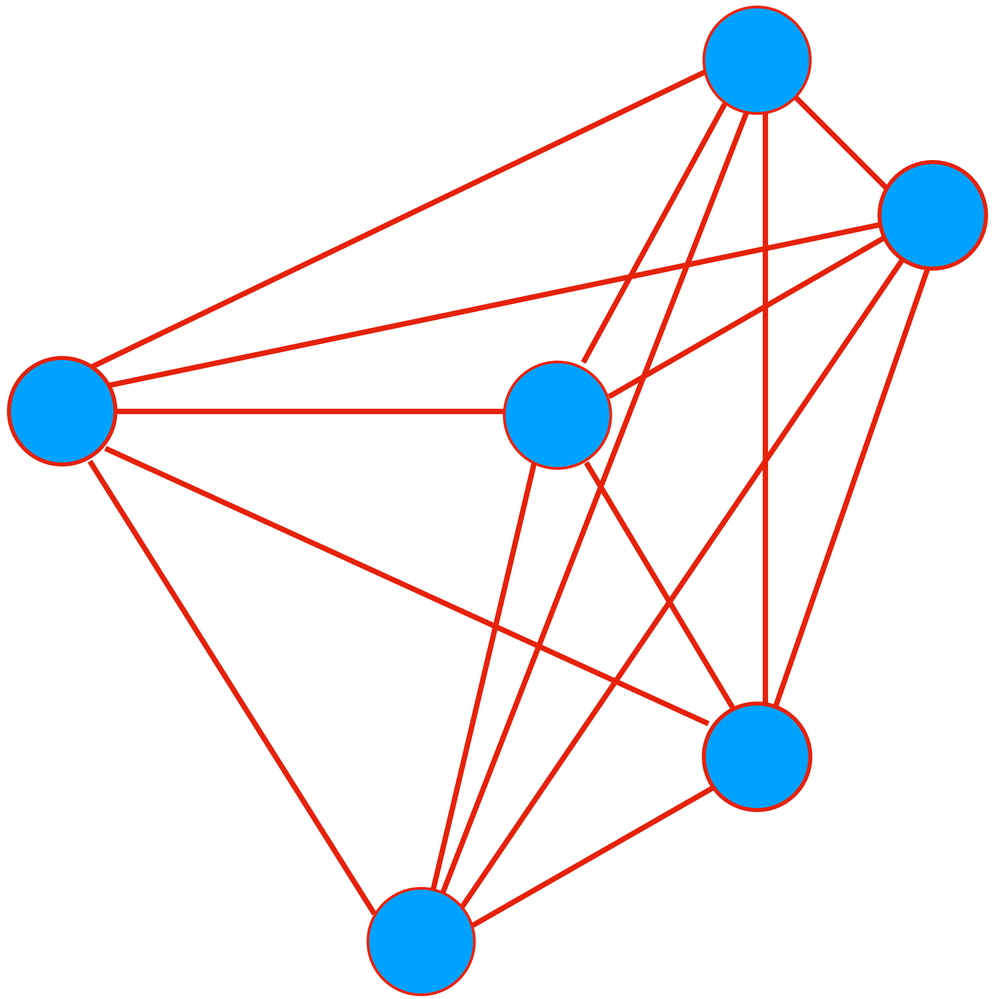

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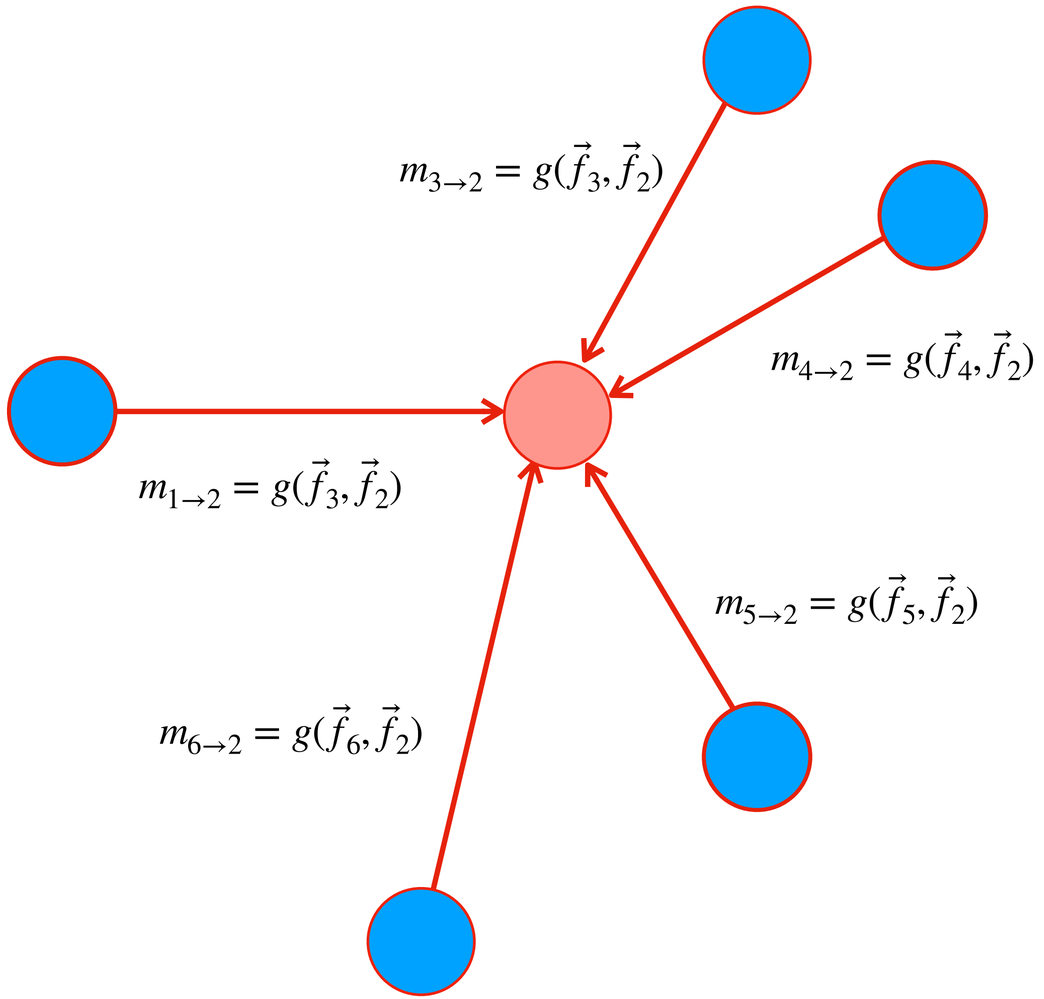
  - ***Messages are passed through links and aggregated on the vertices***



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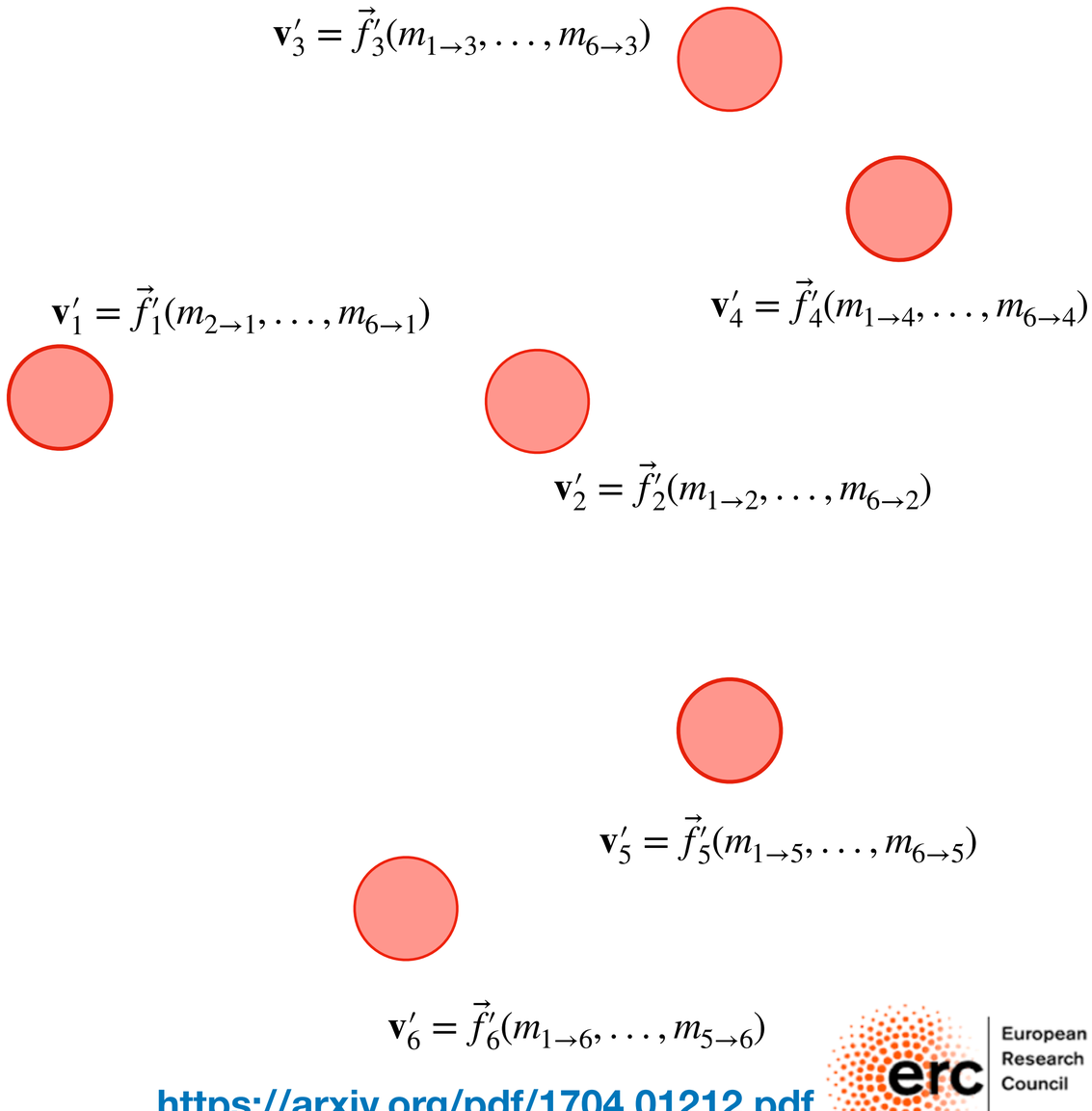
  - *Messages are passed through links and aggregated on the vertices*
  - ***A new representation of each node is created, based on the information gathered across the graph***



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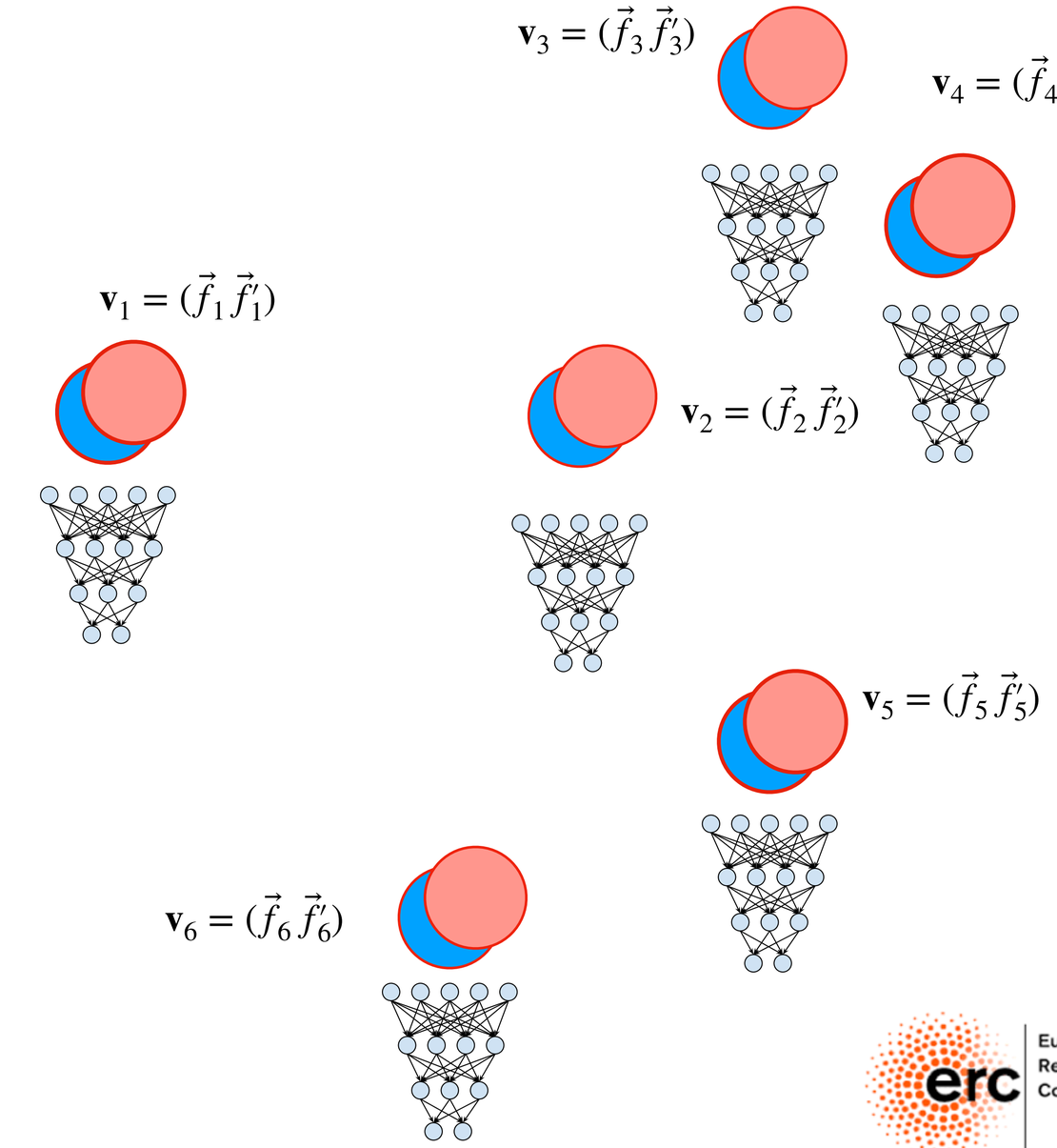
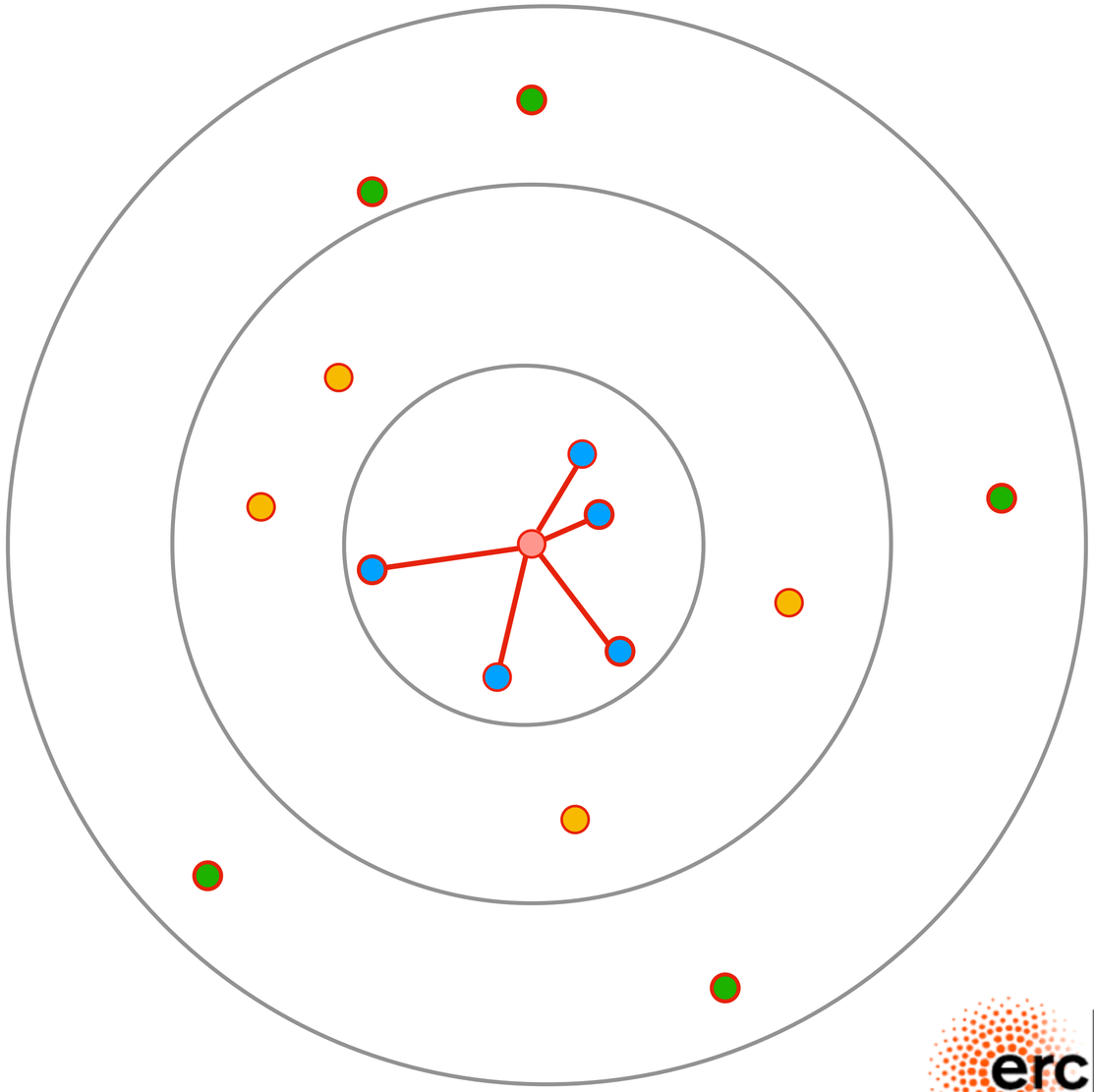
The inference step

- *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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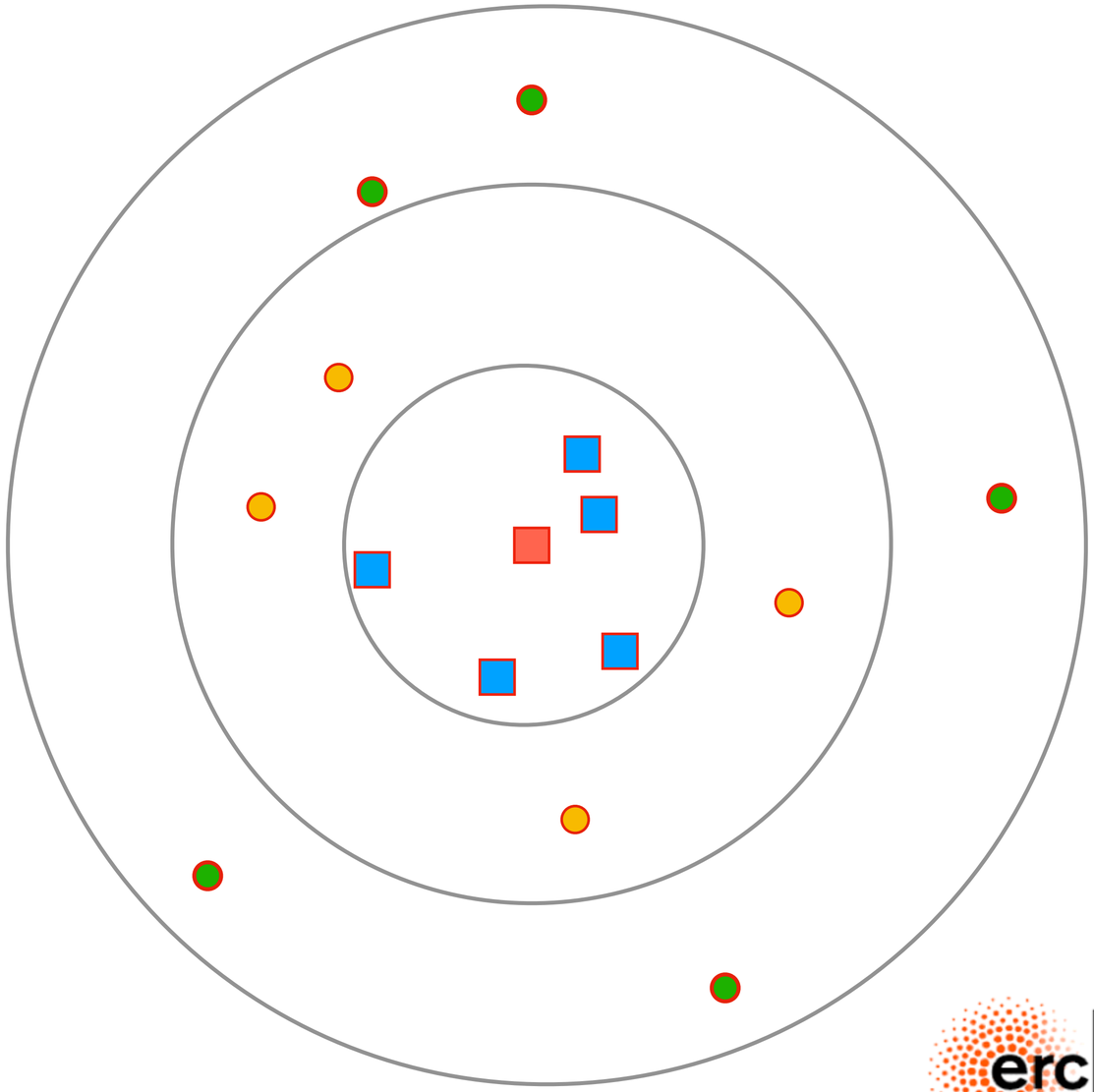

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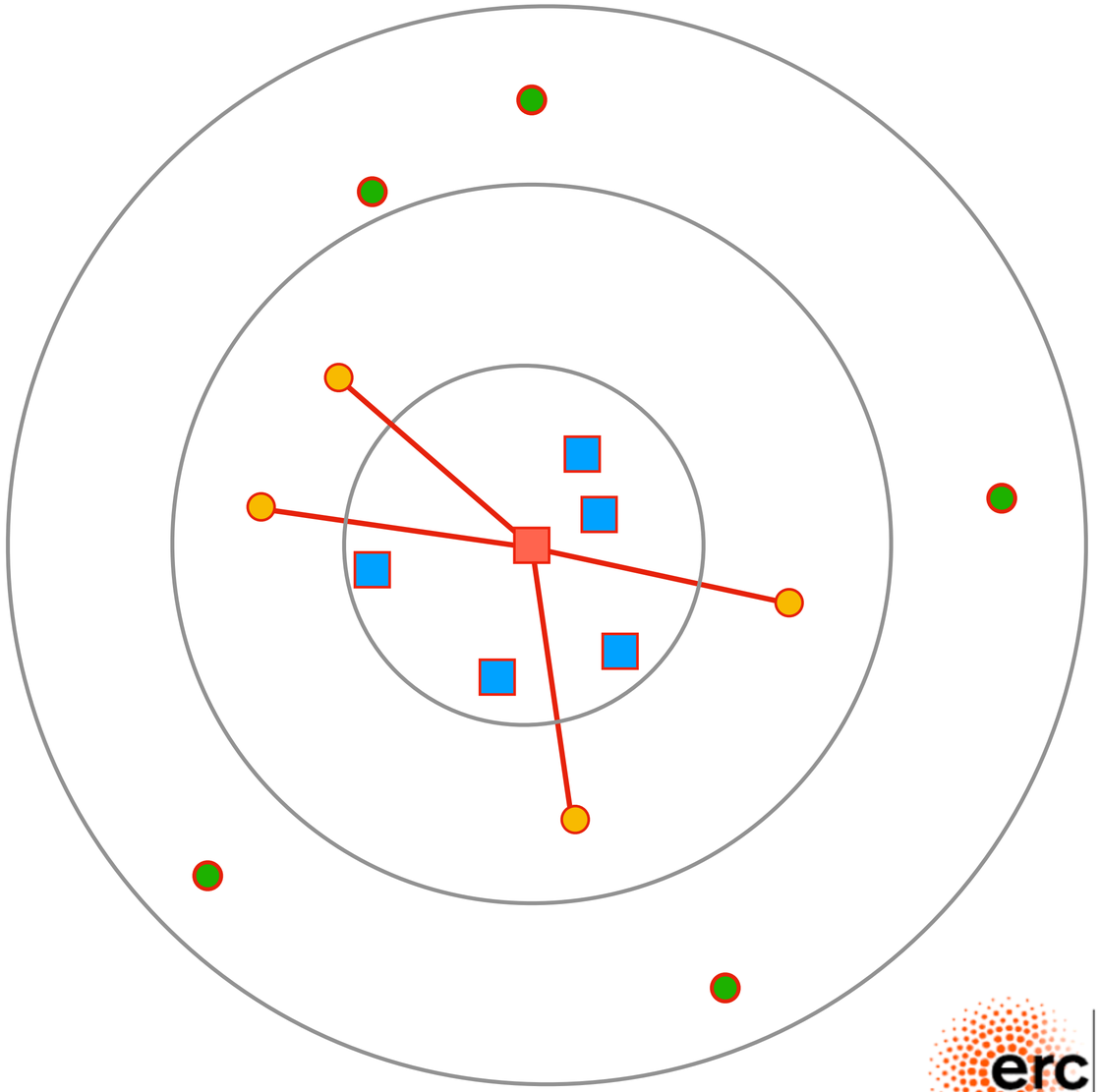

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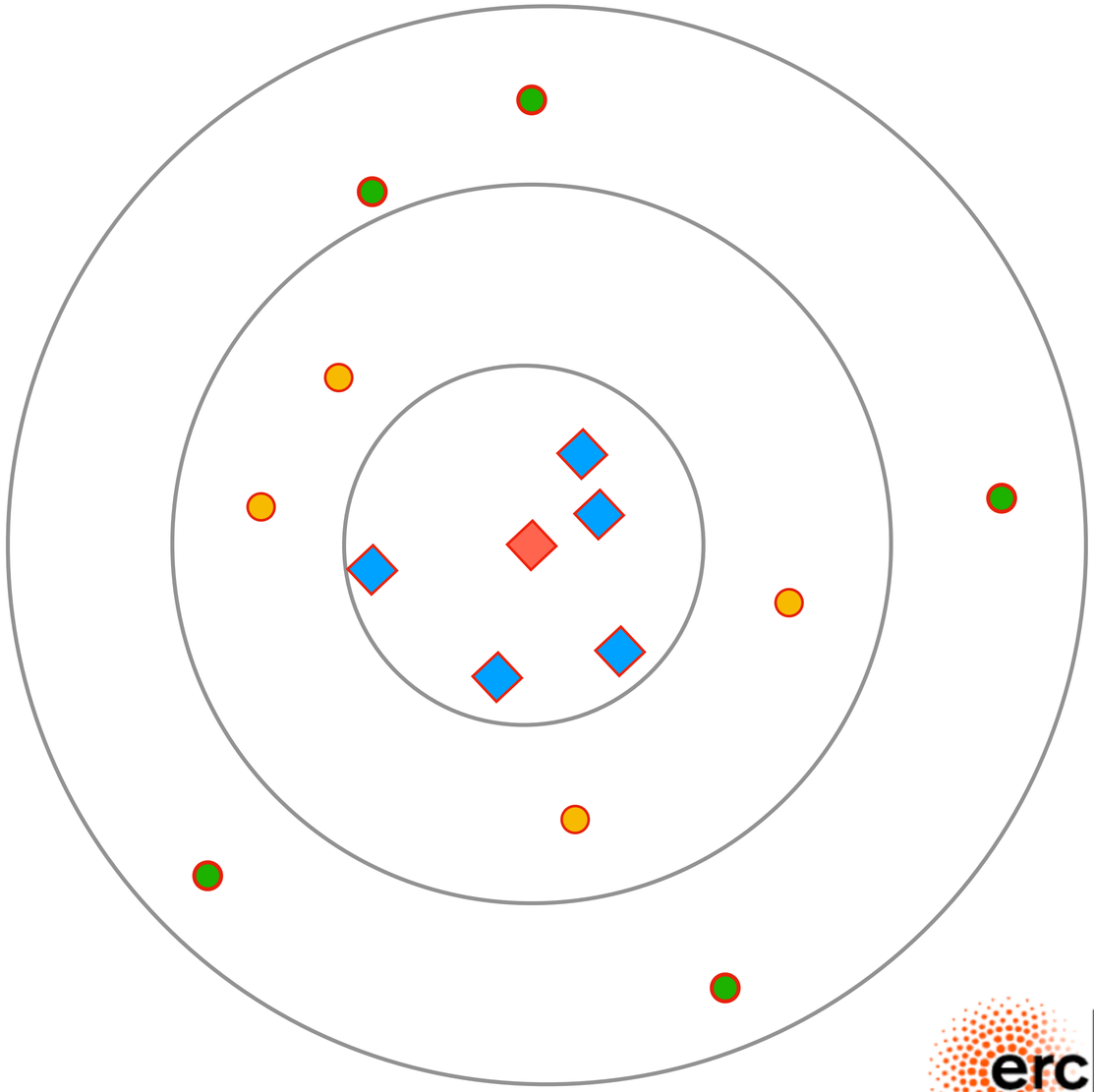

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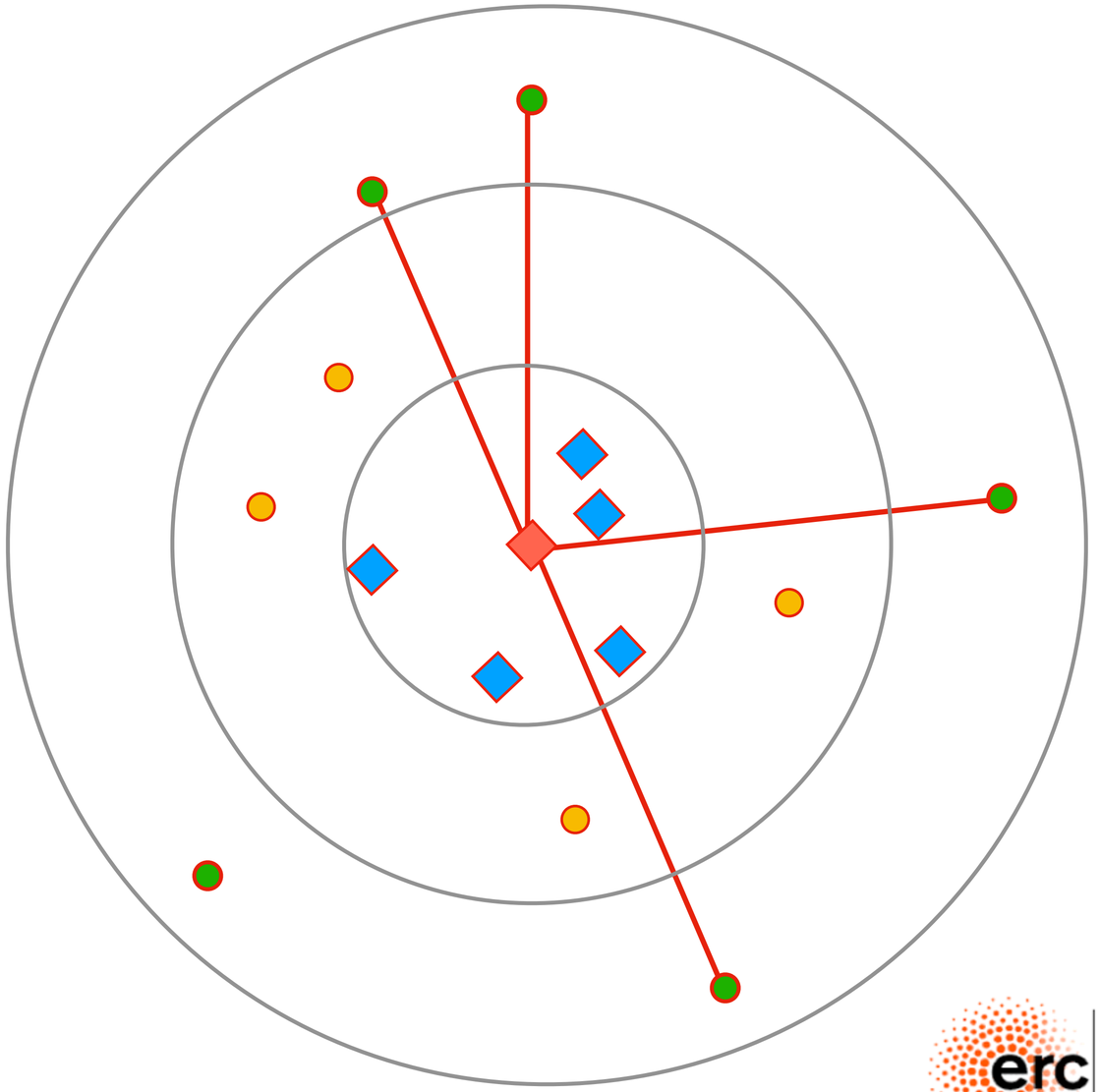
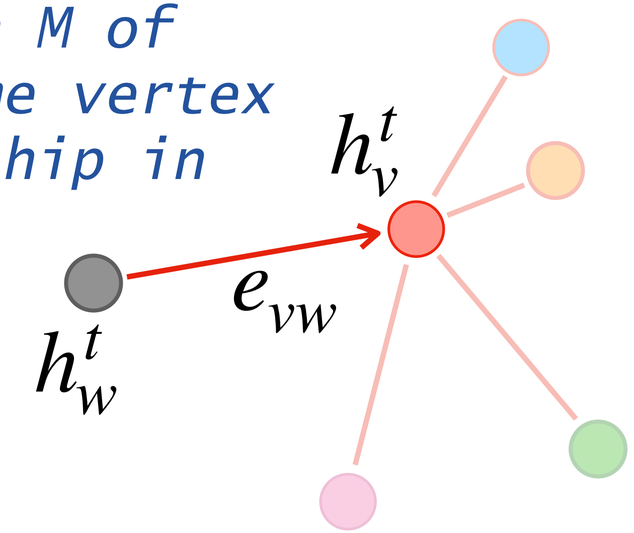


With equations...

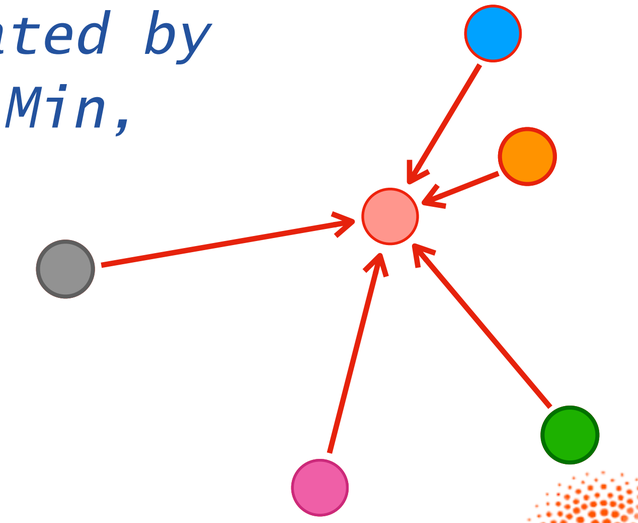
- *Your message at iteration t is some function M of the sending and receiving features, plus some vertex features (e.g., business relation vs friendship in social media)*

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



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

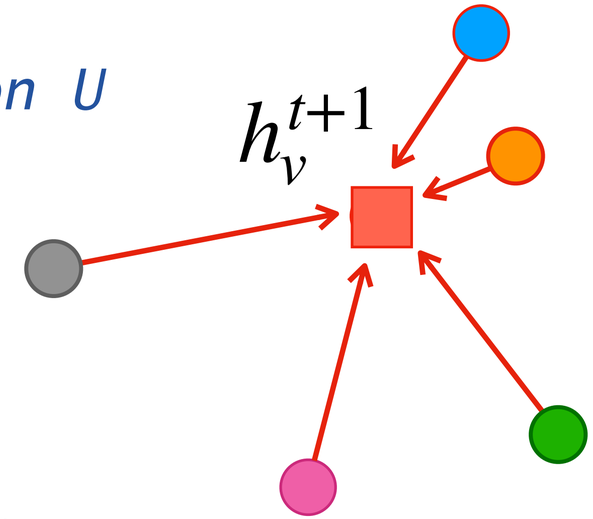
$$m_v^{t+1} = \sum_{w \in G(v)} M_t(h_v^t, h_w^t, e_{vw})$$



With equations...

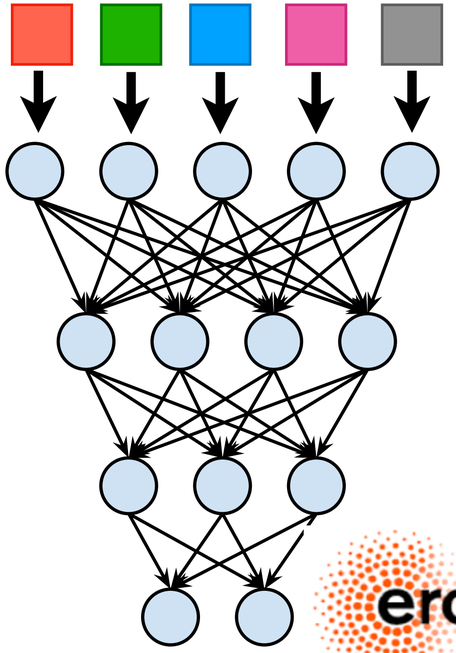
- *The state of vertex v is updated by some function U of the current state and the gathered message*

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



- *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*

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

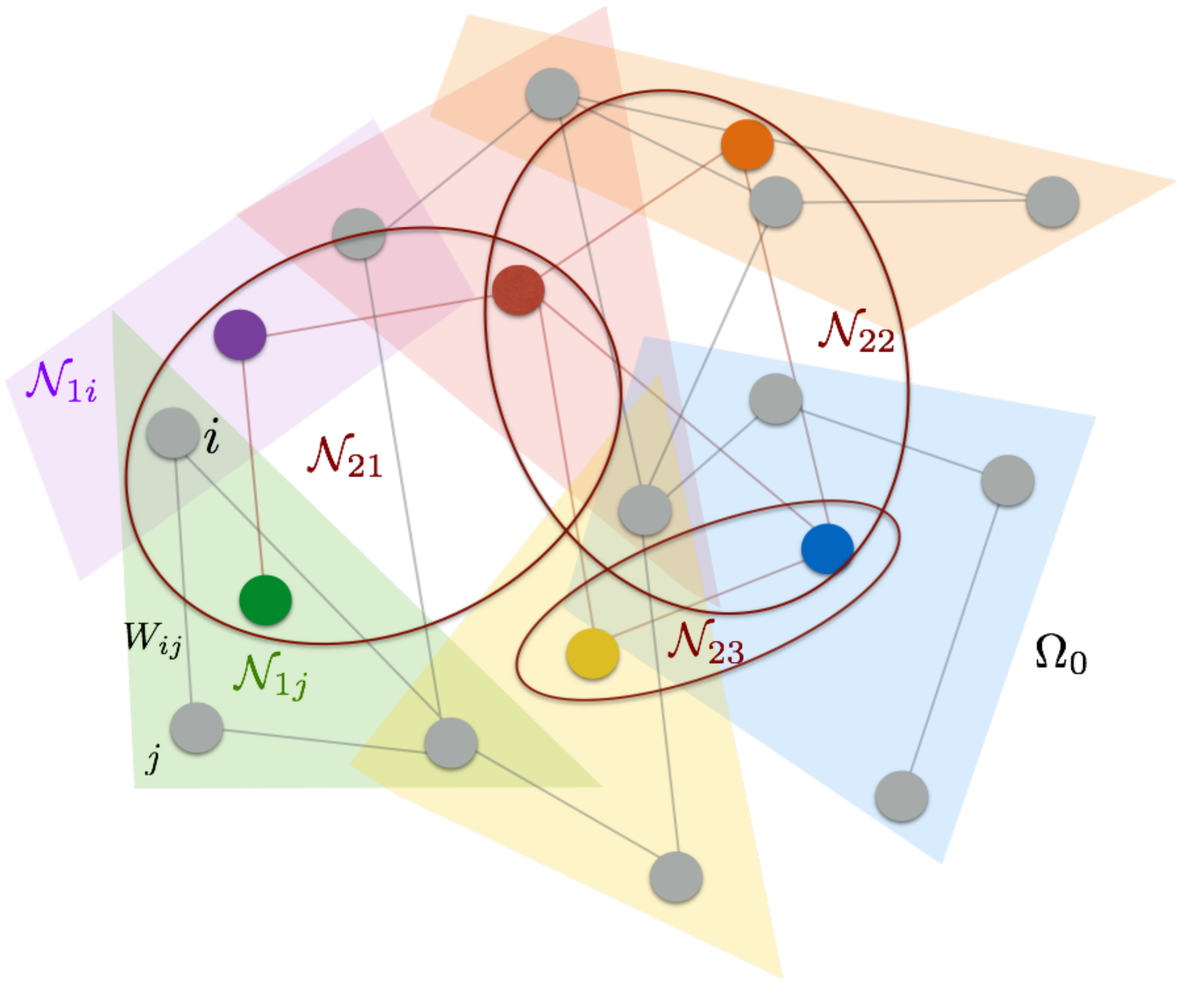


Learning Message

- *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., Netwon's low 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

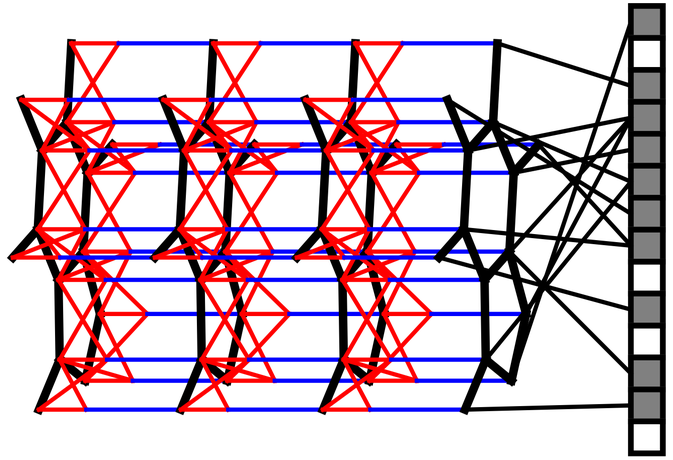
- *(in this millenium) Graph networks started (as often it is the case) with a Yann LeCun et al. paper*
- *They tried to generalise CNNs beyond the regular-array dataset paradigm*
- *They replaced the translation-invariant kernel structure of CNNs with hierarchical clustering*



https://arxiv.org/abs/1312.6203

A little bit of History

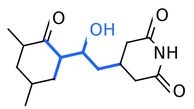
- *The idea of message passing can be tracked to a '15 paper by Duvenaud et al.*
- *The paper introduces "a convolutional neural network that operates directly on graphs"*
- *Language is different, but if you look at the algorithm it is pretty much what we discussed (for specific network architecture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

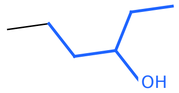


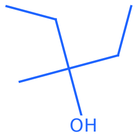
Algorithm 2 Neural graph fingerprints

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

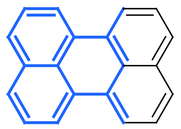
Fragments most activated by pro-solubility feature

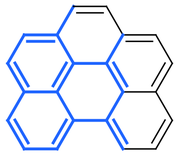






Fragments most activated by anti-solubility feature





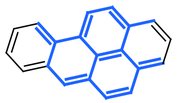
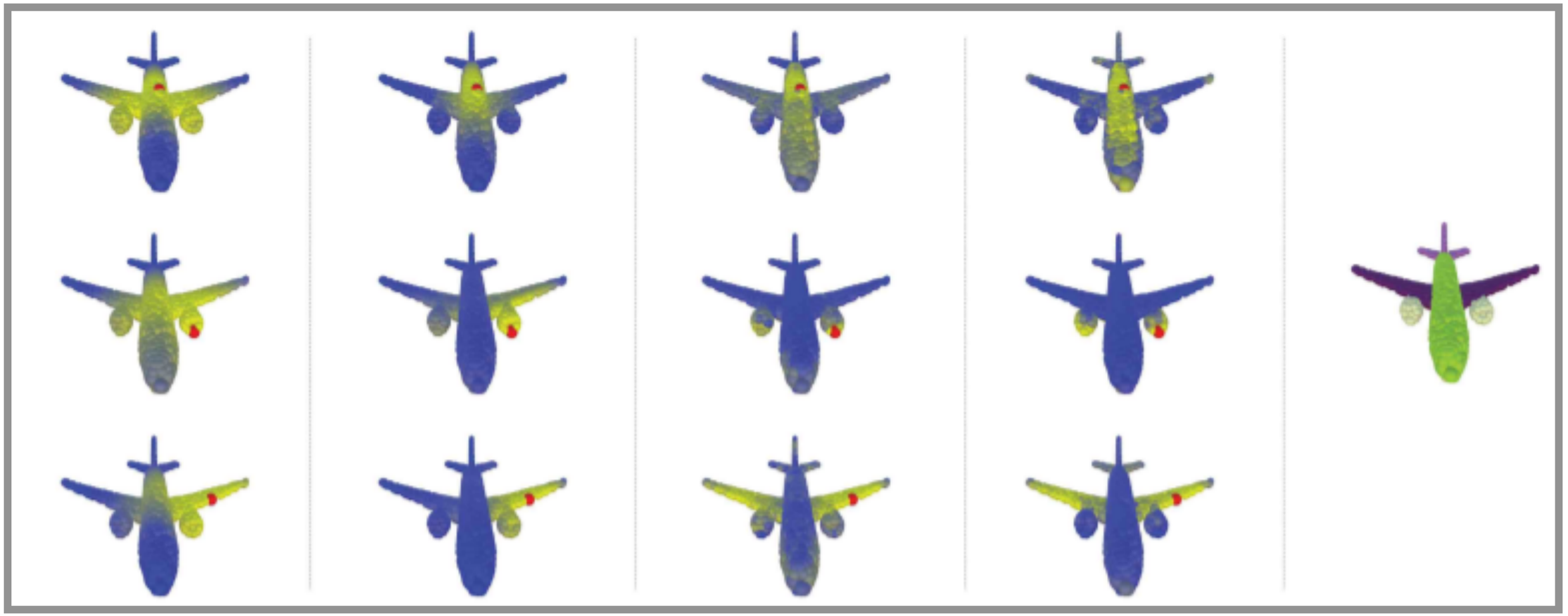


Figure 4: Examining fingerprints optimized for predicting solubility. Shown here are representative examples of molecular fragments (highlighted in blue) which most activate different features of the fingerprint. *Top row:* The feature most predictive of solubility. *Bottom row:* The feature most predictive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

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

Further Reading & Coding

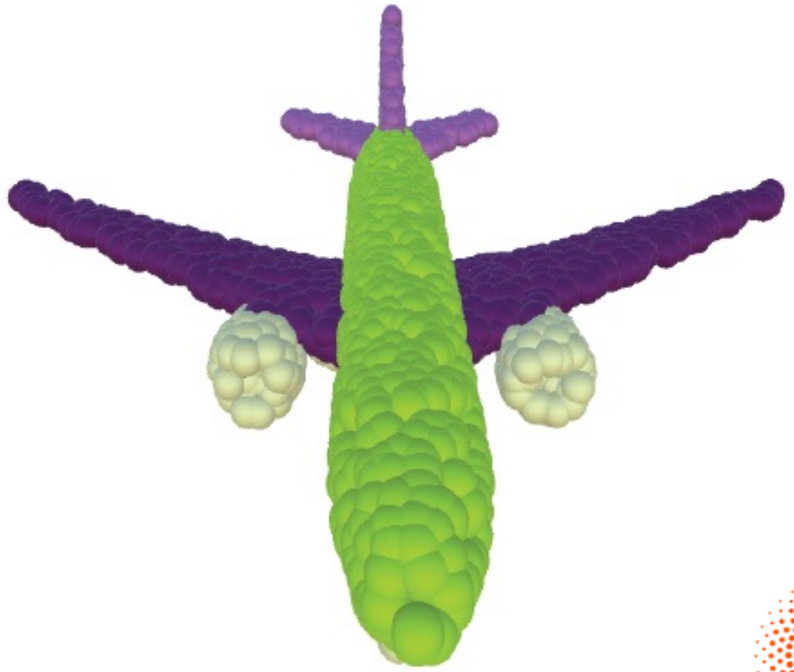
- *A few recent reviews that could guide you through the many applications and networks*
  - *A nice BLOG article on GNNs*
  - *Another nice BLOG article on GNNs*
  - *A generic review*
  - *A particle-physics specific one*
- *A few GitHub entries*
  - *JEDI-net Interaction Networks for jet tagging on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



Edge Conv

EdgeConv

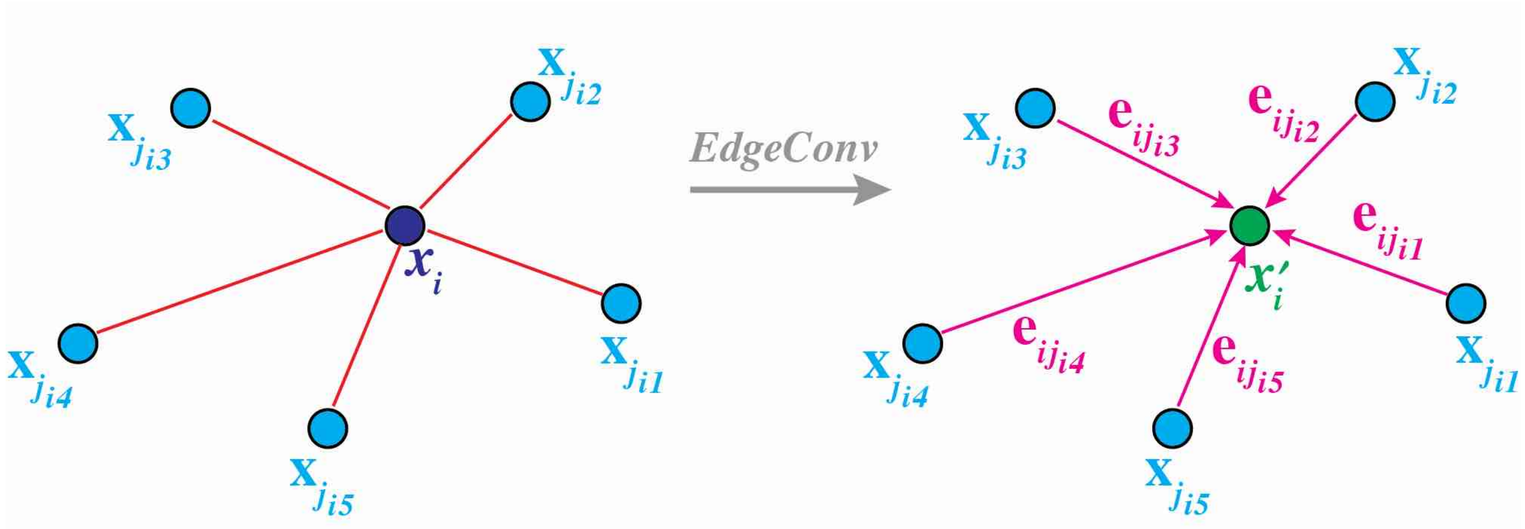
- *Dynamic Graph CNN (DGCNN) is one kind of message-passing neural network*
- *It uses EdgeConv layers to perform point-cloud segmentation*
- *Segmentation is the process of clustering pixels in an image into objects*
- *EdgeConv was capable of extending semantic segmentation beyond nearby-pixel clustering*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

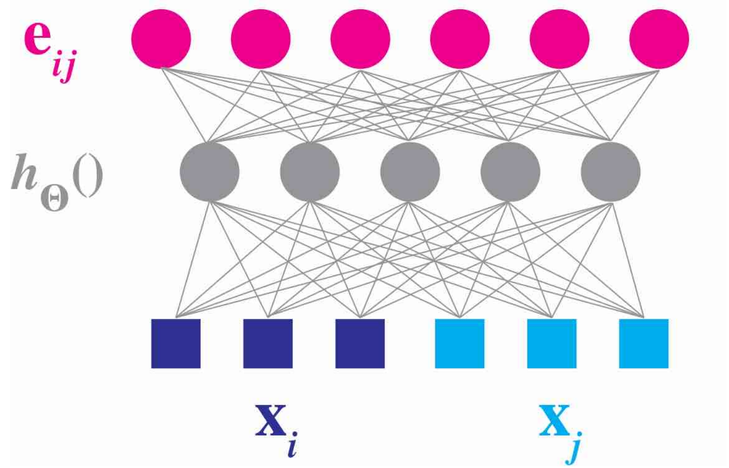


https://arxiv.org/abs/1801.07829

EdgeConv

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

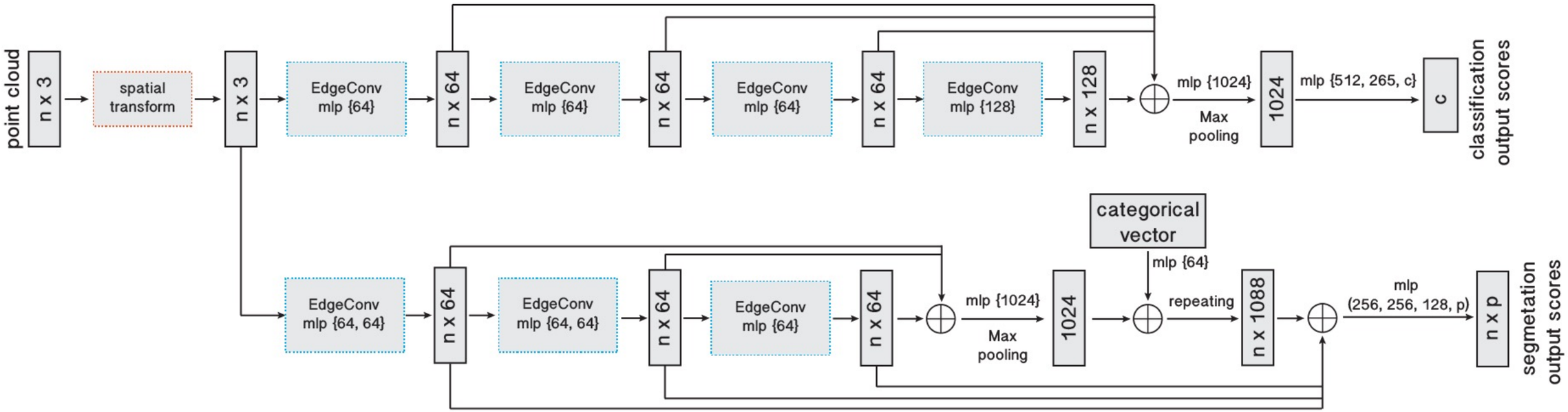




https://arxiv.org/abs/1801.07829

EdgeConv

- *But the actual model is much more complicated than that*



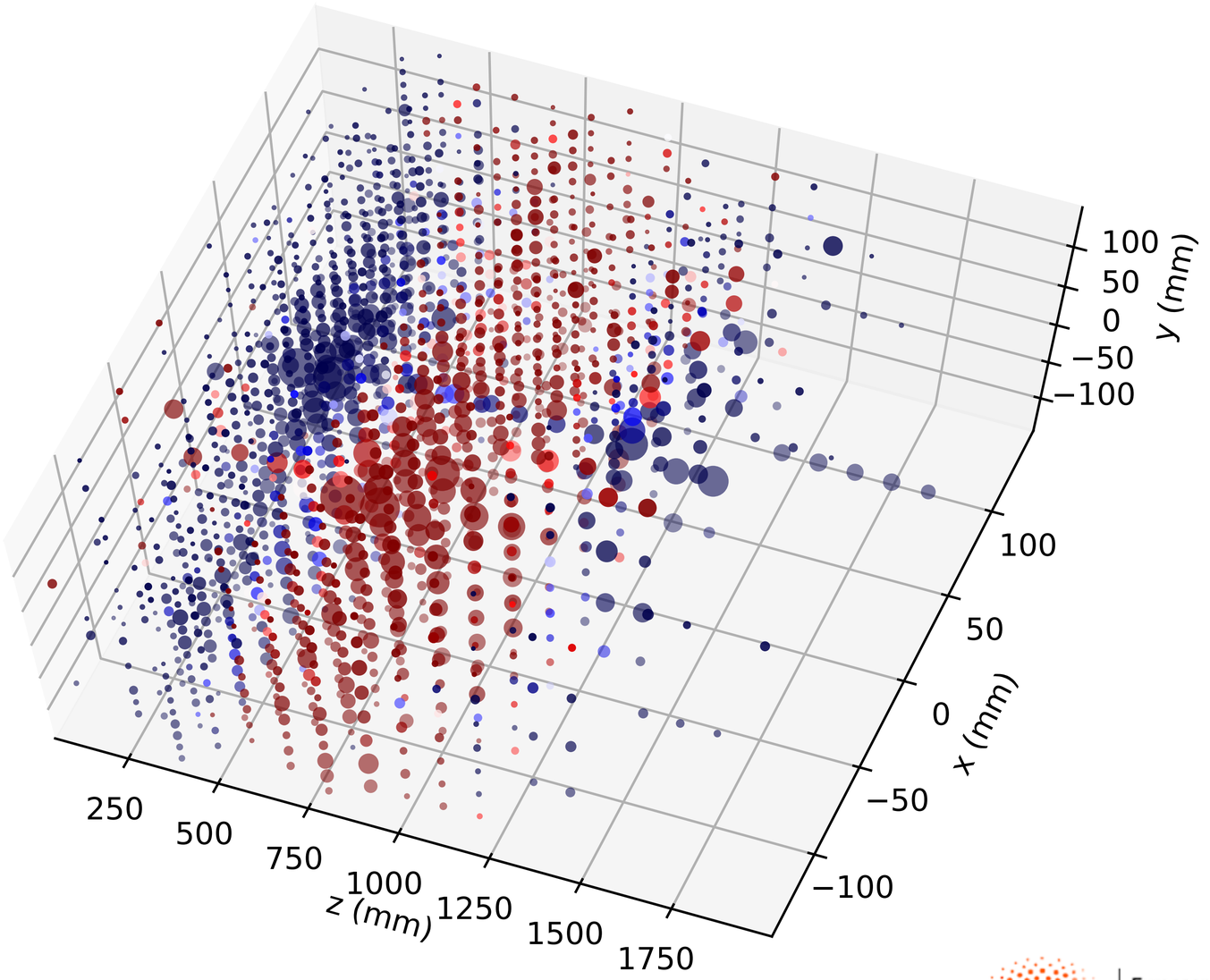
- *Each EdgeConv layer runs a message passing and creates an updated representation of the graph of points*

- *Similar to a CNN, but capable of processing unordered sets of points*

https://arxiv.org/abs/1801.07829

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*



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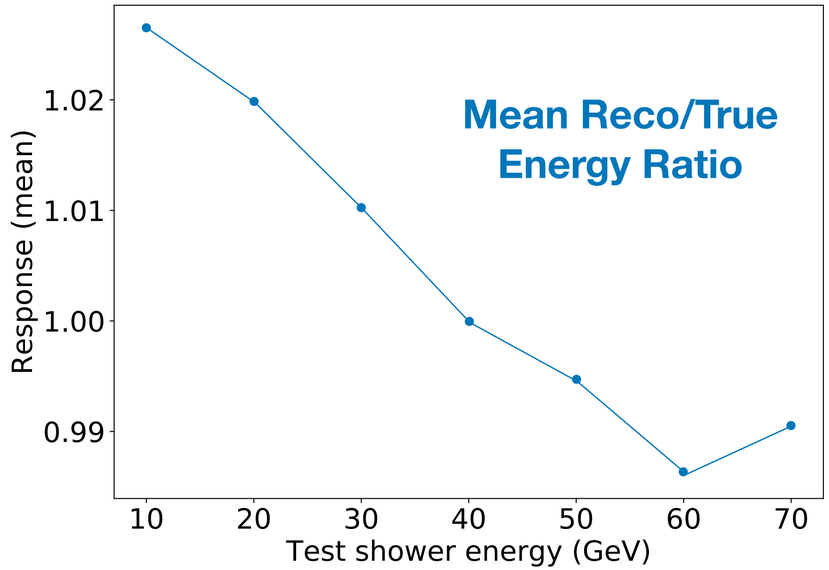
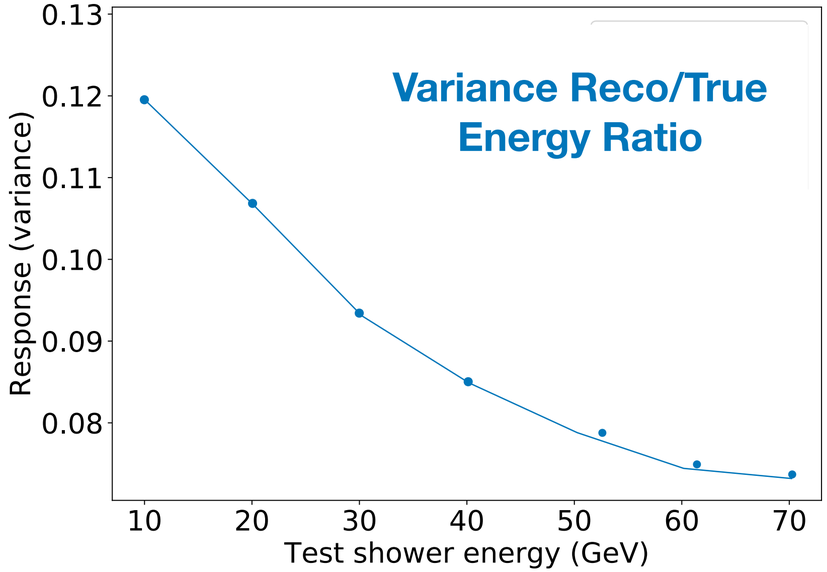
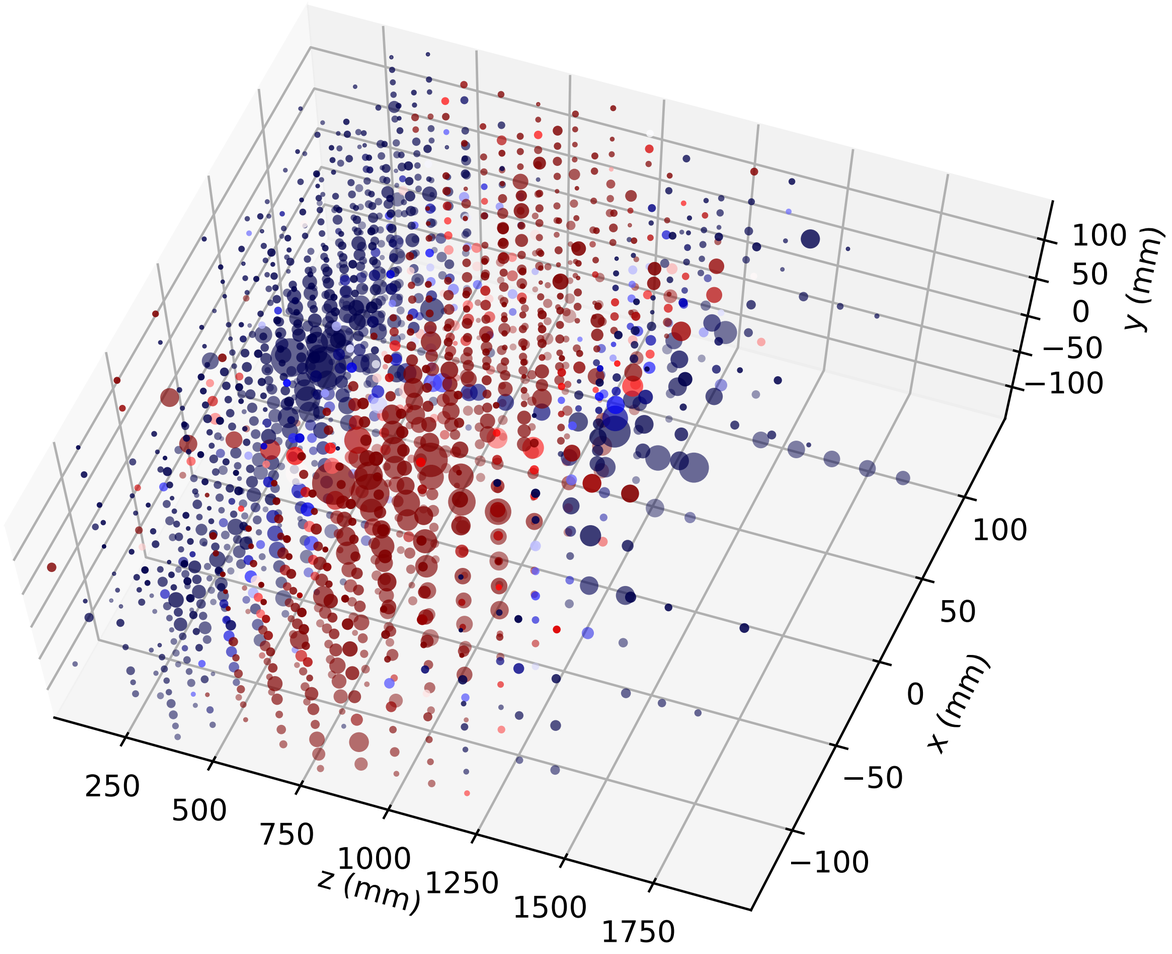
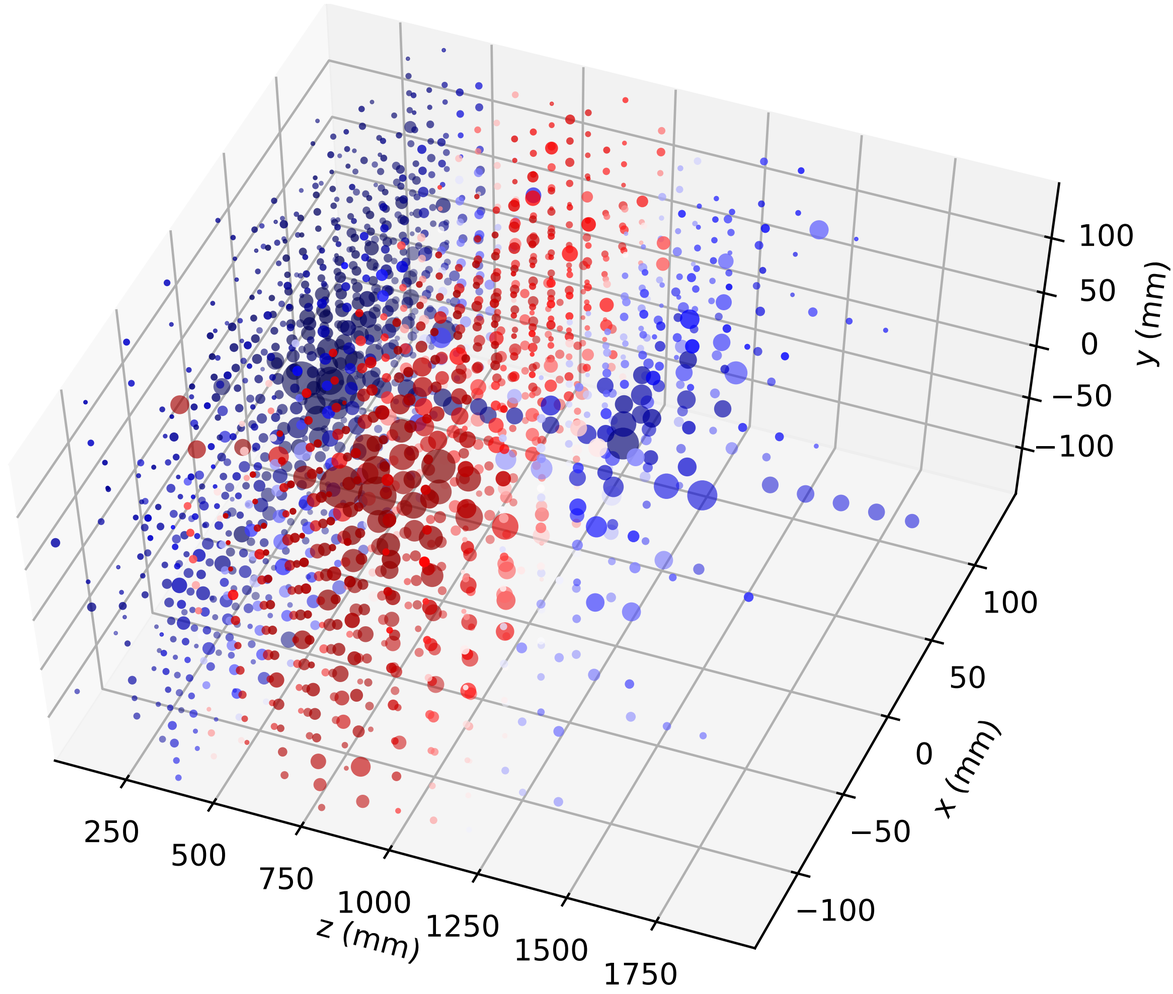




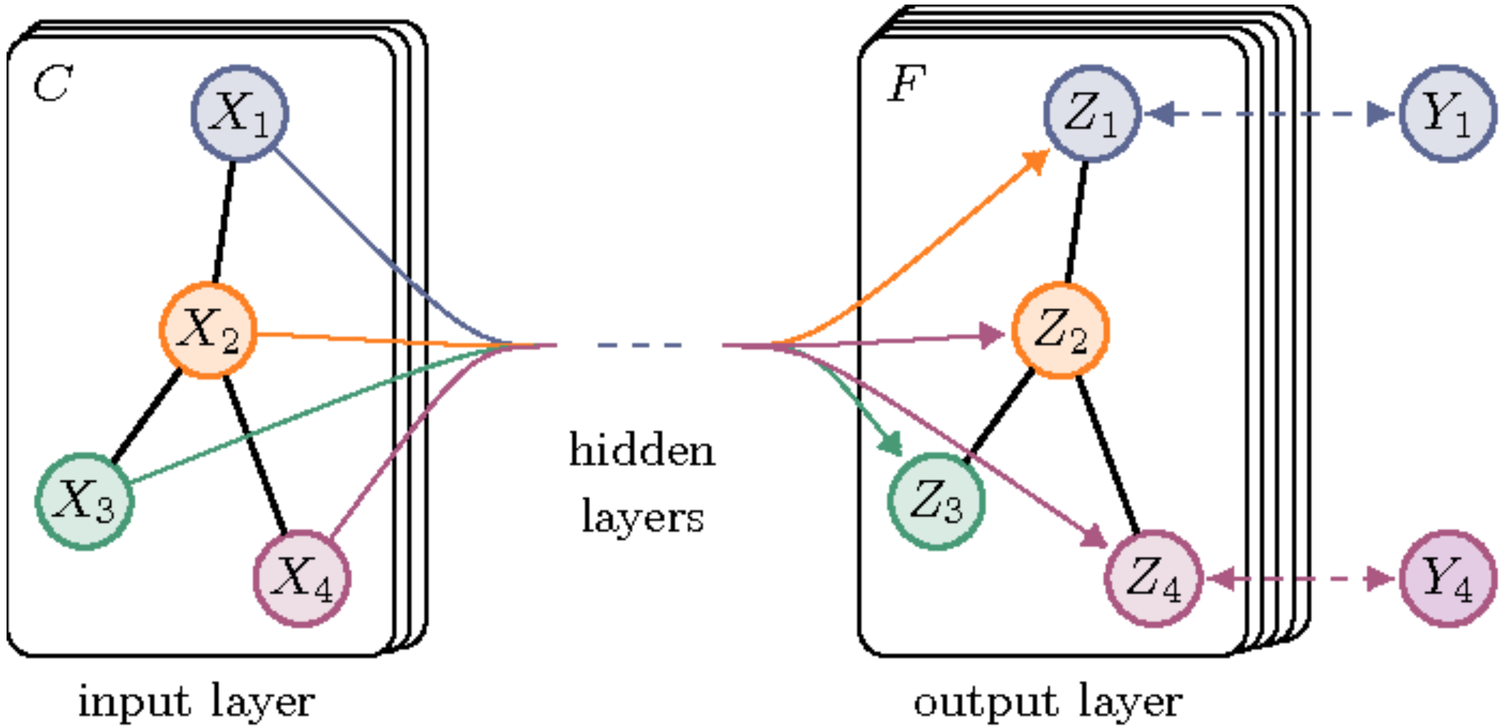
Separating overlapping showers

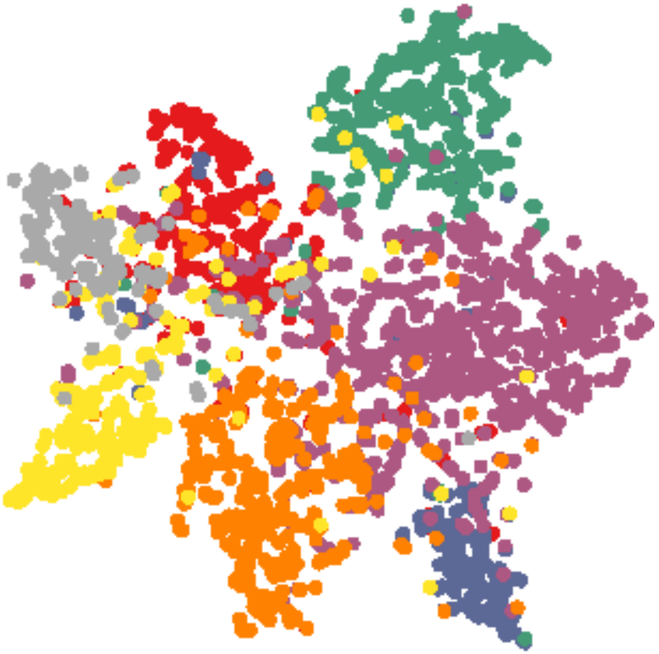


(a) Truth



(b) Reconstructed





Convolutional Graph Neural Networks

European Research Council

Generalising CNN to point clouds

How Graph Convolutions work

CNN on image

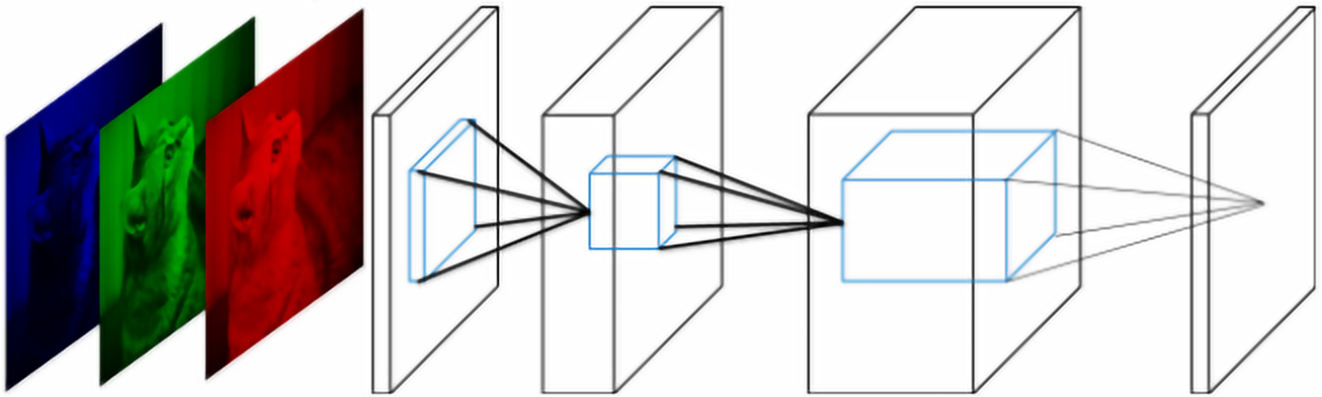
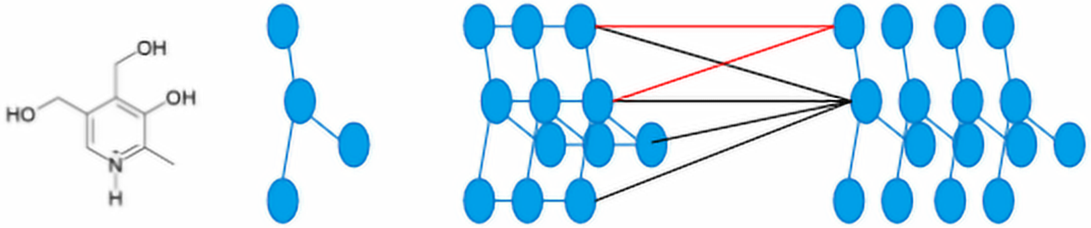


Image
class label

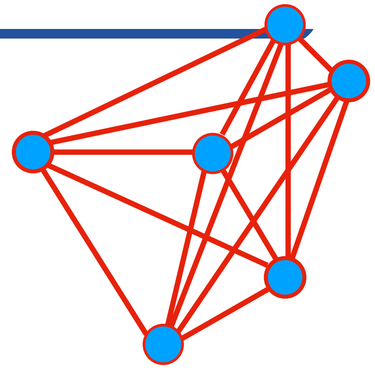
Graph convolution



Chemical
property

Convolution “kernel” depends on Graph structure

The math

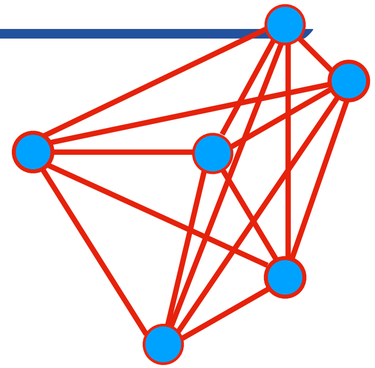


Consider a graph with n nodes, each containing f features.

$$A.X.W = \underbrace{\begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{21} & 0 & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & 0 \end{pmatrix}}_{n \times n \ adjacency} \underbrace{\begin{pmatrix} \vdots & x_{12} & \vdots & \vdots & \vdots \\ x_{21} & x_{22} & x_{23} & \dots & x_{2f} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & x_{n2} & \vdots & \vdots & \vdots \end{pmatrix}}_{n \times f \ (nodes \times features)} \underbrace{\begin{pmatrix} w_{11} & w_{12} & \dots & w_{1c} \\ w_{21} & w_{22} & \dots & w_{2c} \\ \vdots & \vdots & \vdots & \vdots \\ w_{f1} & w_{f2} & \dots & w_{fc} \end{pmatrix}}_{f \times c \ (feature \ weight \times channels)}$$

- *The inputs X*
- *The weights W*
- *The Adjacency matrix*

The Inputs

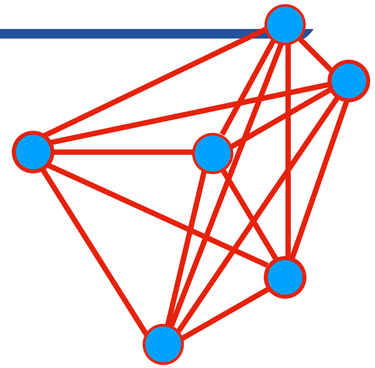


Consider a graph with n nodes, each containing f features.

$$A.X.W = \underbrace{\begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{21} & 0 & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & 0 \end{pmatrix}}_{n \times n \ adjacency} \underbrace{\begin{pmatrix} \vdots & x_{12} & \vdots & \vdots & \vdots \\ x_{21} & x_{22} & x_{23} & \dots & x_{2f} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & x_{n2} & \vdots & \vdots & \vdots \end{pmatrix}}_{n \times f \ (nodes \times features)} \underbrace{\begin{pmatrix} w_{11} & w_{12} & \dots & w_{1c} \\ w_{21} & w_{22} & \dots & w_{2c} \\ \vdots & \vdots & \vdots & \vdots \\ w_{f1} & w_{f2} & \dots & w_{fc} \end{pmatrix}}_{f \times c \ (feature \ weight \times channels)}$$

- *Same as all other networks*
  - *Each vertex (row) is represented as an array of features (columns)*

The Weights



Consider a graph with n nodes, each containing f features.

$$A.X.W = \underbrace{\begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{21} & 0 & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & 0 \end{pmatrix}}_{n \times n \ adjacency} \underbrace{\begin{pmatrix} \vdots & x_{12} & \vdots & \vdots & \vdots \\ x_{21} & x_{22} & x_{23} & \dots & x_{2f} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & x_{n2} & \vdots & \vdots & \vdots \end{pmatrix}}_{n \times f \ (nodes \times features)} \underbrace{\begin{pmatrix} w_{11} & w_{12} & \dots & w_{1c} \\ w_{21} & w_{22} & \dots & w_{2c} \\ \vdots & \vdots & \vdots & \vdots \\ w_{f1} & w_{f2} & \dots & w_{fc} \end{pmatrix}}_{f \times c \ (feature \ weight \times channels)}$$

- *The weight matrix W is used on each vertex to create new function of the inputs x (encoding)*
- *If wij=1, the input representations is used directly in the message passing*

The Adjacency Matrix

Consider a graph with n nodes, each containing f features.

$$A.X.W = \underbrace{\begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{21} & 0 & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & 0 \end{pmatrix}}_{n \times n \ adjacency} \underbrace{\begin{pmatrix} \vdots & x_{12} & \vdots & \vdots & \vdots \\ x_{21} & x_{22} & x_{23} & \dots & x_{2f} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & x_{n2} & \vdots & \vdots & \vdots \end{pmatrix}}_{n \times f \ (nodes \times features)} \underbrace{\begin{pmatrix} w_{11} & w_{12} & \dots & w_{1c} \\ w_{21} & w_{22} & \dots & w_{2c} \\ \vdots & \vdots & \vdots & \vdots \\ w_{f1} & w_{f2} & \dots & w_{fc} \end{pmatrix}}_{f \times c \ (feature \ weight \times channels)}$$

- *Embeds graph structure: says which vertex is connected to which.*
- *The value could be 1 (0 for no connection) or it could be a weight*
- *Could be used with attention mechanism: the fixed weights are replaced by learnable parameters. In training, the graph decides which connections are relevant*

The Message Passing

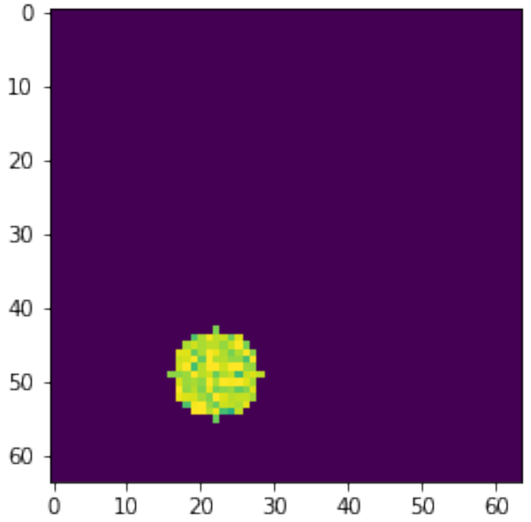
Consider a graph with n nodes, each containing f features.

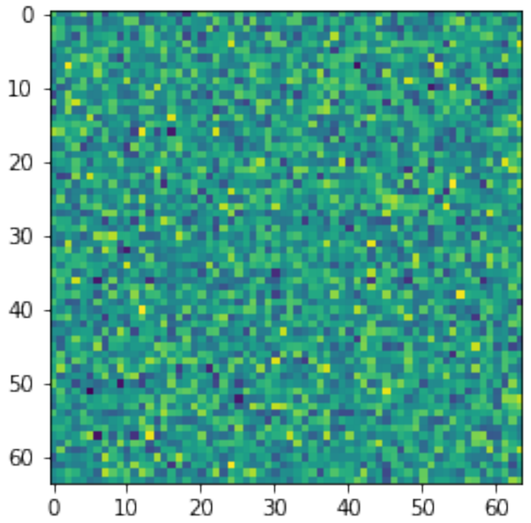
$$A.X.W = \underbrace{\begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{21} & 0 & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & 0 \end{pmatrix}}_{n \times n \ adjacency} \underbrace{\begin{pmatrix} \vdots & x_{12} & \vdots & \vdots & \vdots \\ x_{21} & x_{22} & x_{23} & \dots & x_{2f} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & x_{n2} & \vdots & \vdots & \vdots \end{pmatrix}}_{n \times f \ (nodes \times features)} \underbrace{\begin{pmatrix} w_{11} & w_{12} & \dots & w_{1c} \\ w_{21} & w_{22} & \dots & w_{2c} \\ \vdots & \vdots & \vdots & \vdots \\ w_{f1} & w_{f2} & \dots & w_{fc} \end{pmatrix}}_{f \times c \ (feature \ weight \times channels)}$$

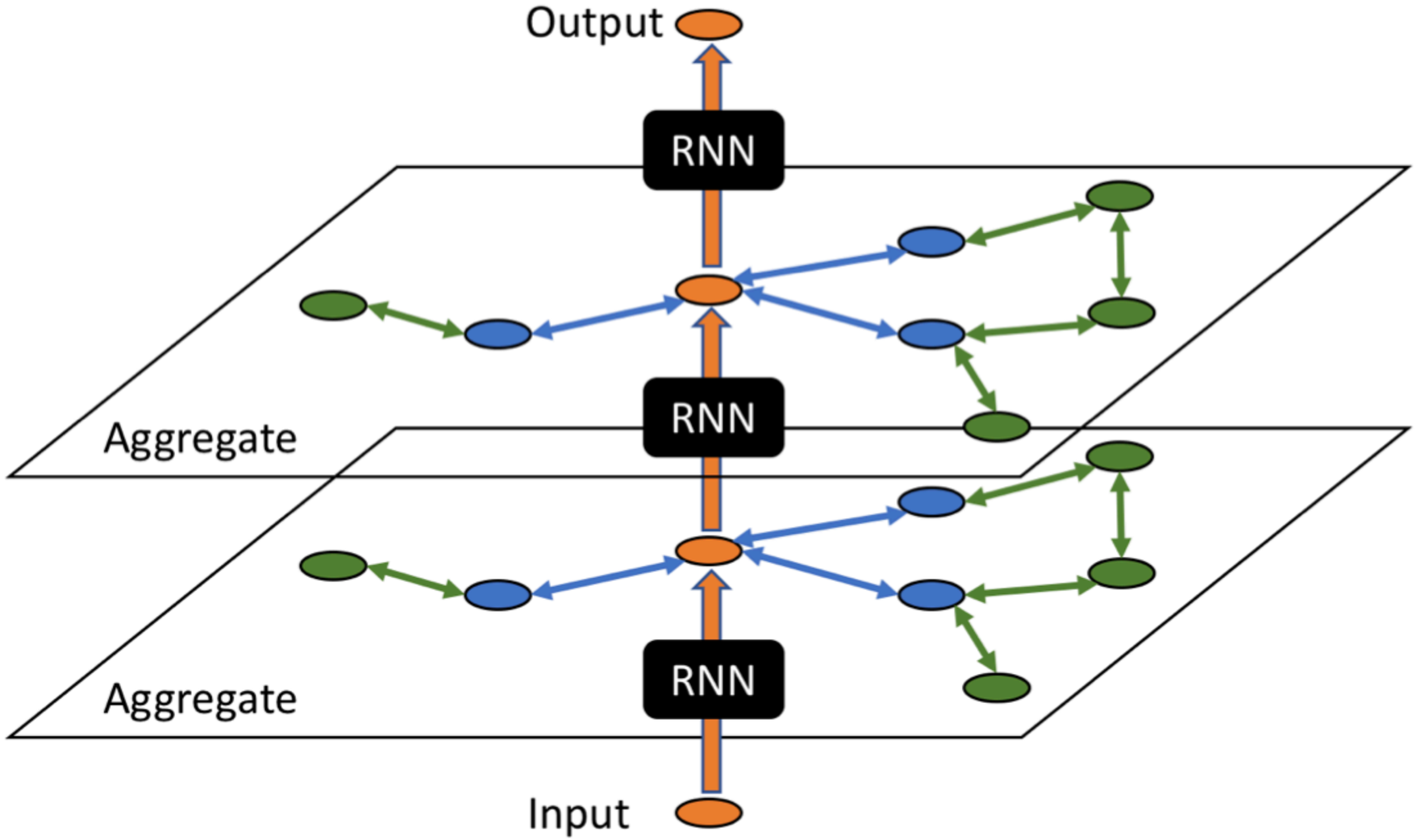
- *By performing a standard matrix product, one builds the message*
- *This is for one filter. One can have multiple filters, as for CNNs*

We will use GCNs for exercise

- *Images of 64x64x1 pixels*
  - *Class 1: a sample of circles in grey scale (one channel, pixels filled with value in [0,1])*
    - *Fill pixels with Gaus(0.9,0.1)*
  - *Class 0: a noise sample, filled with G(m,0.1) (m =0.3 or 0.7)*
- *Take the 100 pixels closer to 1*
- *Represent the event as a (100,3) list, the three features being (iX, iY, GrayScale)*



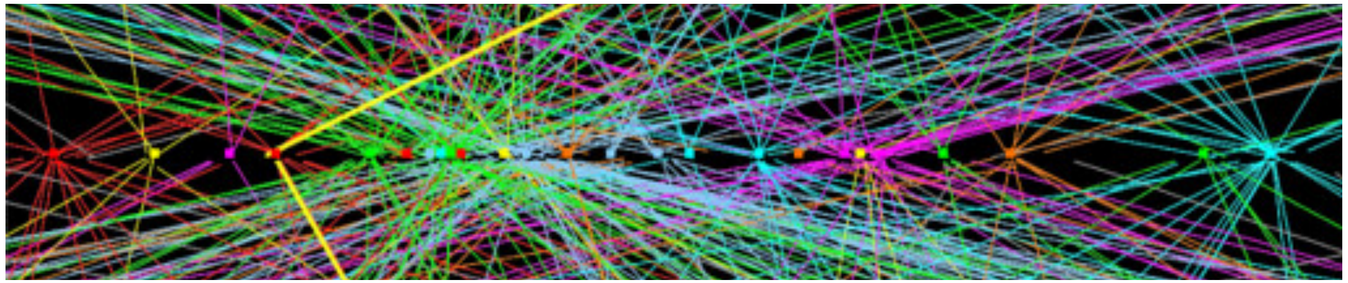


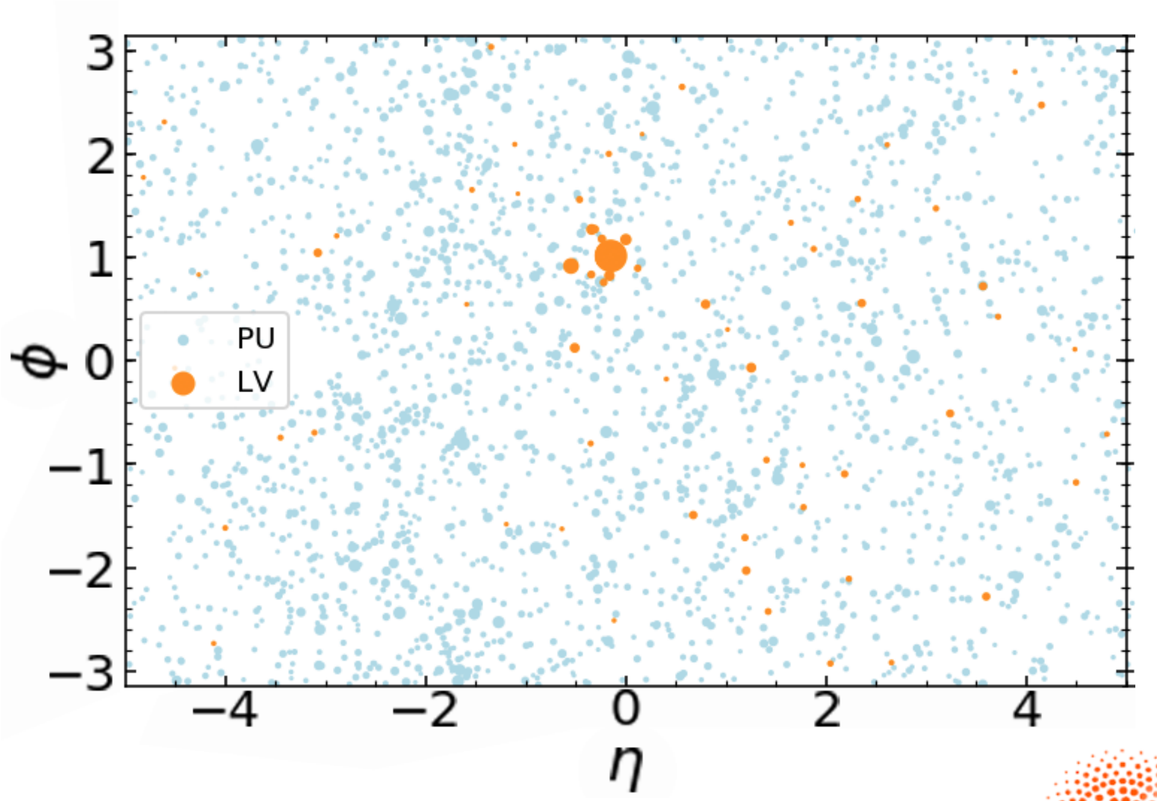


Gated Graph Neural Networks

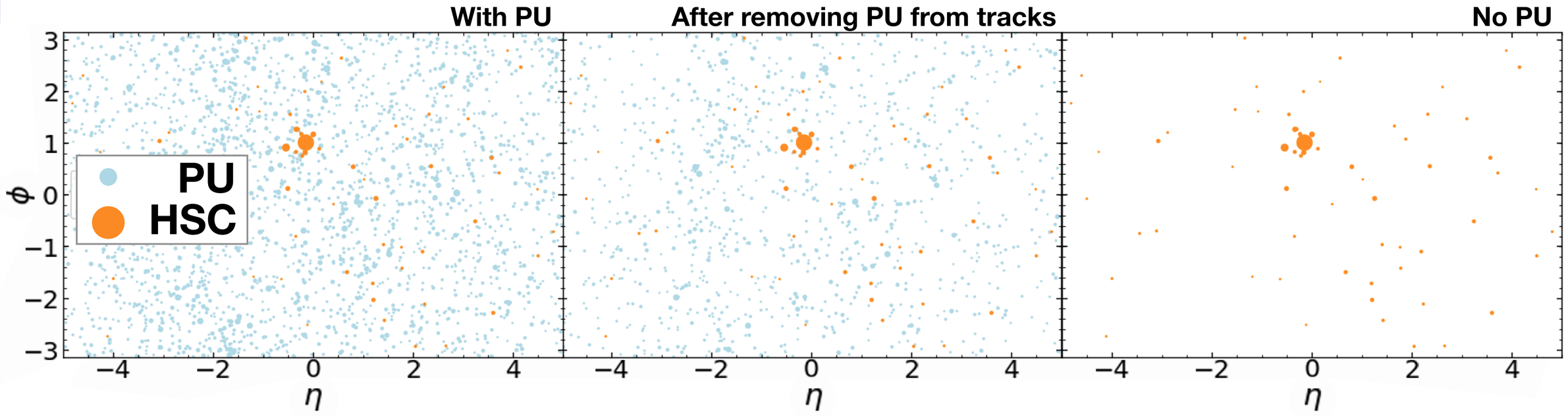
Example: pileup removal

- *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*



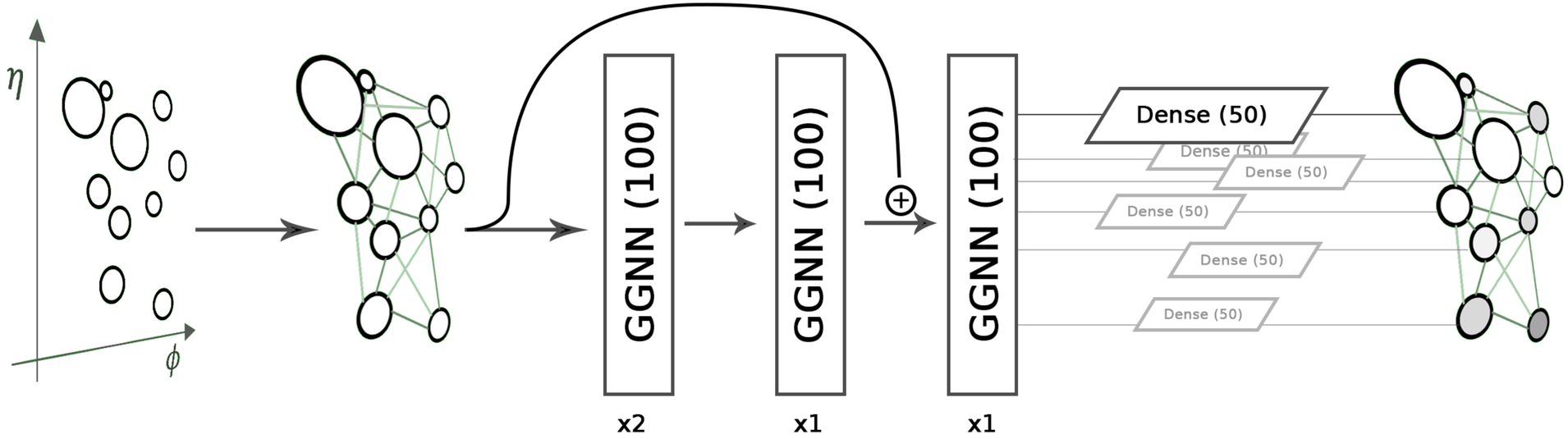


Example: pileup removal



- *We want to learn if a given neutral comes from PU of 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*

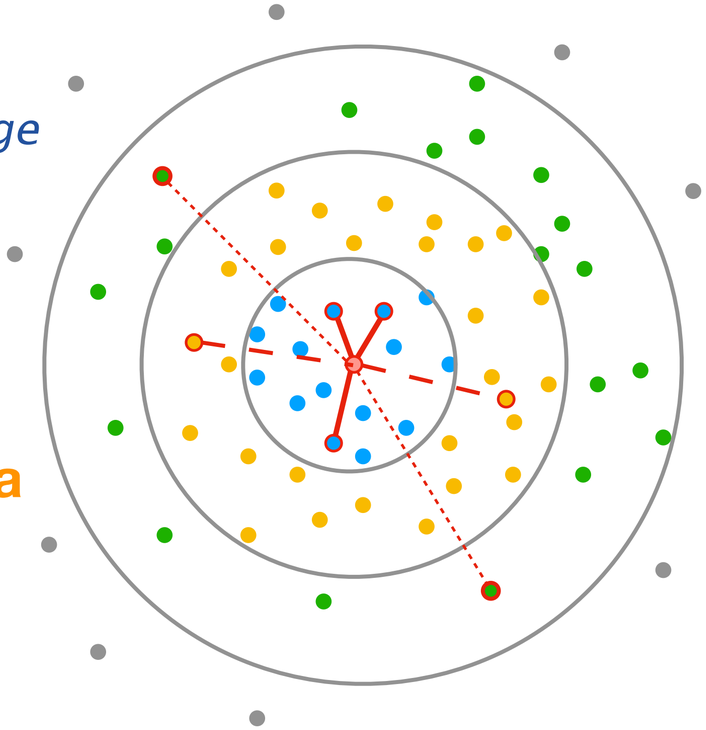
Graph Networks for PU removal



- *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<R0) 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



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

$$m_j = \frac{1}{N}\sum_{j}^{N} m_{v,v_j} = \sum_{j} \mathbf{A} \times f_j$$

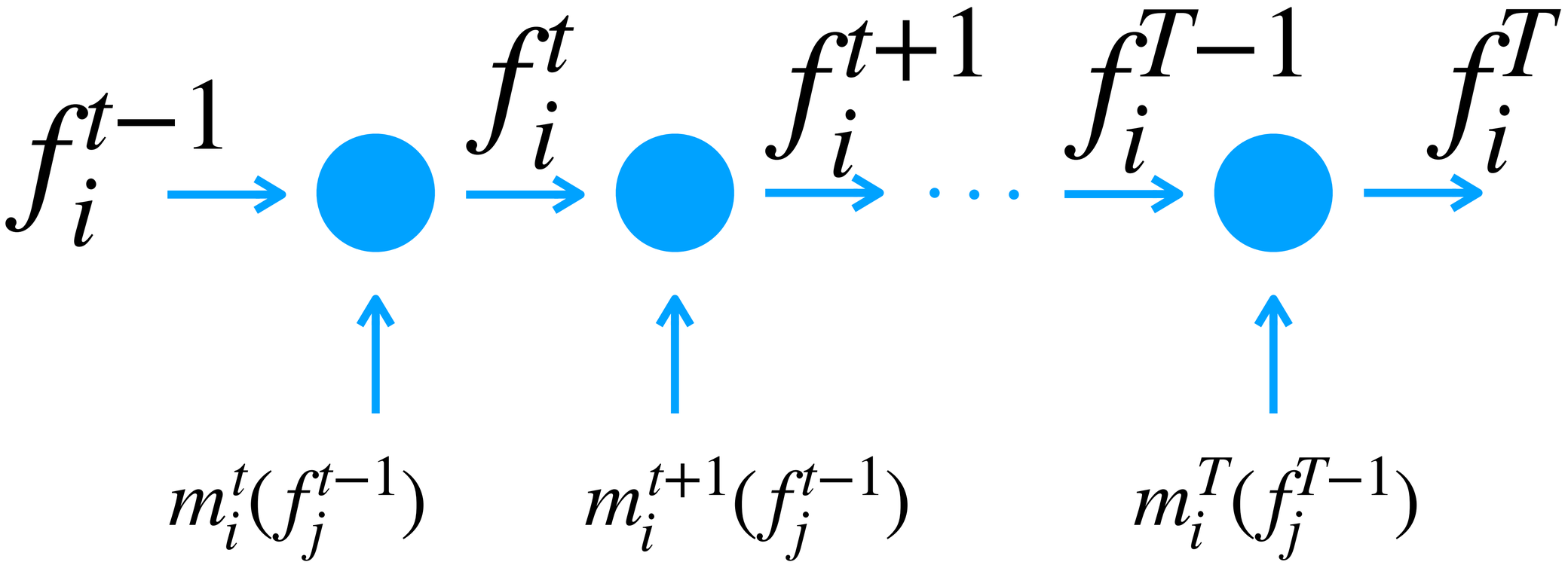
Gathered message

Messages

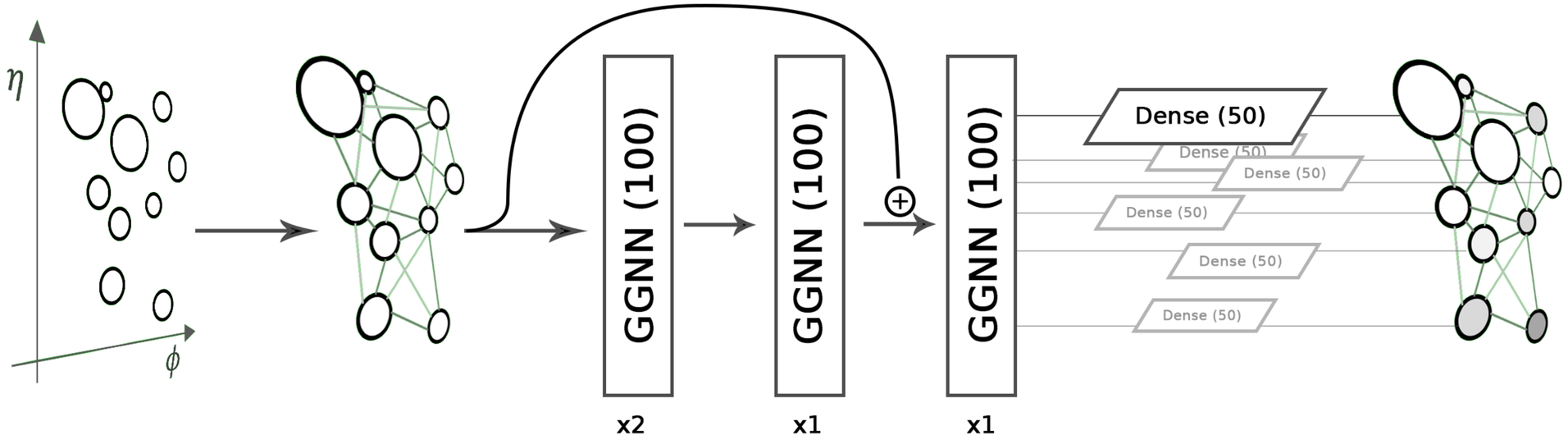
features of the j-th vertex

Multiple message passing

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



Done 3 times (for 3 GRU layers)

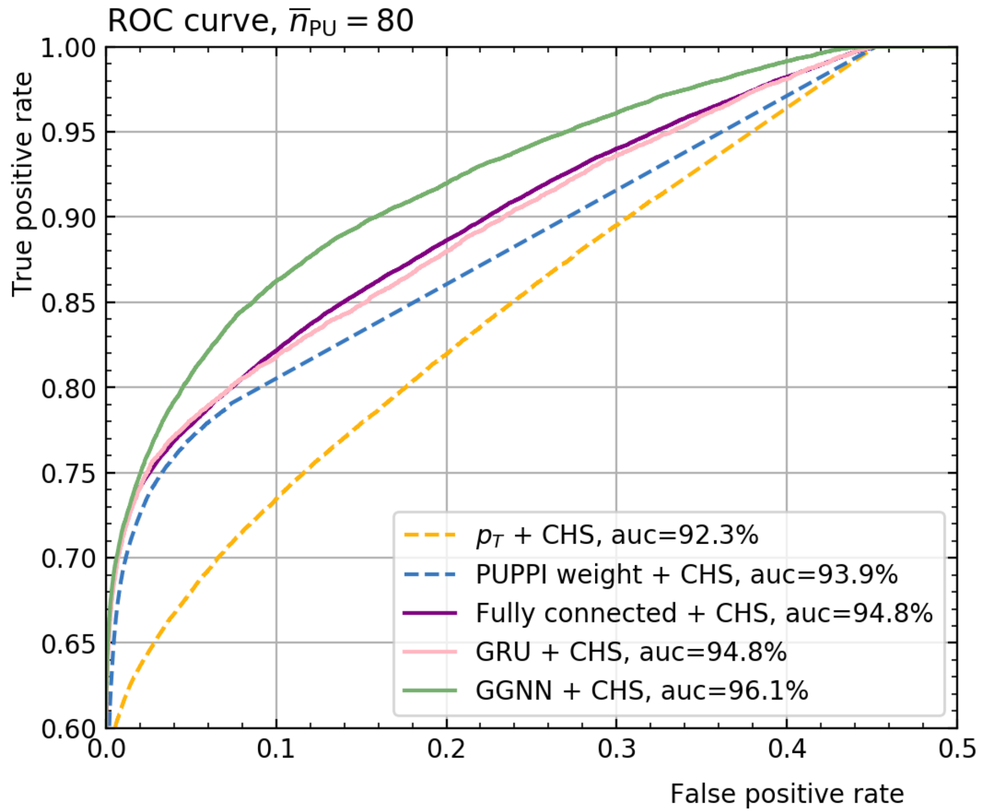


- *The representation created by each layer is passed to the next*
- *A ResNet-like skip connection is implemented (input -> last layer)*
- *The per-particle outcome set of features (function of the features of the connected particles) is used to train a dense classifier: PU vs interesting particle?*

PUPPIML: Graph Nets for PU subtraction

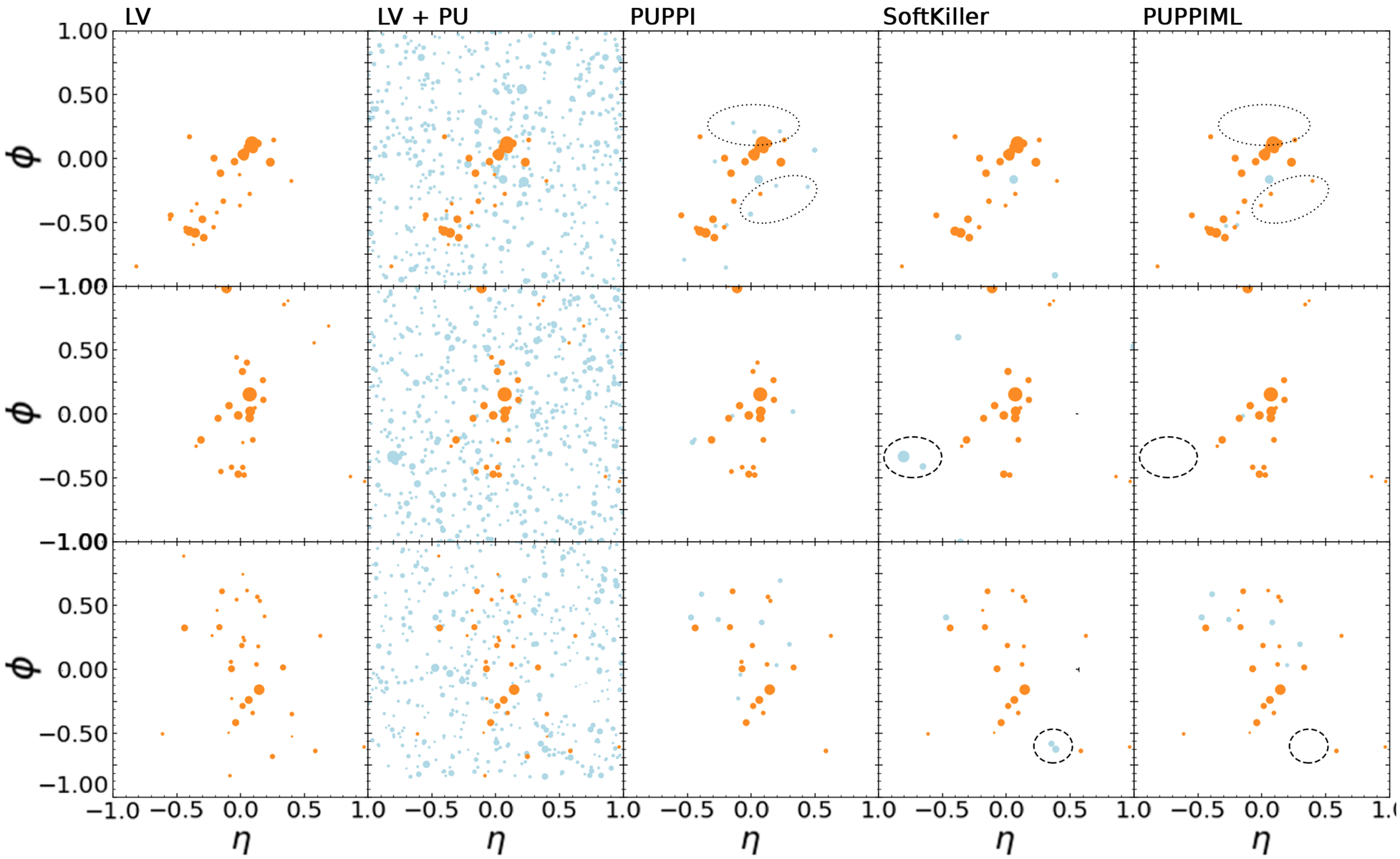
- *Improve state-of-the-art algorithms substantially*
- *Little dependence of algorithm tuning on pileup conditions*
- *Small/No performance loss with average number of PU collisions*
- *Outperforms alternative particle-based architectures (DNNN, simple GRU)*

$\overline{n}_{\mathrm{PU}}$	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

PUPPIML: Graph Nets for PU subtraction



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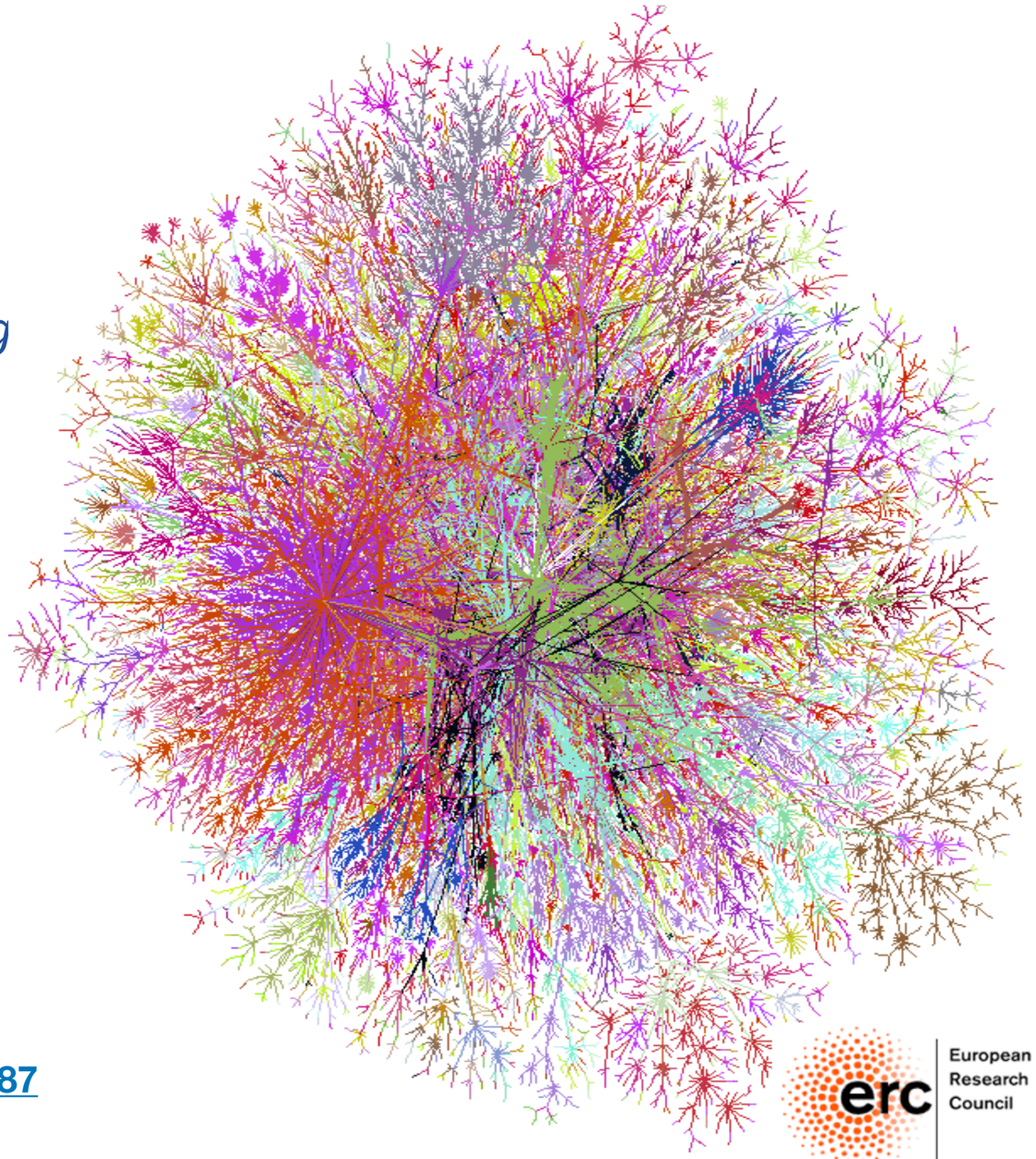
Distance-Weighted Graph Networks

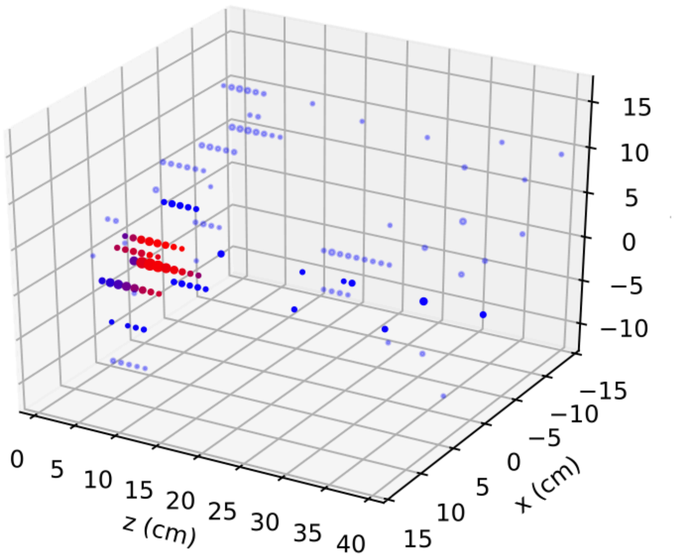
Reducing memory consumption

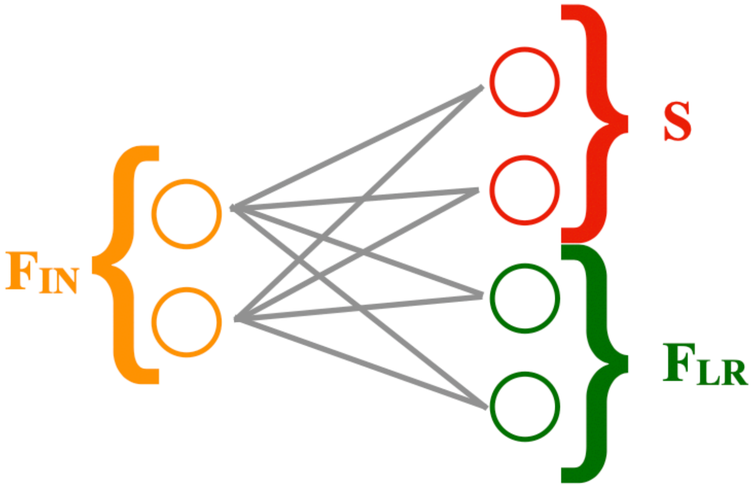
- *When building a graph of N vertices, number of edges (and number of computing operations) scale with N^2*
- *This might clash with computing resource limitations (both for training and inference)*
- *Certainly, this is the case at the LHC*
  - *real-time event selection runs in short time*
  - *most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

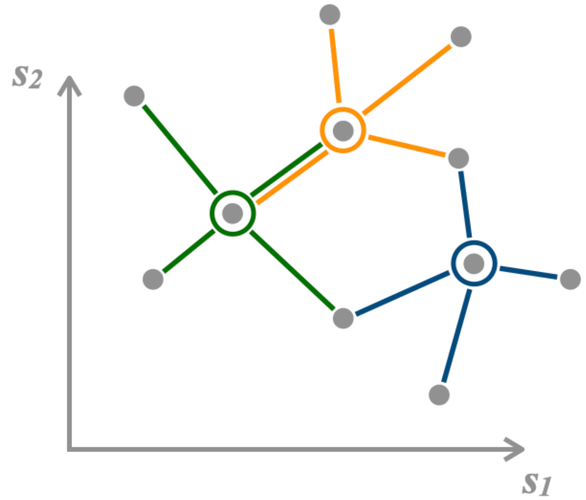


GravNet

https://arxiv.org/abs/1902.07987







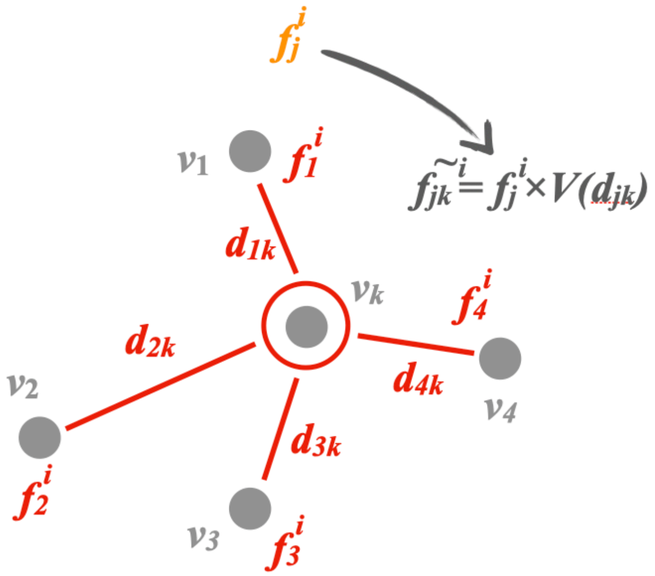
1) Start with a graph in geometric space. Each vertex feature vector F_{IN} is characterized by coordinates and features

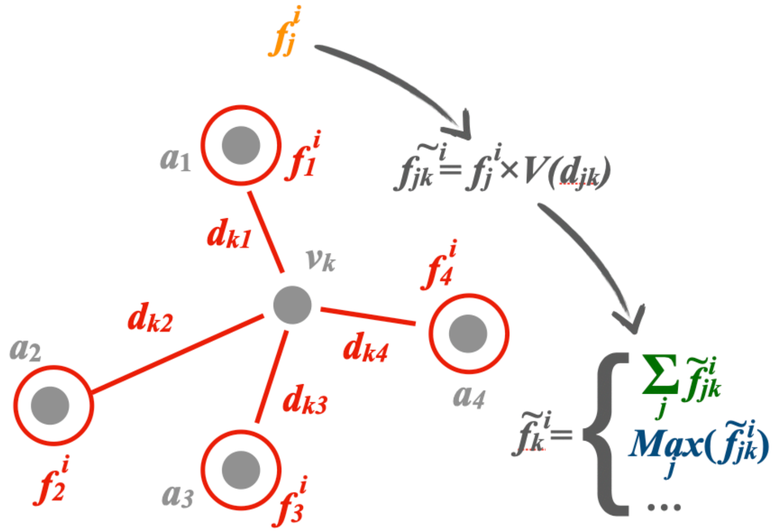
2) Each F_{IN} is processed by a linear network, returning two outputs: a coordinate vector s & a learned representation F_{LR}

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

GravNet

https://arxiv.org/abs/1902.07987



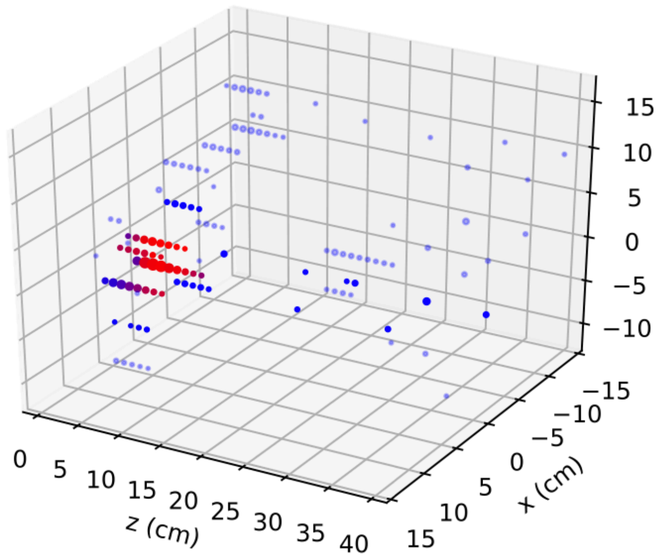


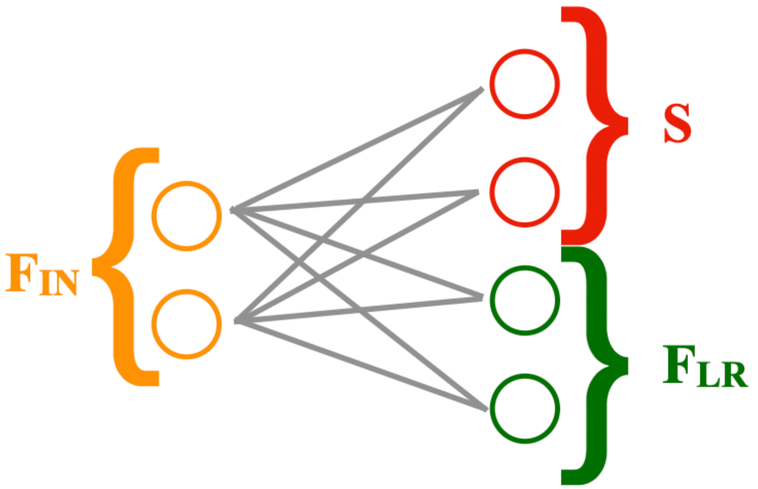
4) Unlike DGCNN, the message function is a potential function (we use e^{-d^2} where d is the Euclidean distance in learned space)

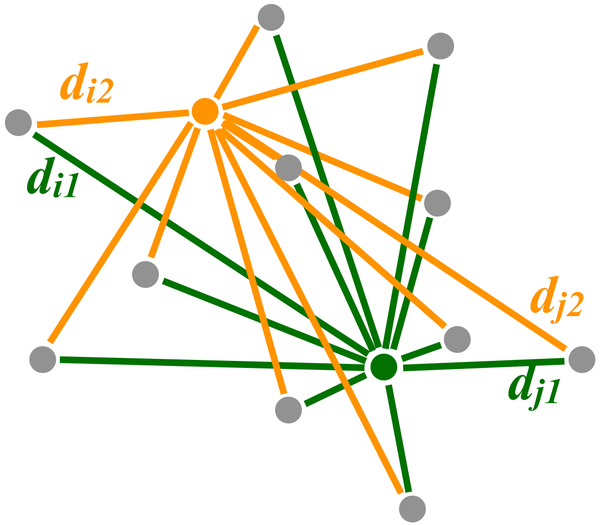
5) Message aggregated with different functions (Max, Average,…)

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 Ns aggregators

https://arxiv.org/abs/1902.07987

https://arxiv.org/pdf/2008.03601.pdf

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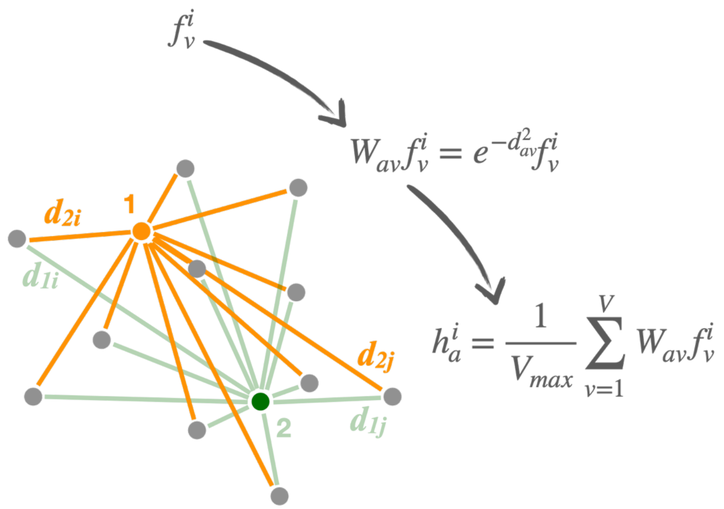
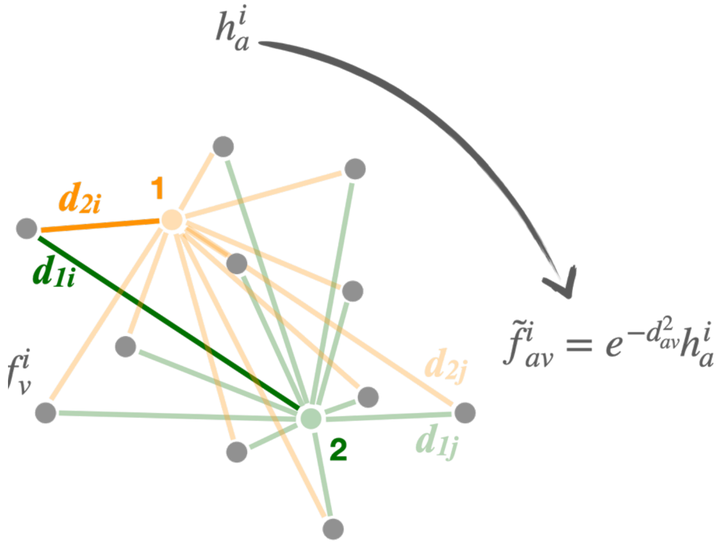
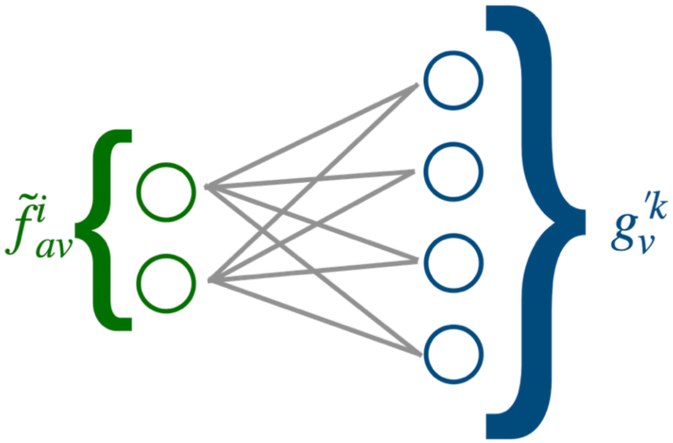
(simplified) GarNet



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 $W_{ab} = e^{-d_{ab}}$)



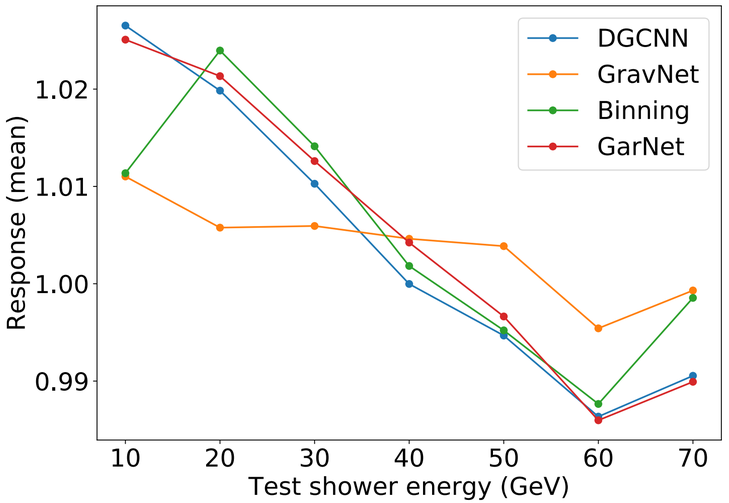
6) Final representation is learned from the engineered features and the original ones

https://arxiv.org/abs/1902.07987

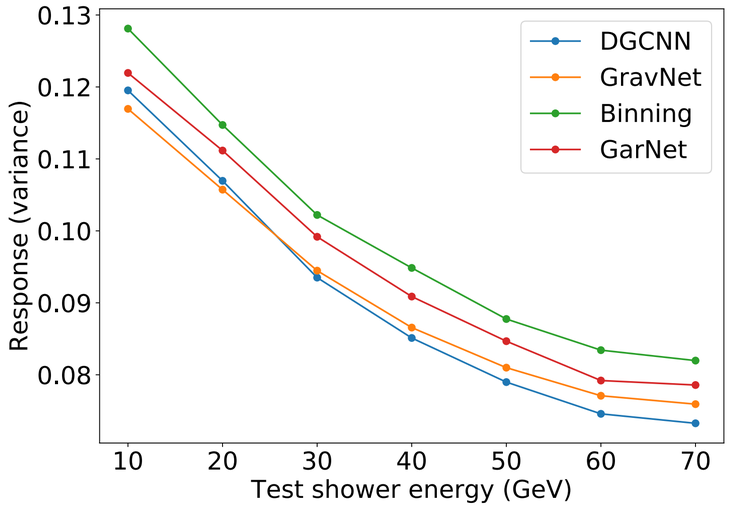
https://arxiv.org/pdf/2008.03601.pdf

GarNet & GravNet for Calorimetry

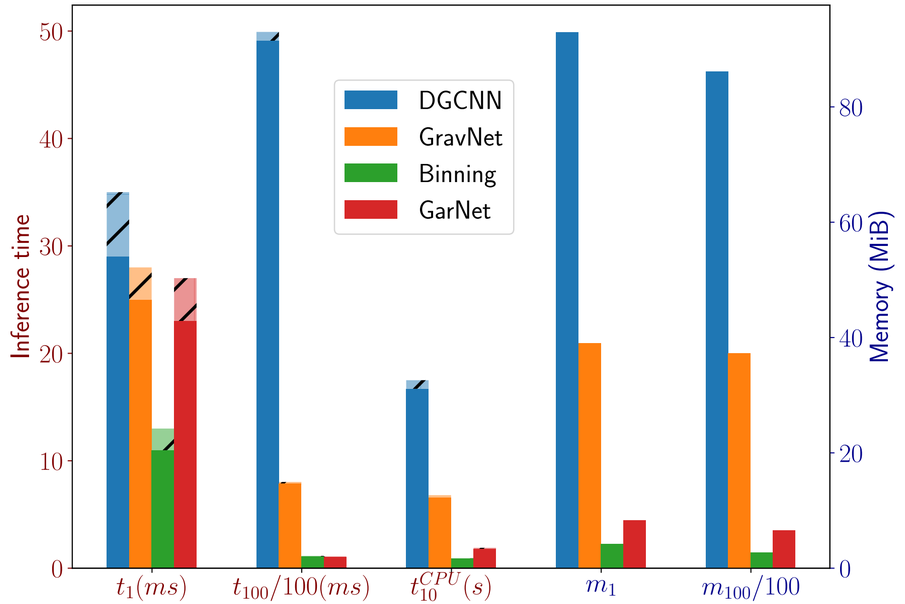
- *Good performance achieved, comparable to DGCNN and traditional approaches*
- *Using a potential (V(d)) to weight up the near neighbours allows to keep memory footprint under control (with respect to other graph approaches)*



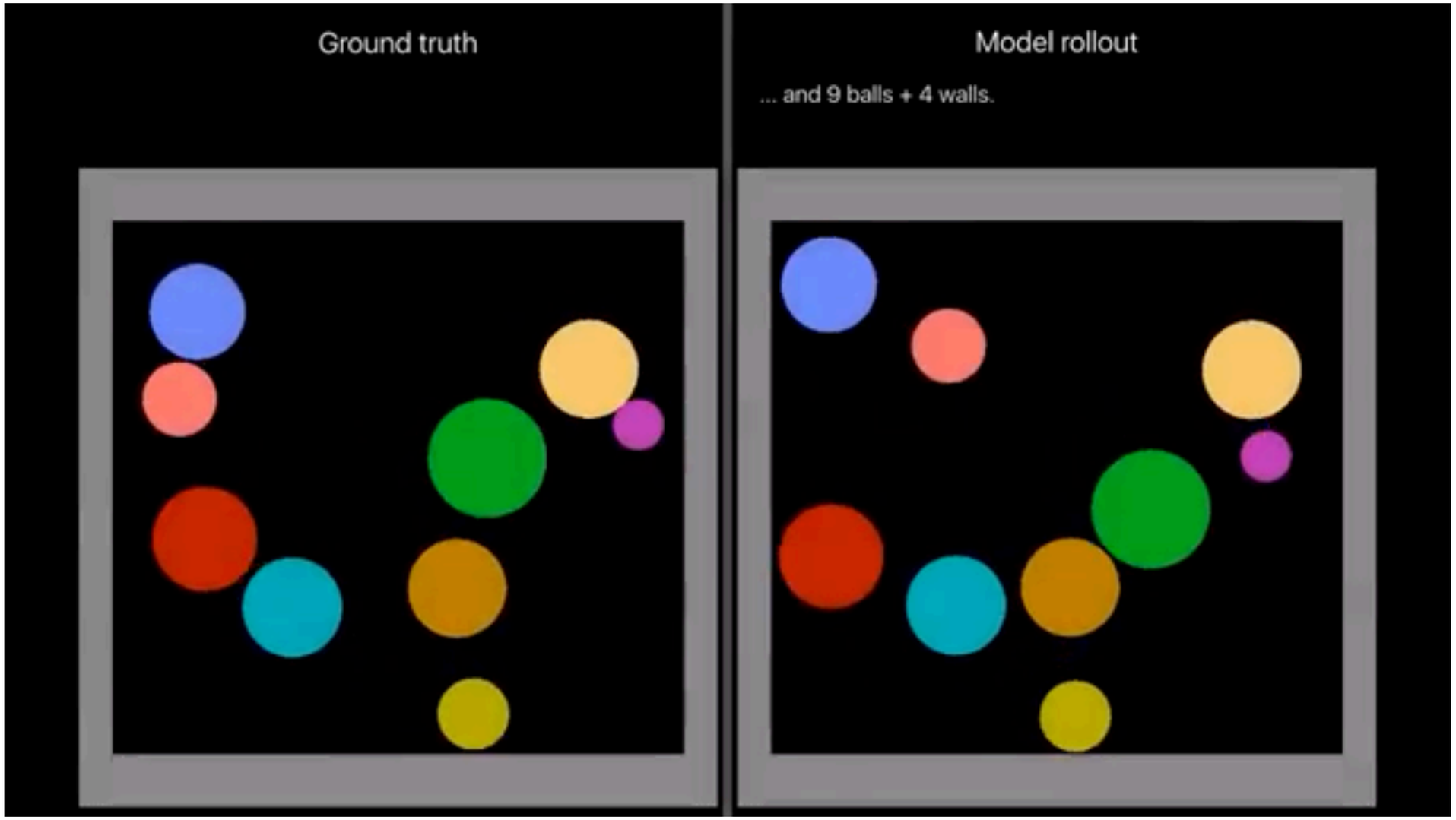
(c) Mean



(d) Variance



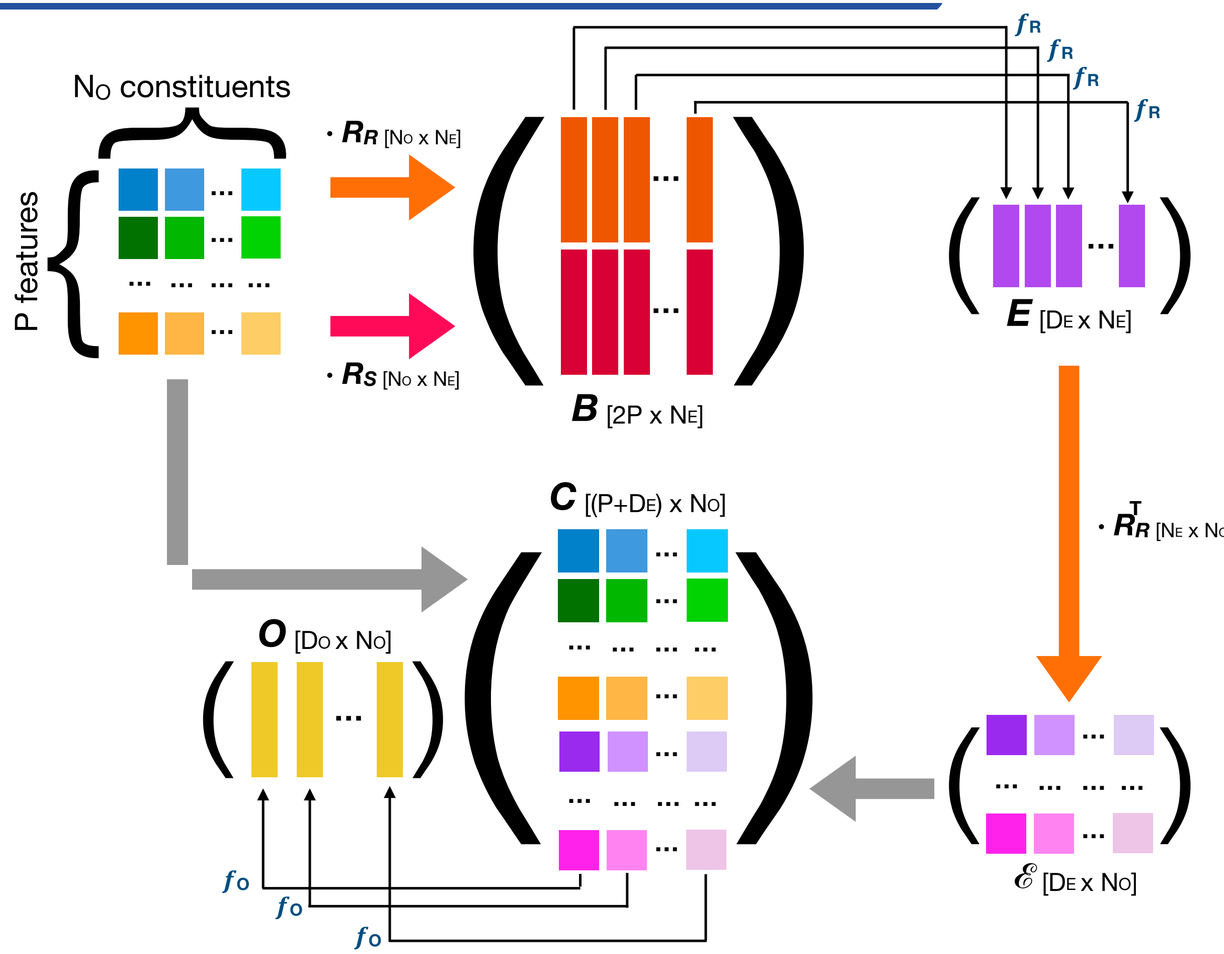
Interaction Networks



https://arxiv.org/abs/1612.00222

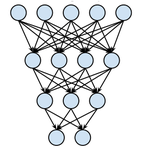
Interaction Networks

- *INs process a list of No x P inputs in pairs, through Receiving and Sending matrices*



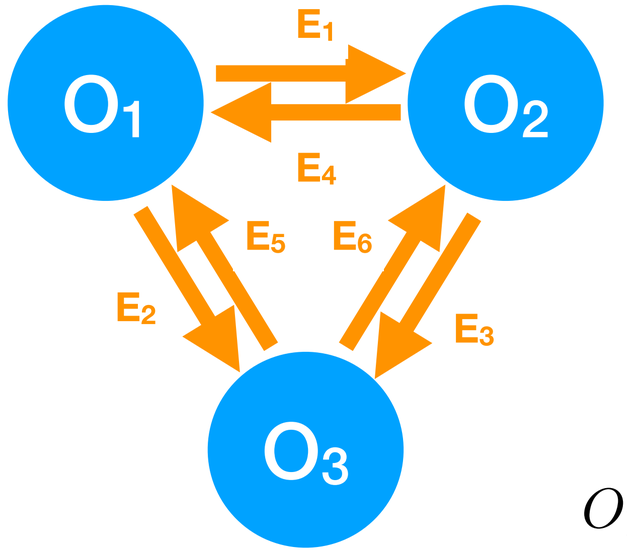
NO: # of constituents
P: # of features
NE = NO(NO-1): # of edges
DE: size of internal representations
DO: size of post-interaction internal representation

ϕC, fO, fR parameterized as neural networks



Interaction Networks

- *INs process a list of No x 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*

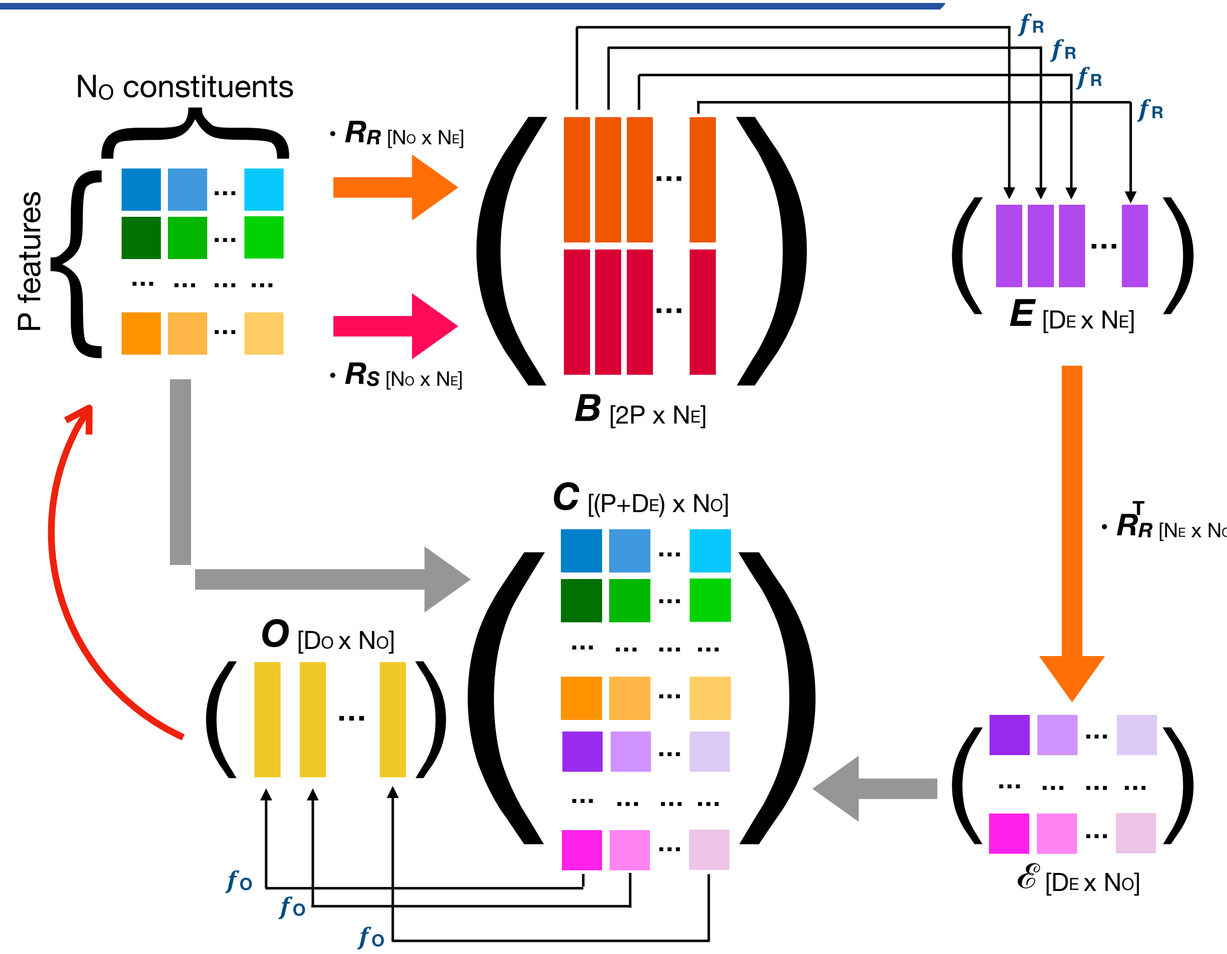


$$R_R = \begin{array}{c} \\ O_1 \\ O_2 \\ O_3 \end{array} \begin{array}{c} \begin{array}{cccccc} E_1 & E_2 & E_3 & E_4 & E_5 & E_6 \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

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

Interaction Networks

- *INs process a list of No x 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*
- *The procedure can then be iterated to produce further steps i the interactions*

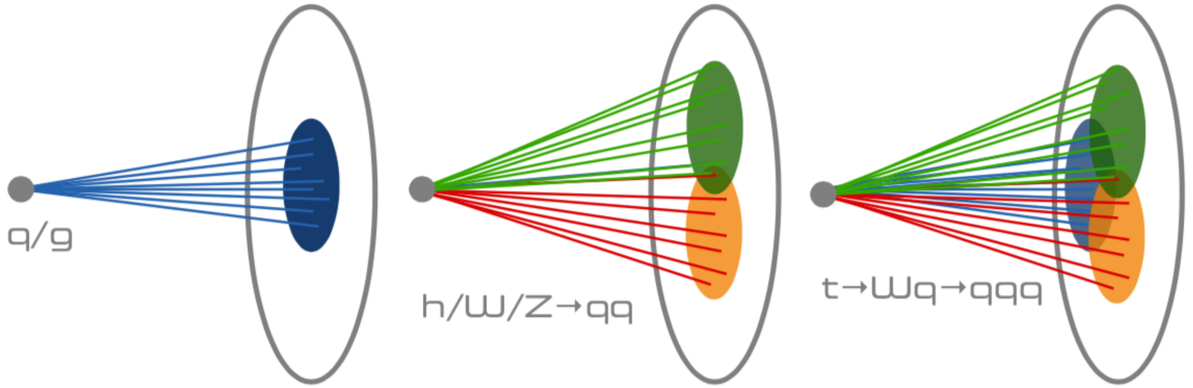


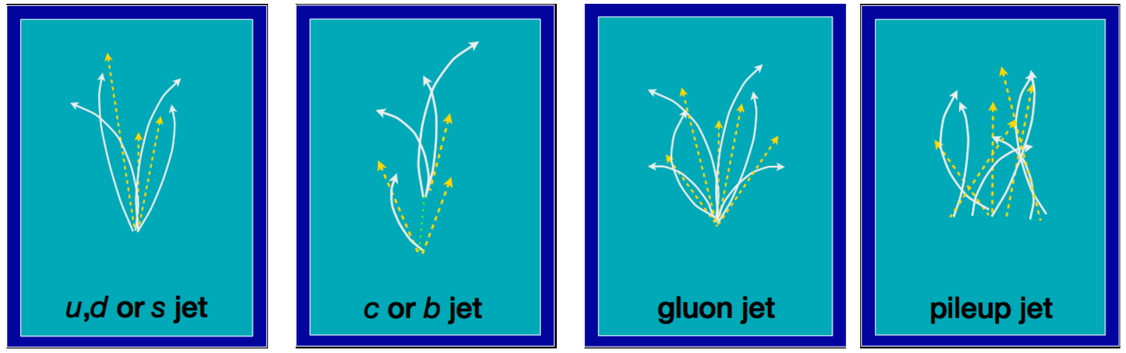
NO: # of constituents
P: # of features
NE = NO(NO-1): # of edges
DE: size of internal representations
DO: size of post-interaction internal representation

ϕC, fO, fR parameterized as neural networks

Example: jet tagging

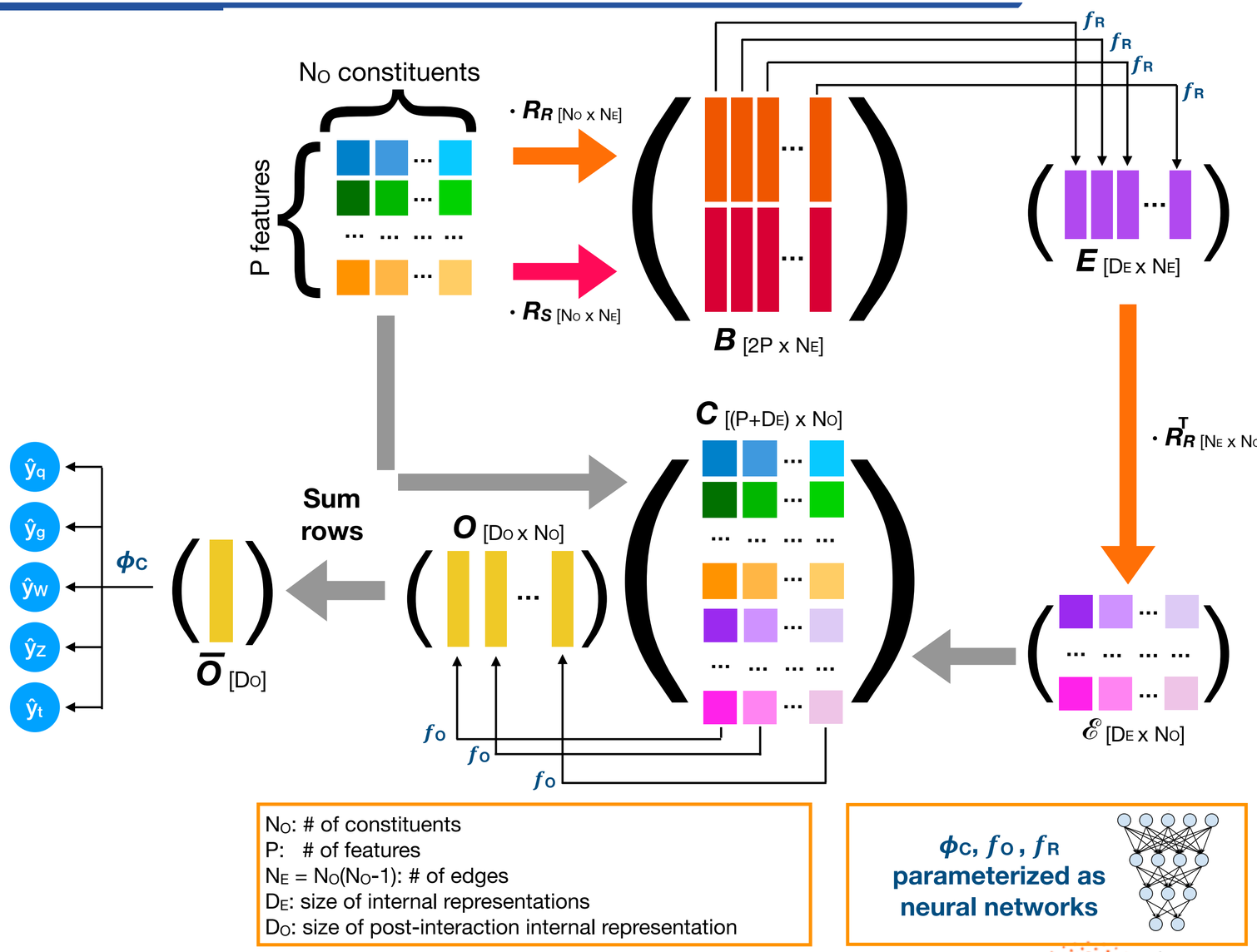
- *You have a jet at LHC: spray of hadrons coming from a "shower" initiated by a fundamental particle of some kind (quark, gluon, W/Z/H bosons, top quark)*
- *You have a set of jet features whose distribution depends on the nature of the initial particle*
- *You can train a network to start from the 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

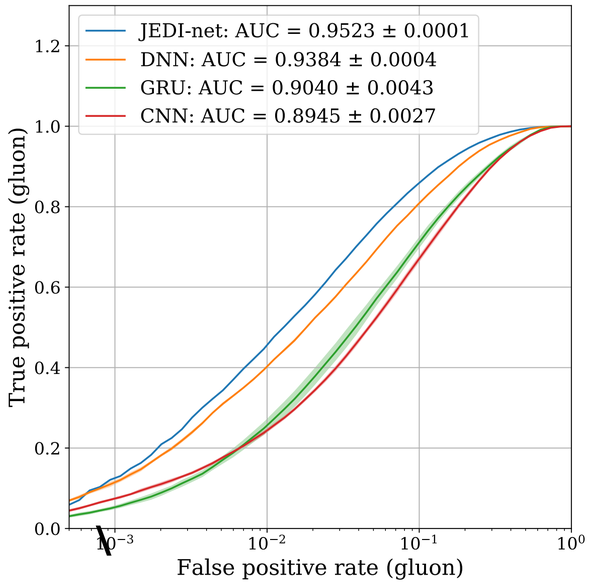
- *In this case, there is no system update needed (i.e., no cycle)*
- *It is sufficient to use the post-interaction representation as input to a classifier that returns the jet category*
- *The three networks are simultaneously optimized: the learned representation is chosen to help the classification*

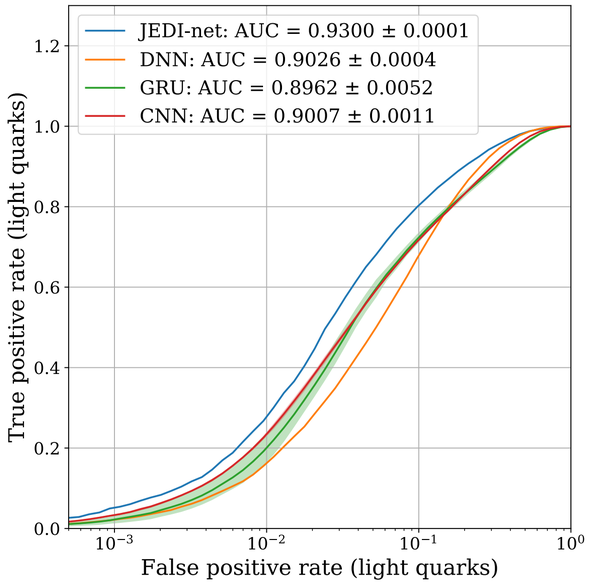


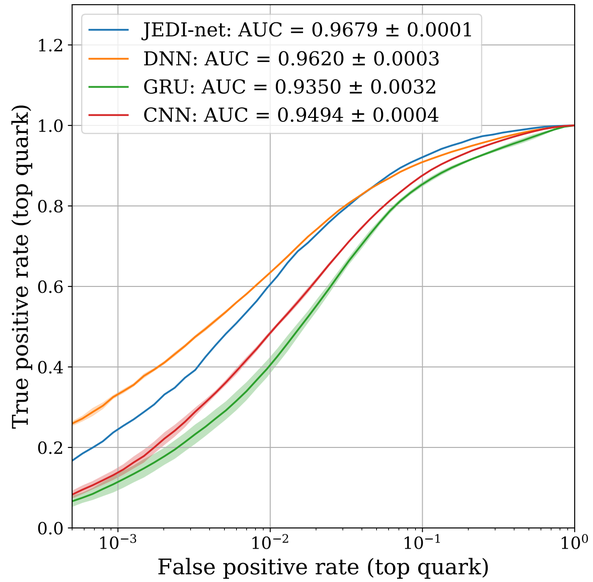
N_O: # of constituents
P: # of features
$N_E = N_O(N_O-1)$: # of edges
D_E: size of internal representations
D_O: size of post-interaction internal representation

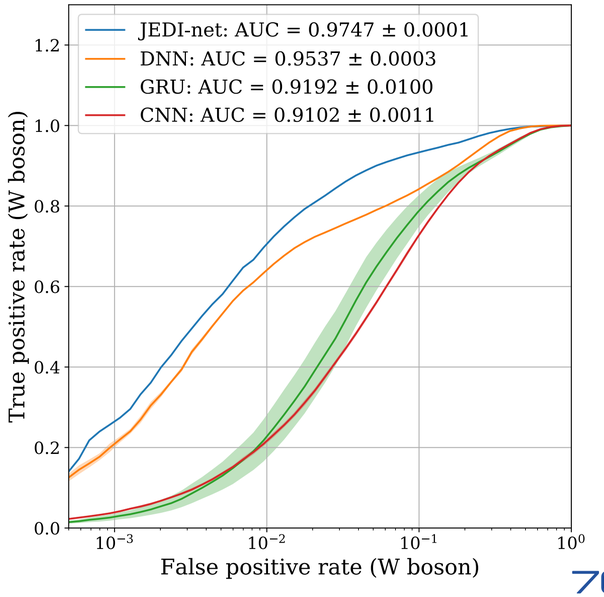
ϕ_C, f_O, f_R parameterized as neural networks

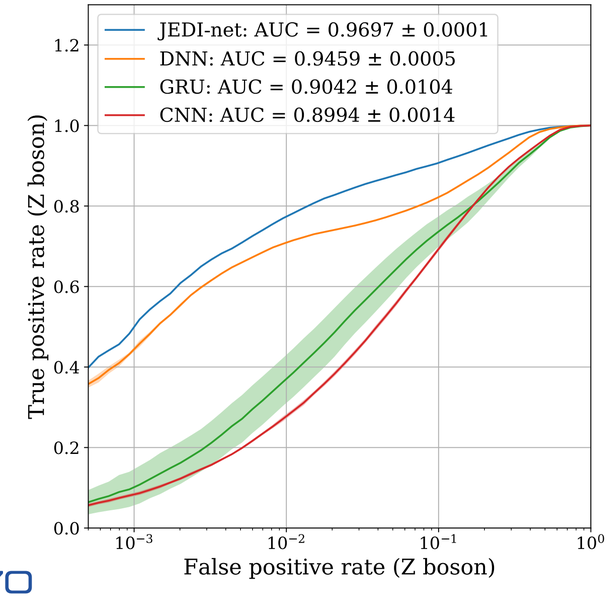
A comparison











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*