Neural Networks for Network-like structures

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ICL

Common examples so far

- Plain features (tables)
- Image
- Text
- Time series

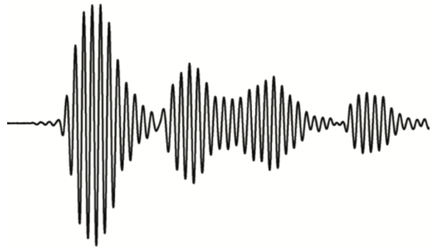
Таблица умножения в упрощенном виде

Фактически для запоминания **только 36 комбинаций !**
Остальные либо простые (например, умножение на 1 или 10),
либо обратимые (например 2*4 = 4*2).

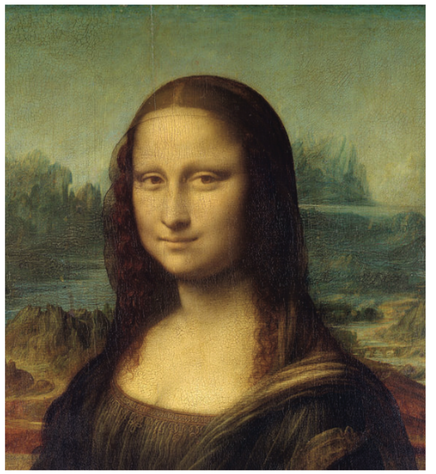
	2	3	4	5	6	7	8	9	
2	4	6	8	10	12	14	16	18	2
3	6	9	12	15	18	21	24	27	3
4	8	12	16	20	24	28	32	36	4
5	10	15	20	25	30	35	40	45	5
6	12	18	24	30	36	42	48	54	6
7	14	21	28	35	42	49	56	63	7
8	16	24	32	40	48	56	64	72	8
9	18	27	36	45	54	63	72	81	9
	2	3	4	5	6	7	8	9	

Doubt thou the stars are fire,
Doubt that the sun doth move,
Doubt truth to be a liar,
But never doubt I love...

Text



Audio signals

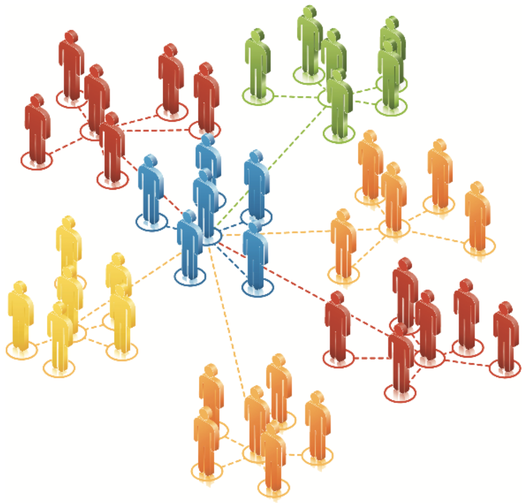


Images

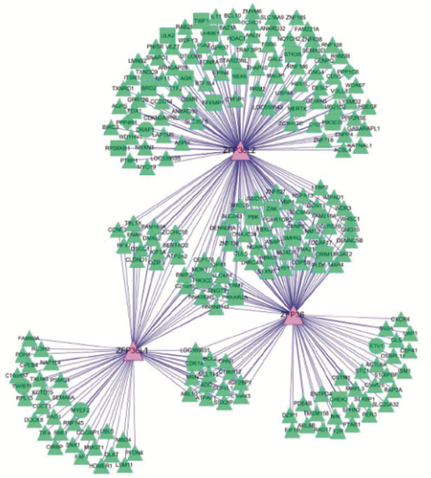
What about those?

Geometry
Manifolds
Graphs

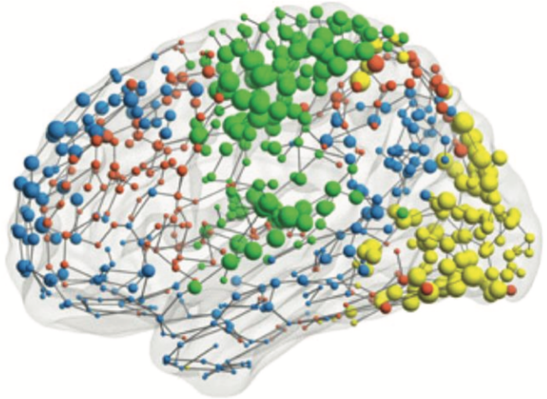
Non-euclidean distance,
twisted connectivity



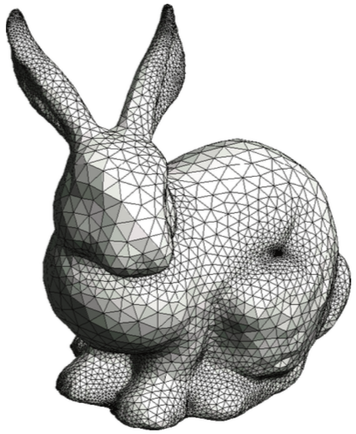
Social networks



Regulatory networks



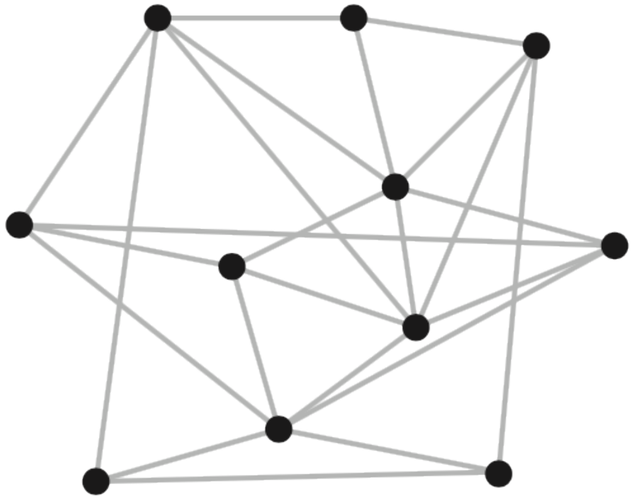
Functional networks



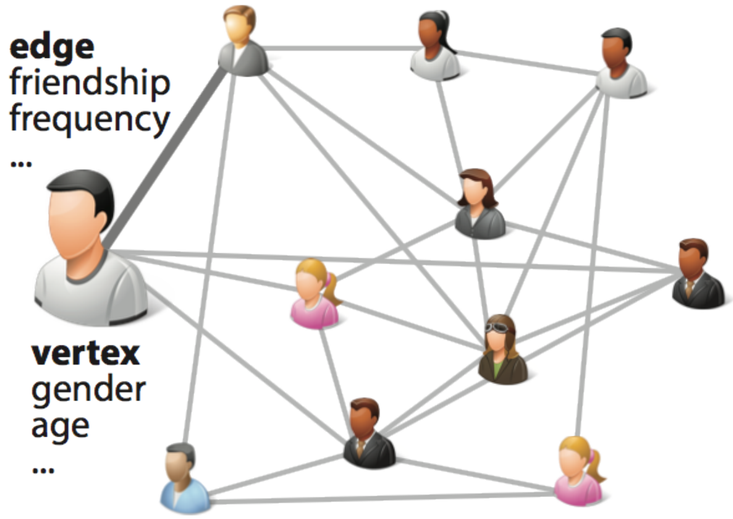
3D shapes

Formalization

- **Graph (structure):**
  - G(V, E), A – adjacency matrix
- **Features (data):**
  - Vertex (node) features
  - Edge features



Domain structure



Data on a domain

From hits to graph

K-nearest neighbors, euclidean distance

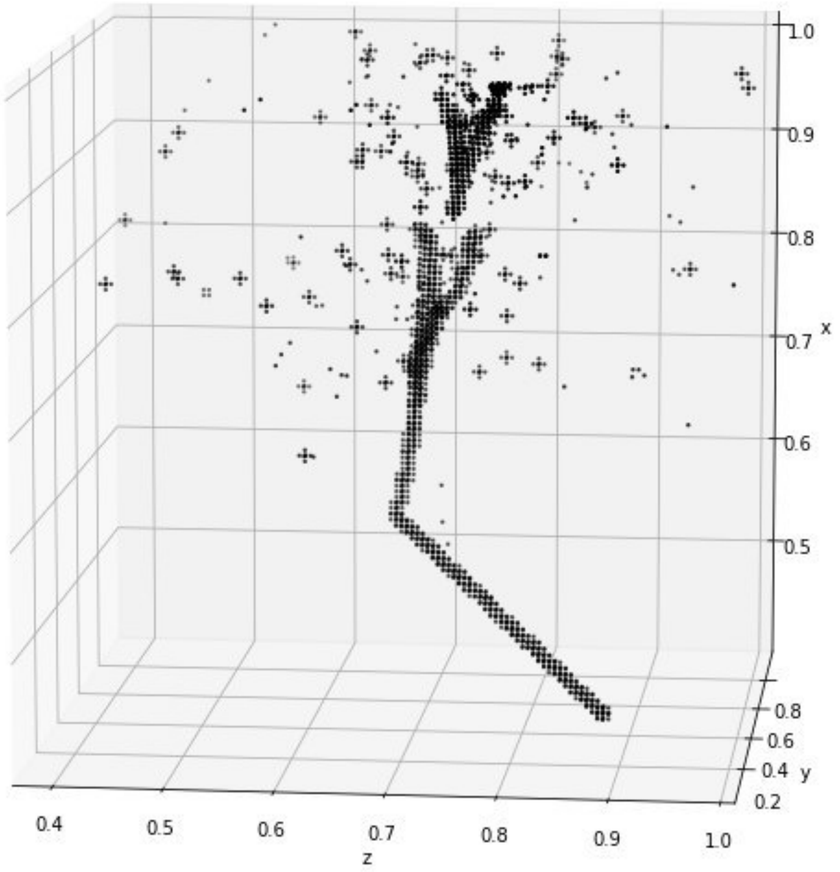
- Iterate by hits

1. Find K closest hits for each hit
2. Connect with edges

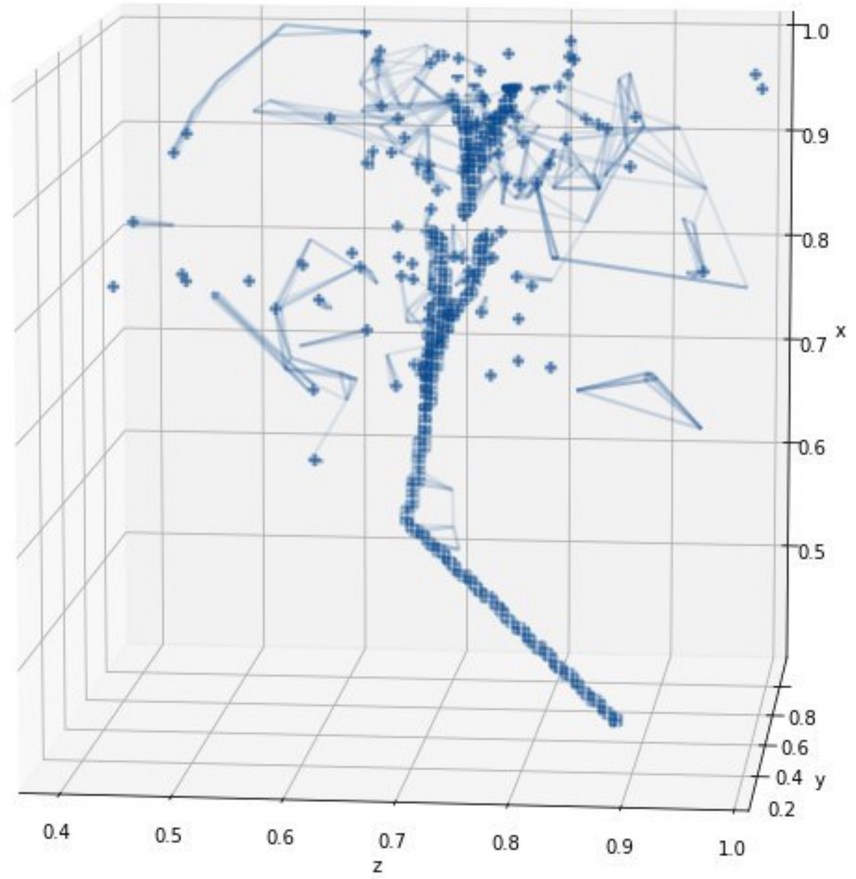
Radius graph, euclidean distance

- Iterate by hits

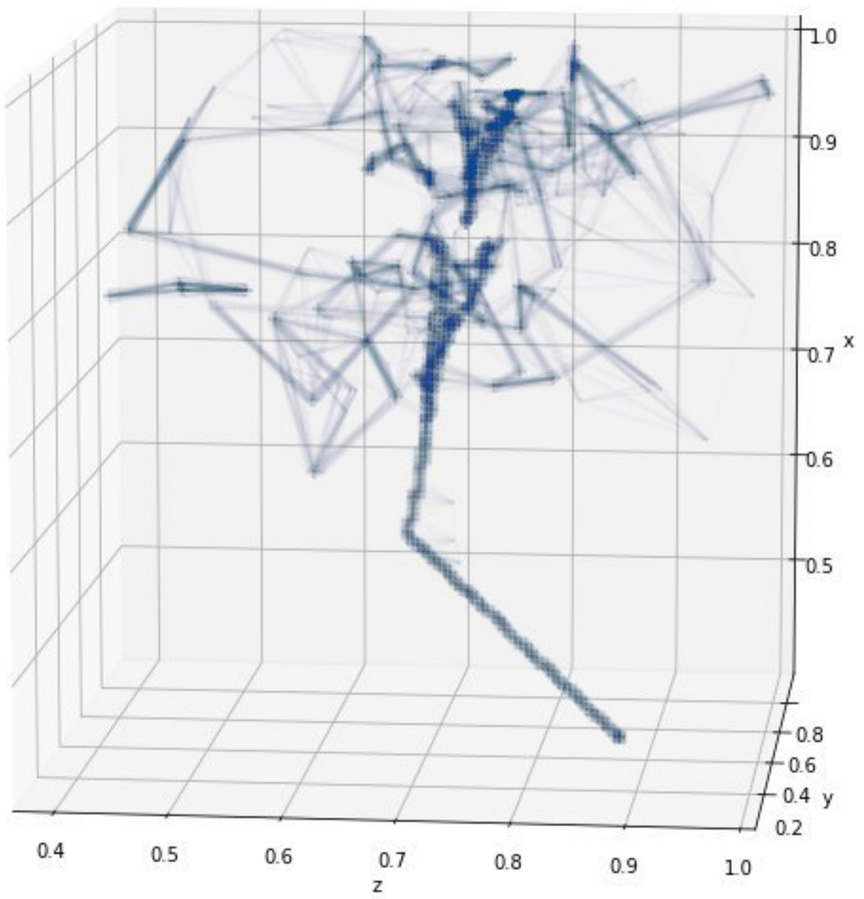
1. Find nodes within given radius and connect with an edge



After graph-ication



Neighbors = 5



Neighbors = 20

Neural Networks over graph

We want to learn some structural patterns in nodes adjacency (connectivity), that correlate with labels we want to predict for every node.

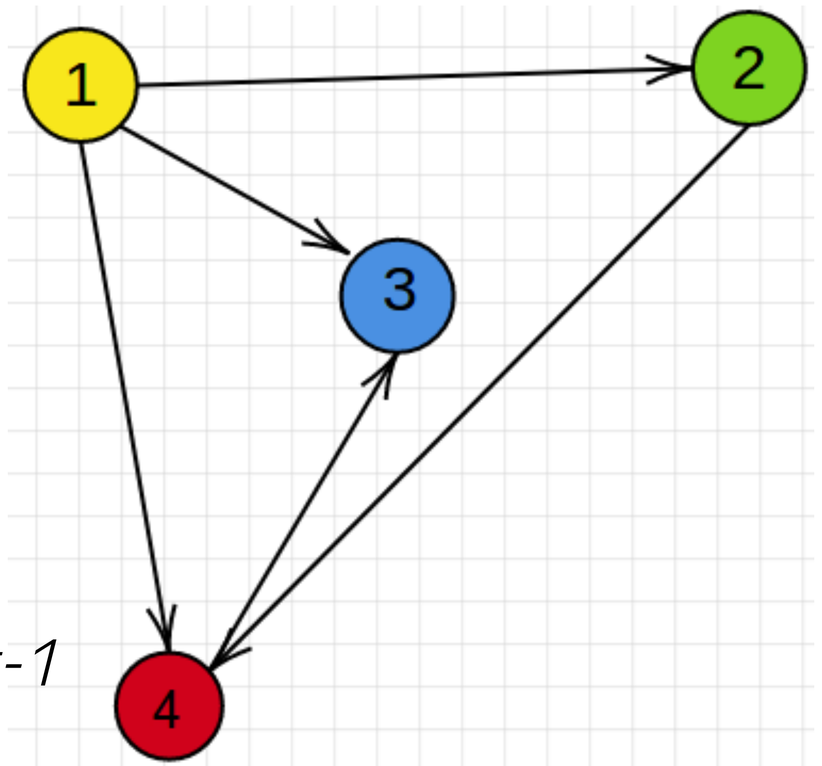
Connectivity patterns correspond to some structure in adjacency matrix. How can we reveal it using neural network?

Let’s assume that labels we want to predict correlate with certain computable function over incoming/outgoing edges of each node

Message Passing Neural Networks

We want to predict label for each node
Let's assume the following :

- Each *node has a state* (node features) at time *t*
- Each *edge has a state* (edge features) at time *t*
- *Message* is a **function** of source node state, destination node state and edge state at *t-1*
- Node state is a **function** of incoming messages at *t-1*
- Node *label* is a **function** of its state at *t* (*readout*)



Trivial Example

Step 0: pick random node states h_i^0
Step 1. Messages pass node state:

$m_{13} = h_1^0, m_{43} = h_4^0$

Step 2. Messages are aggregated:

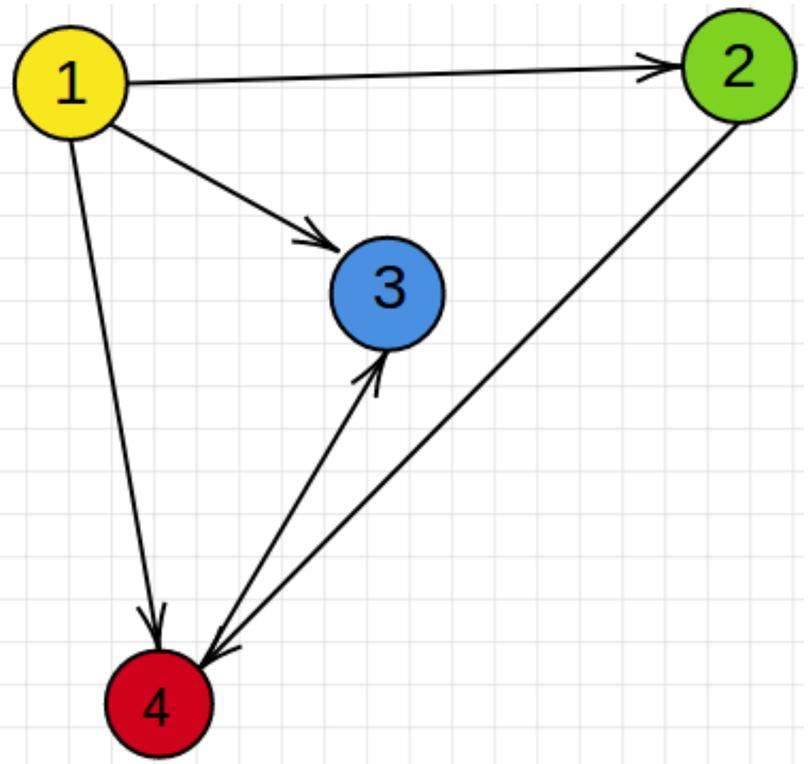
$M_3 = (m_{13} + m_{43})/2$

Step 3. Node updates its state:

$h_3^1 = (h_3^0 + M_3)/2$

Step 4. Estimate prediction (readout):

$R_3 = ||h_3^1||$



Starter Kit MPNN baseline

Ideas for improvement

- Clustering algorithm type, parameters
- Depth of messages (number of steps)
- State updater and message passer can have longer memory GRU/LSTM
- Use batches of events
- Different optimizers / learning rates
- Data augmentation

References

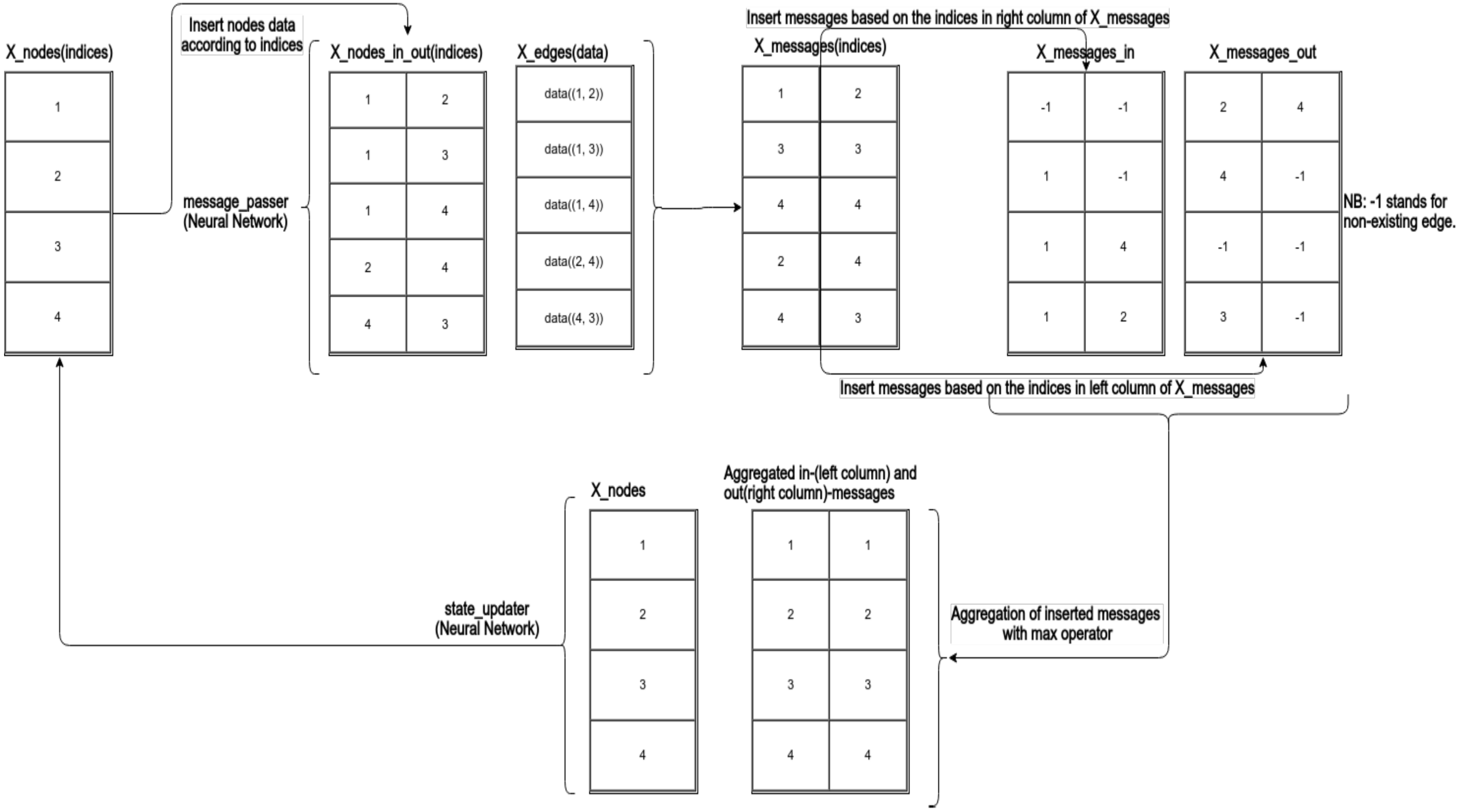
Plot event as a graph:
https://gist.github.com/SchattenGenie/28204a1135c3b7bca06162b7b2adf073

Neural Message Passing for Quantum Chemistry, arXiv:1704.01212,

Neural Message Passing for Jet Physics,
https://orbi.uliege.be/bitstream/2268/226446/1/nips_dlps_2017_29.pdf

http://geometricdeeplearning.com

Backup


X_nodes(indices)
1
2
3
4
Insert nodes data according to indices
message_passer (Neural Network)
X_nodes_in_out(indices)
1 2
1 3
1 4
2 4
4 3
X_edges(data)
data((1, 2))
data((1, 3))
data((1, 4))
data((2, 4))
data((4, 3))
Insert messages based on the indices in right column of X_messages
X_messages(indices)
1 2
3 3
4 4
2 4
4 3
X_messages_in
-1 -1
1 -1
1 4
1 2
X_messages_out
2 4
4 -1
-1 -1
3 -1
NB: -1 stands for non-existing edge.
Insert messages based on the indices in left column of X_messages
Aggregated in-(left column) and out(right column)-messages
1 1
2 2
3 3
4 4
Aggregation of inserted messages with max operator
X_nodes
1
2
3
4
state_updater (Neural Network)