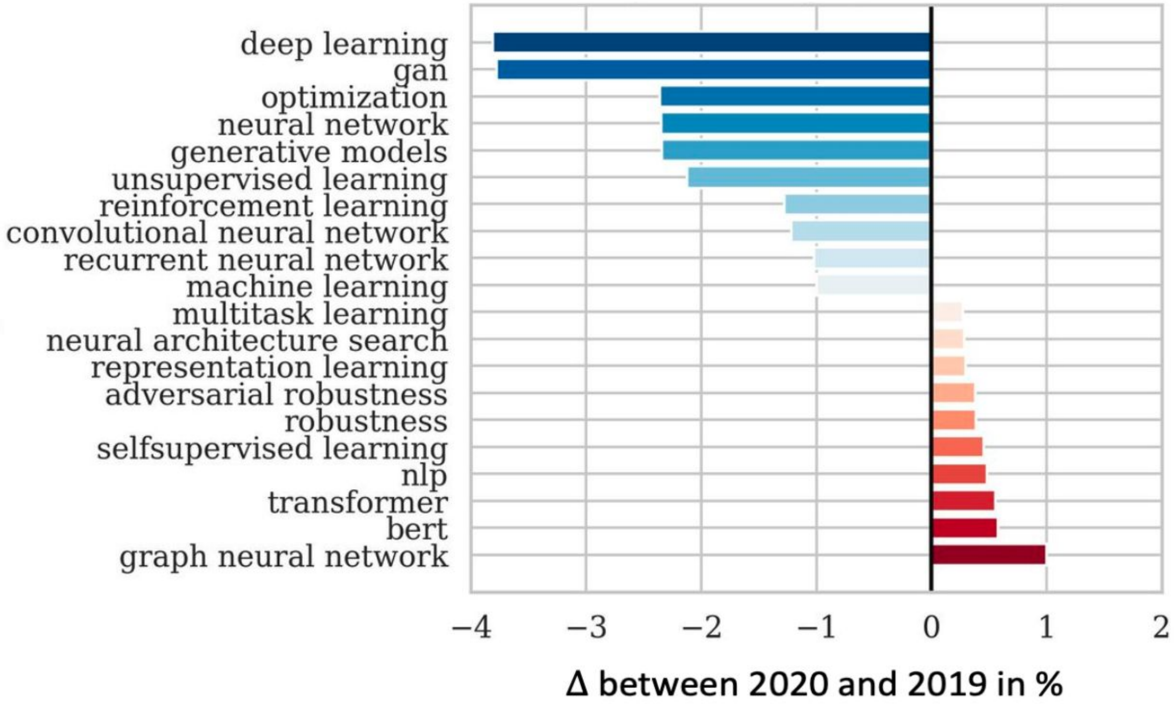
TGN: Temporal Graph Networks for Dynamic Graphs

Emanuele Rossi, Twitter

In collaboration with Ben Chamberlain, Fabrizio Frasca, Davide Eynard, Federico Monti and Michael Bronstein

Background

Graph Neural Networks are a Hot Topic in ML!

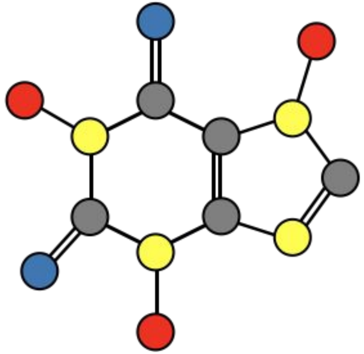


ICLR 2020 submissions keyword statistics

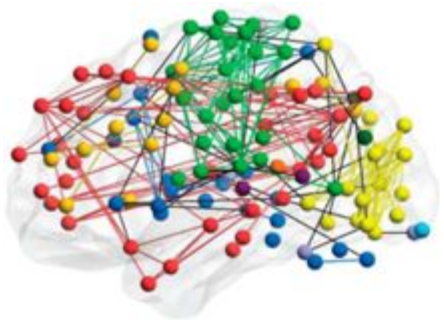
Plot: Pau Rodríguez López

Graphs are everywhere

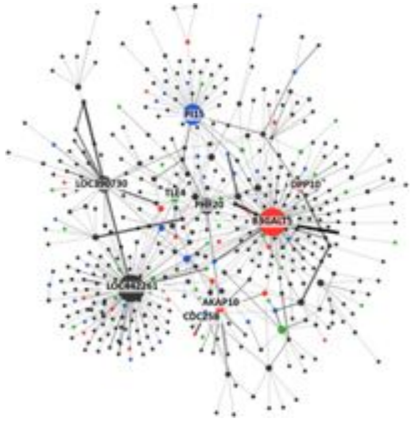
Social Networks



Molecules

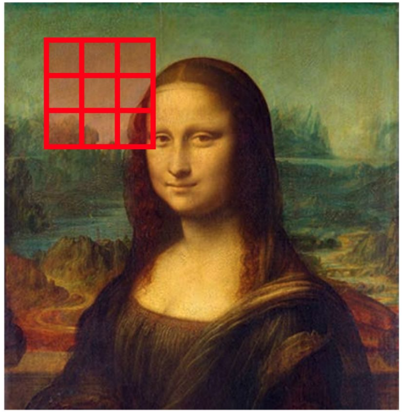


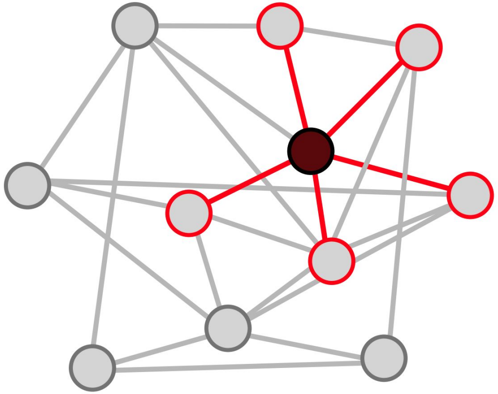
Functional Networks



Interaction Networks

From Images to Graphs



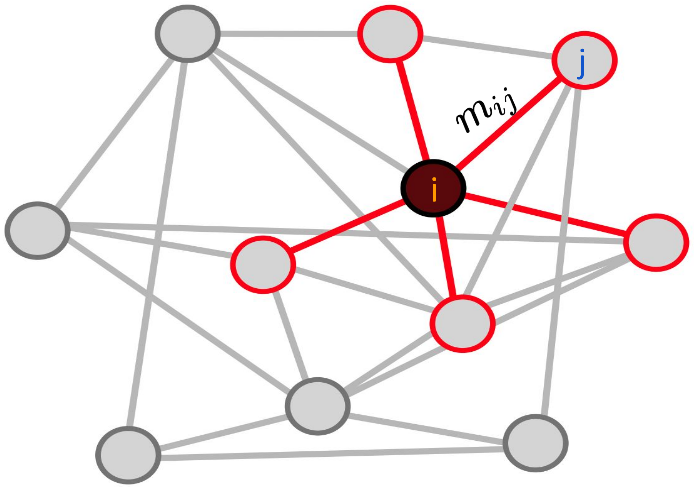


- Constant number of neighbors
- Fixed ordering of neighbors

- Different number of neighbors
- No ordering of neighbors

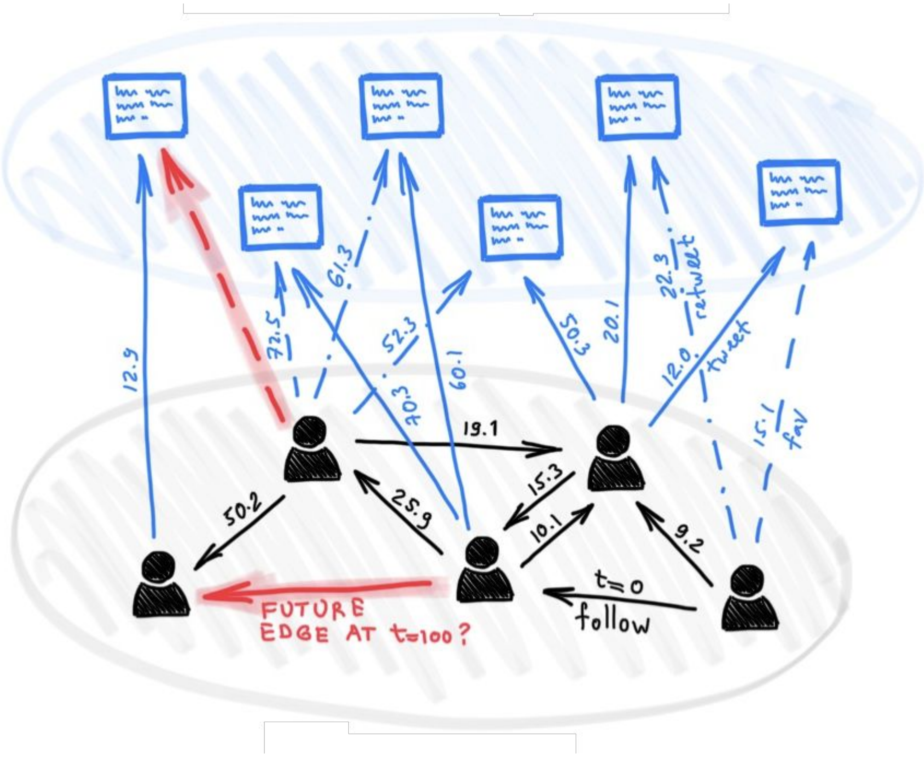
Graph Neural Networks

$$\mathbf{m}_{ij} = \mathrm{msg}(\mathbf{v}_i, \mathbf{v}_j, \mathbf{e}_{ij}),$$
$$\mathbf{z}_i = \sum_{j \in \mathcal{N}_i} h(\mathbf{m}_{ij}, \mathbf{v}_i)$$



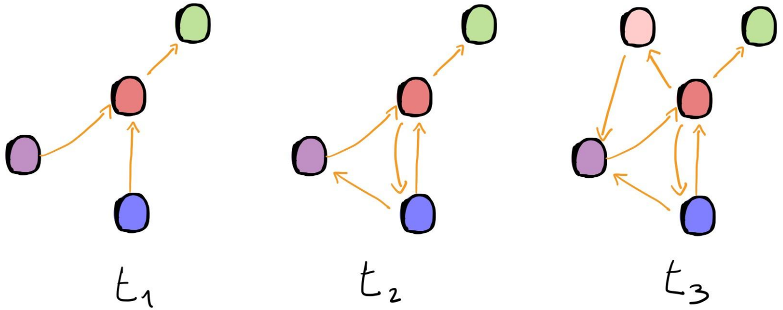
Gilmer et al. 2017

Problem: Many Graphs are Dynamic

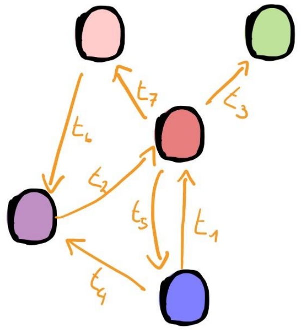


Dynamic Graphs

- *Discrete-time dynamic graphs*: sequence of snapshots
- *Continuous-time dynamic graphs*: sequence of timed-events



Discrete-time dynamic graphs

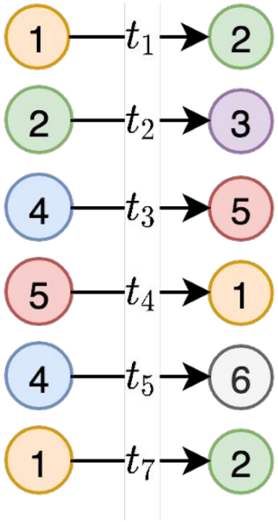


Continuous-time dynamic graphs

Learning on Dynamic Graphs

$$t_1 \leq t_2 \leq t_3 \leq t_4 \leq t_5 \leq t_6 \leq t_7$$

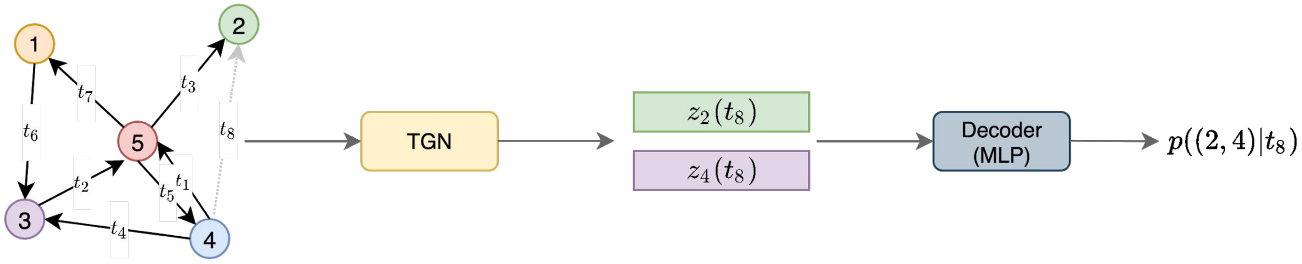
- Data is a **sequence of ordered timed events** (eg. edge addition)
- An epoch goes through the events in chronological order
- Model is **trained self-supervised**, predicting future edges using all information from previous edges



Model

TGN: Temporal Graph Networks

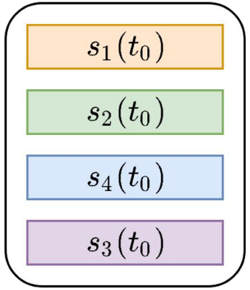
- Model for dynamic graphs is an encoder-decoder pair
- TGN is an encoder model which is able to generate **temporal node embeddings** $z_i(t) = f(i, t)$ for any node *i* and time *t*. Decoder is task-dependent, eg. MLP from two node embeddings to edge probability
- **General theoretical framework**, which consists of **5 different modules**
- Generalizes existing models such as *Jodie*[1] and *TGAT*[2]



[1]Kumar et al. 2019, [2]Xu et al. 2019

Modules: Memory

- State (vector) for each node the model has seen so far
- **Compressed representation** of all past interactions of a node
- Analogous to RNN hidden state, for one for each node
- **Not a parameter** $\rightarrow$ updated also at test time
- Initialized at 0, it can handle new nodes (inductive)

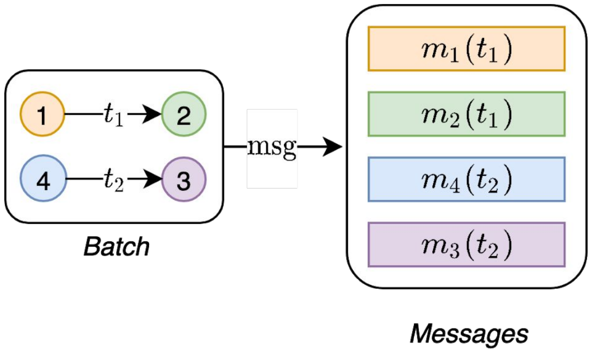


Memory

Modules: Message Function

- **Given an interaction** (i, j), **computes messages** for the source and the destination
- **Messages** will be used to **update the memory**

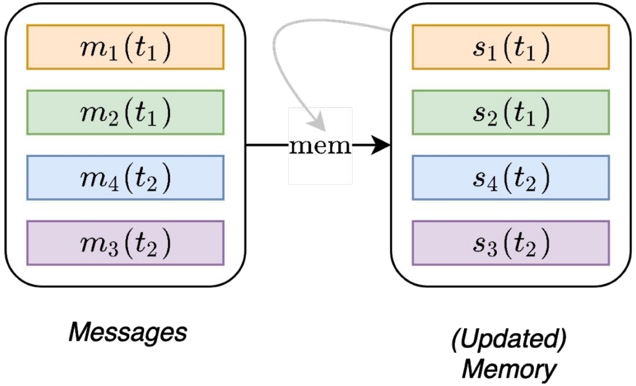
$$\mathbf{m}_i(t) = \operatorname{msg}\left(\mathbf{s}_i(t^-), \mathbf{s}_j(t^-), t, \mathbf{e}_{ij}(t)\right),$$
$$\mathbf{m}_j(t) = \operatorname{msg}\left(\mathbf{s}_j(t^-), \mathbf{s}_i(t^-), t, \mathbf{e}_{ij}(t)\right)$$



Modules: Memory Updater

- **Updates memory** using new messages

$$\mathbf{s}_i(t) = \mathrm{mem}\left(\bar{\mathbf{m}}_i(t), \mathbf{s}_i(t^-)\right)$$

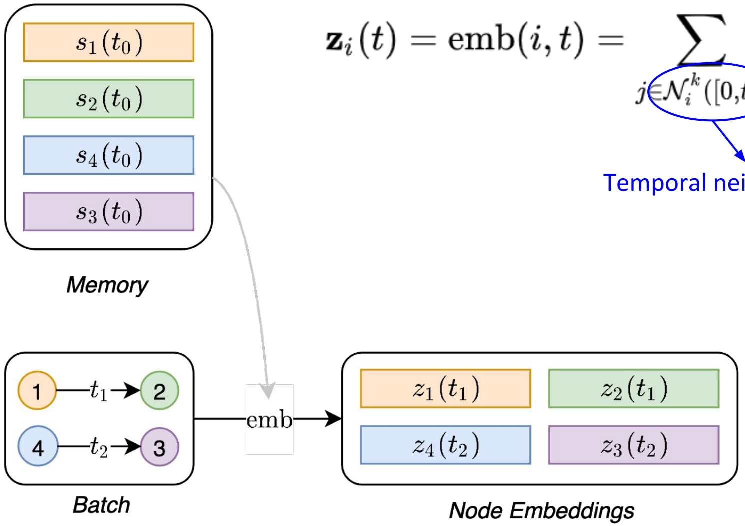


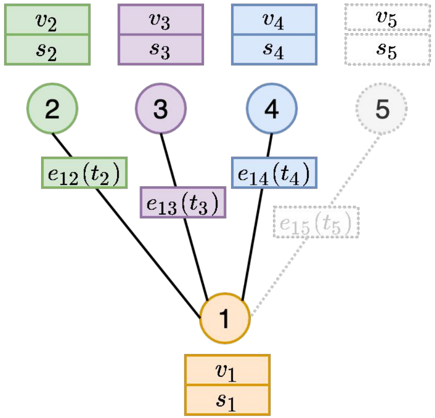
Modules: (Graph) Embedding

- **Computes** the **temporal embedding** of a node (which can be then used for prediction) using the graph
- **Solves** the **staleness problem** (memory becoming out of date)

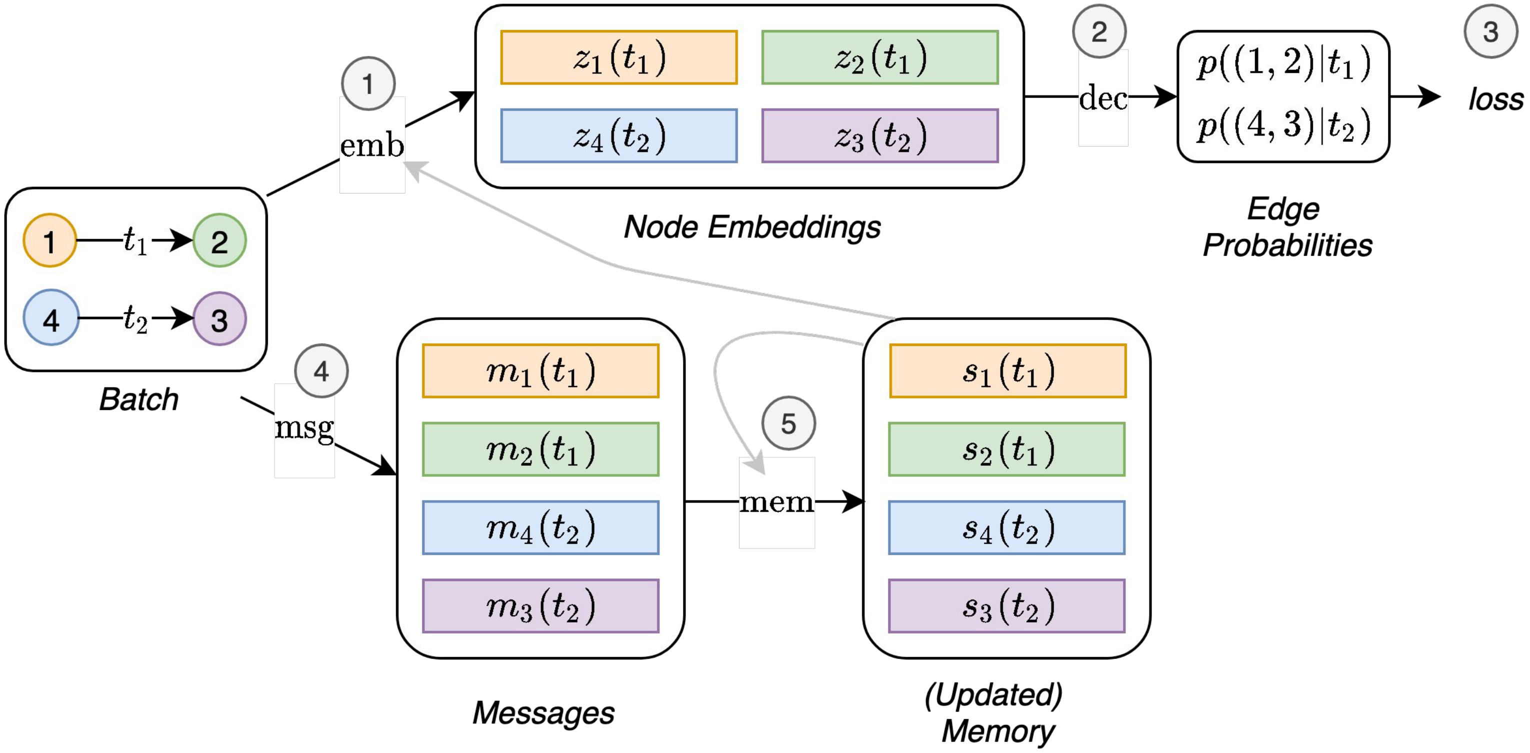
$$\mathbf{z}_i(t) = \mathrm{emb}(i,t) = \sum_{j \in \mathcal{N}_i^k([0,t])} h\left(\mathbf{s}_i(t), \mathbf{s}_j(t), \mathbf{e}_{ij}, \mathbf{v}_i(t), \mathbf{v}_j(t)\right),$$

Temporal neighborhood





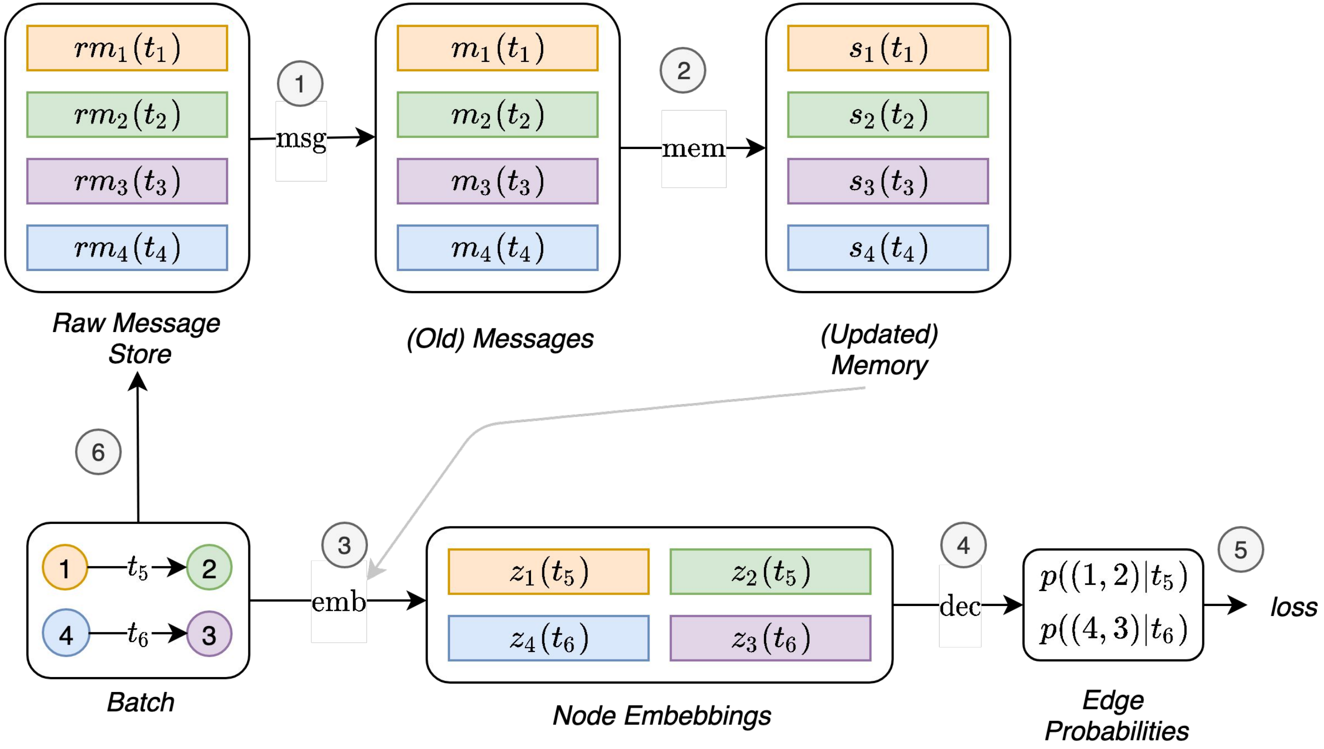
TGN: Overview



Learning TGN

- **Problem**: Given a batch, interaction serves both as our training target and as information to update the memory
- If we first update the memory (with the ground truth interactions), and then predict the same interactions, the memory would contain information about what we want to predict
- However, predicting before updating the memory causes all memory-related modules not to receive a gradient
- **Solution**: Update memory first, but using **interactions** from **previous batch**

Learning TGN - Diagram



Scalability

- **Memory** is **not a parameter** and we can just think of it as an additional feature vector for each node which we change over time
- **Only memory for nodes involved in a batch** is in GPU memory at any time
- Model is as scalable as GraphSage → **Can scale to very large graphs** (even if we don't show this in the paper)

Experiments

Experiments: Future Edge Prediction

	Wikipedia		Reddit		Twitter	
	Transductive	Inductive	Transductive	Inductive	Transductive	Inductive
GAE*	91.44 ± 0.1	†	93.23 ± 0.3	†	—	†
VAGE*	91.34 ± 0.3	†	92.92 ± 0.2	†	—	†
DeepWalk*	90.71 ± 0.6	†	83.10 ± 0.5	†	—	†
Node2Vec*	91.48 ± 0.3	†	84.58 ± 0.5	†	—	†
GAT*	94.73 ± 0.2	91.27 ± 0.4	97.33 ± 0.2	95.37 ± 0.3	67.57 ± 0.4	62.32 ± 0.5
GraphSAGE*	93.56 ± 0.3	91.09 ± 0.3	97.65 ± 0.2	96.27 ± 0.2	65.79 ± 0.6	60.13 ± 0.6
CTDNE	92.17 ± 0.5	†	91.41 ± 0.3	†	—	†
JODIE	94.33 ± 0.4	91.29 ± 0.5	96.36 ± 0.5	94.62 ± 0.5	62.05 ± 1.0	52.72 ± 1.6
TGAT	95.34 ± 0.1	93.99 ± 0.3	98.12 ± 0.2	96.62 ± 0.3	67.84 ± 0.6	62.21 ± 0.6
TGN-attn	$\mathbf{98.64} \pm 0.1$	$\mathbf{98.05} \pm 0.1$	$\mathbf{98.80} \pm 0.1$	$\mathbf{97.71} \pm 0.1$	$\mathbf{93.66} \pm 1.3$	$\mathbf{90.16} \pm 2.4$

Experiments: Dynamic Node Classification

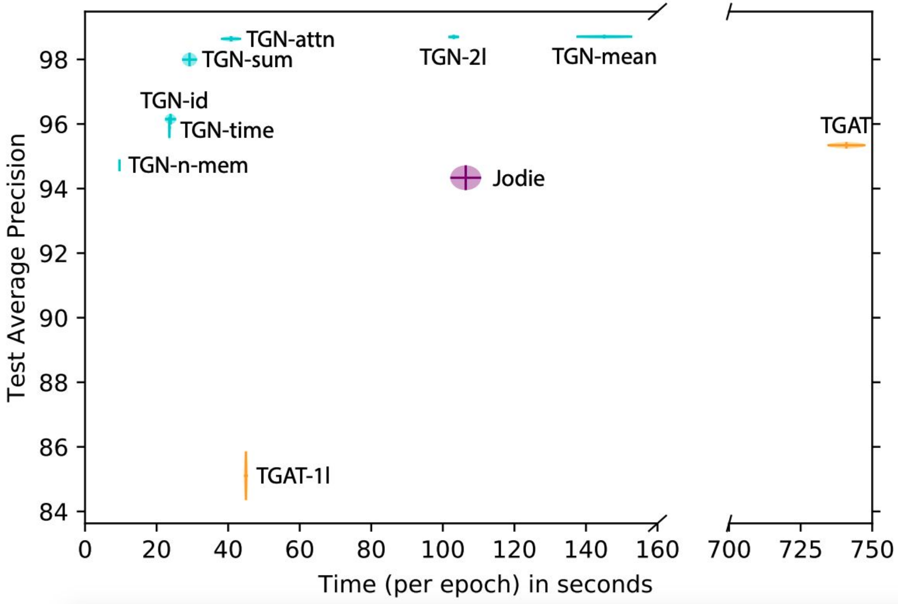
	Wikipedia	Reddit
GAE*	74.85 ± 0.6	58.39 ± 0.5
VAGE*	73.67 ± 0.8	57.98 ± 0.6
GAT*	82.34 ± 0.8	64.52 ± 0.5
GraphSAGE*	82.42 ± 0.7	61.24 ± 0.6
CTDNE	75.89 ± 0.5	59.43 ± 0.6
JODIE	87.17 ± 0.5	59.50 ± 2.1
TGAT	83.69 ± 0.7	65.56 ± 0.7
TGN-attn	$\mathbf{88.56} \pm 0.3$	$\mathbf{68.63} \pm 0.7$

Ablation Study

(Future edge prediction)

- **Faster** and **more accurate** than other approaches
- **Memory** (*TGN-att* vs *TGN-n-mem*) leads to a **vast improvement** in performance
- **Embedding** module is also extremely **important** (*TGN-attn* vs *TGN-id*) and **graph attention performs best**
- Last message aggregator, while discarding some information, performs extremely well while being very fast (*TGN-attn* vs *TGN-mean*)
- Using the memory makes it enough to have 1 graph attention layer

	Mem.	Mem. Update	Embedding	Mess. Agg.	Mess. Func.
JODIE	node	RNN	time	—[†]	id
TGAT	—	—	attn (2l, 20n)*	—	—
TGN-attn	node	GRU	attn (1l, 10n)	last	id
TGN-2l	node	GRU	attn (2l, 10n)	last	id
TGN-no-mem	—	—	attn (1l, 10n)	—	id
TGN-time	node	GRU	time	last	id
TGN-id	node	GRU	id	last	id
TGN-sum	node	GRU	sum (1l, 10n)	last	id
TGN-mean	node	GRU	attn (1l, 10n)	mean	id



Future Work

- **Benchmark datasets** for dynamic graphs (see OGB)
- **Global** (graph-wise) **memory**
- Investigate **scalability** and propose methods which scale better (possibly combining with literature on graph sampling, but not trivial)
- **Applications**: anomaly detection, molecular pathways, financial transactions, and more?

Conclusion

- **Dynamics graphs** are very common, but have received **little attention so far**
- We propose **TGN**, which **generalizes existing models** and achieves **SOTA results** on a variety of benchmarks
- We design an **efficient algorithm for training** the memory-related modules
- The ablation study shows the **importance of the different modules**

Questions?

@emaros96