TGN: Temporal Graph Networks for Dynamic Graphs

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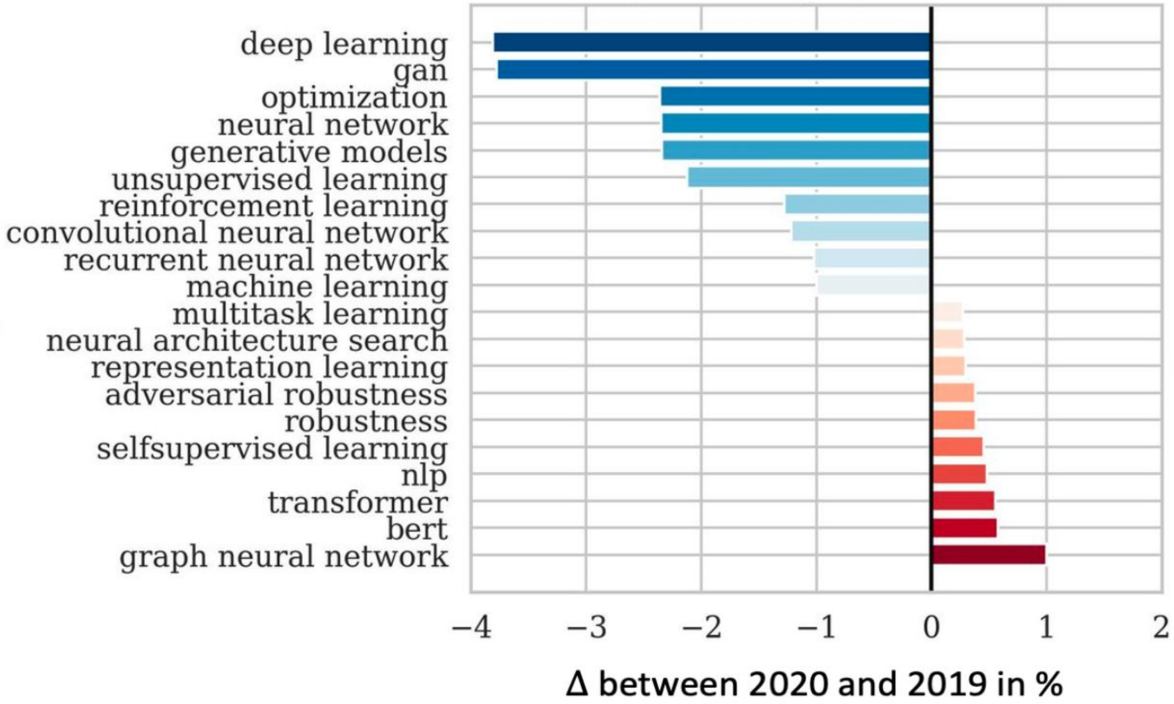
Background

Graph Neural Networks are a Hot Topic in ML!

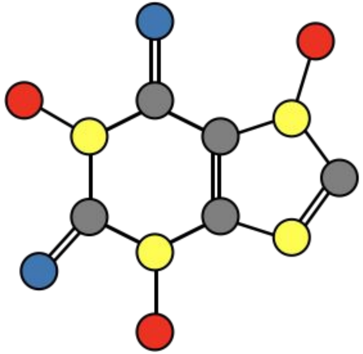


ICLR 2020 submissions keyword statistics

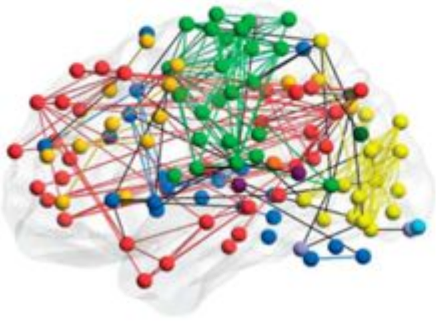
Plot: Pau Rodríguez López

Graphs are everywhere

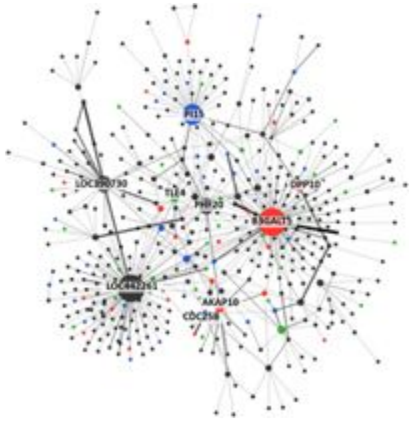
Social Networks



Molecules

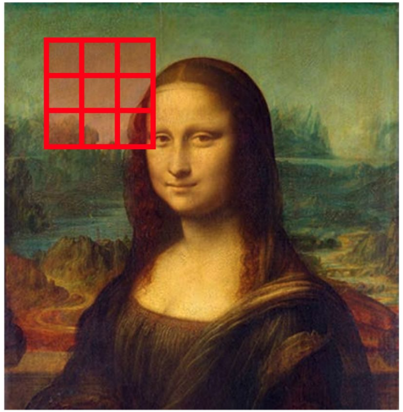


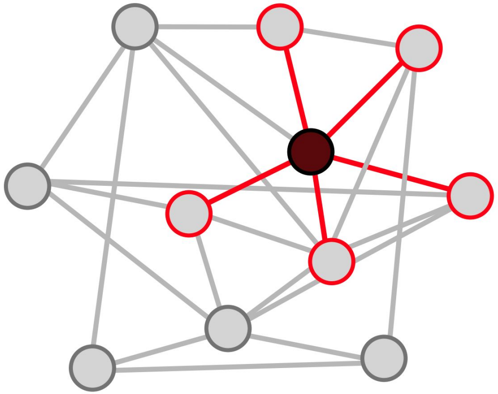
Functional Networks



Interaction Networks

From Images to Graphs



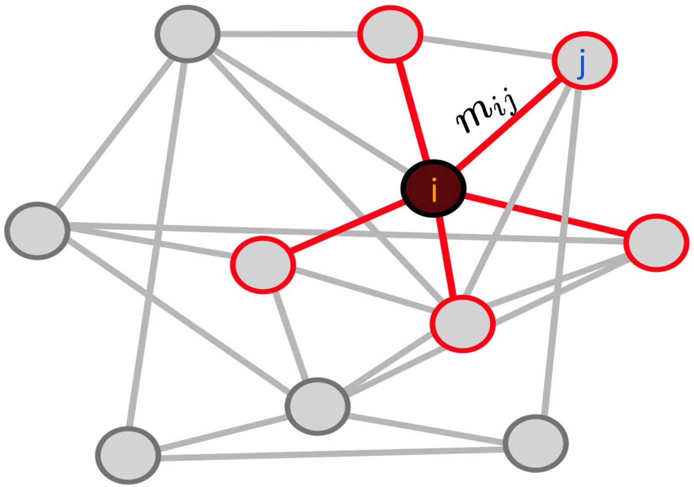


- Constant number of neighbors
- Fixed ordering of neighbors

- Different number of neighbors
- No ordering of neighbors

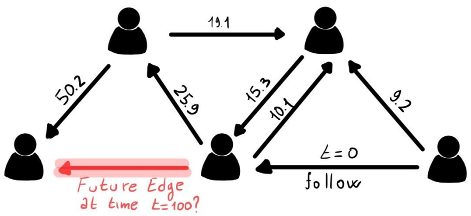
Graph Neural Networks

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

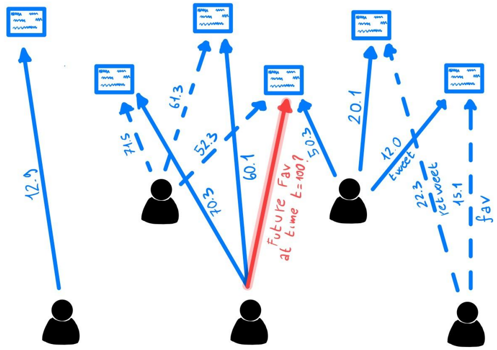


Gilmer et al. 2017

Problem: Many Graphs are Dynamic



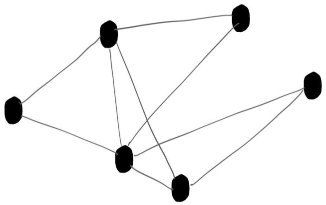
Social Networks



Interaction Networks

From Static to Dynamic Graphs

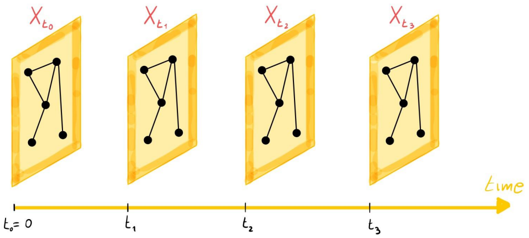
$G = (V, E, X)$



Static Graph

- No notion of time

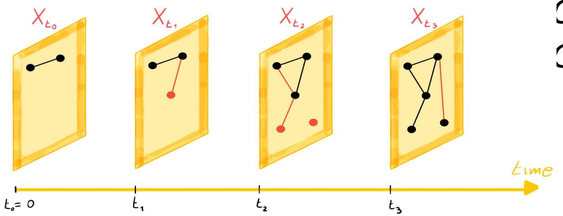
$G_t = (V, E, X_t)$



Spatio-Temporal Graph

- Topology is fixed, but features change over time
- (Usually) observed at regular intervals
- Examples: *traffic forecasting*, *covid-19 forecasting*

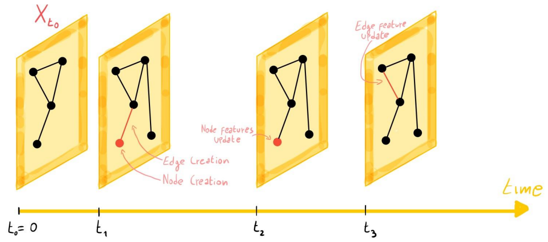
$G_t = (V_t, E_t, X_t)$



Discrete-Time Dynamic Graph (DTDGs)

- Both topology and features change over time
- However, graph is observed at regular intervals (no information about what happens in between)
- Examples: Any system which is observed at regular intervals

$G(t) = \{x_{t_1}, x_{t_2}, \ldots\} \quad 0 \leq t_1 \leq t_2 \leq \cdots \leq t$



Continuous-Time Dynamic Graph (CTDGs)

- Most general formulation
- Each change (‘*event*’) in the graph is observed individually with its timestamp
- Examples: Recommender Systems

Less General *More General*

CTDGs: Many Types of Events

	Node	**Edge**
Creation	User joins platform	User follows another user
Deletion	User leaves platform	User unfollows another user
Feature Change	User updates their bio	User changes retweet message

Why is Learning on Dynamic Graphs Different?

Model needs to:

- *Support addition* / *deletion* of node and edges, as well as *feature changes*
- Make *predictions* (eg. classify a node) at *any point in time*

Using a static *GNN* would mean:

- *Inefficiency: computation is repeated* each time we want to make a prediction
- *Loss of information*: Model would work on a snapshot of the graph, but not able to take into account how the graph evolved

Problem Setup

Tasks

- *Dynamic Node Classification*
- ***Future Link Prediction***
- *Dynamic Graph Classification*

(Encoder) Model Specification

- *model.observe(event, t)*
  - Incrementally observe and incorporate information from a new event
- *model.predict(node_idx, t)*
  - Produce an embedding for a node at a given timestamp, utilizing all the information previously observed
  - In contrast to static GNNs, this operation is called multiple times for each node as we need the embedding at different point in time → It needs to be efficient and avoid repeating computation

Evaluation

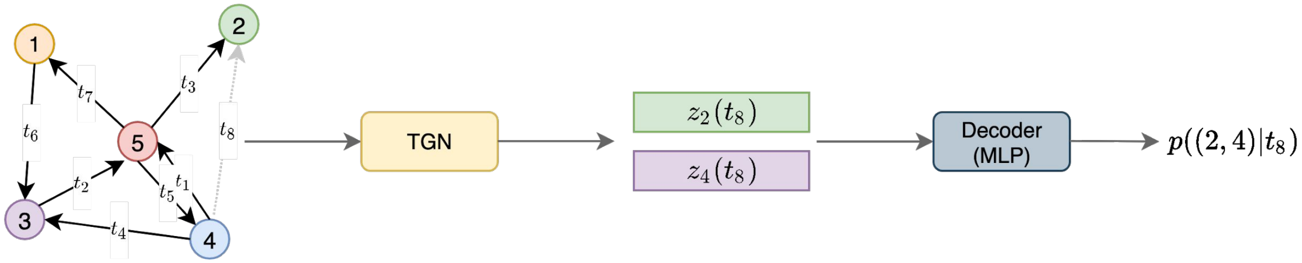
- Data is *split chronologically*
  - Eg. if data spans 1 year → First 10 months train set, 11th month validation and 12th month test set
- Model predicts events sequentially

```
for event, t in events:
  (u, v) = event
  # Predict probability of the next event
  u_embedding = model.predict(u, t)
  v_embedding = model.predict(v, t)
  link_prob   = sigmoid(np.dot(u, v))

  ### Also compute prob. of some negatively
  ### sampled events, and compute eval metric

  # Observe that ground truth event
  model.observe(event, t)
```

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], *TGAT*[2] and DyRep[3]



[1]Kumar et al. 2019, [2]Xu et al. 2019, [3]Trivedi et a. 2018

TGN Modules

Observe:

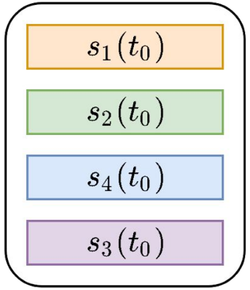
- *Memory*
- *Message Function*
- *Memory Updater*

Predict:

- *Graph Embedding*

Observe 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, one for each node
- **Not a parameter** $\rightarrow$ updated also at test time
- Initialized at 0, it can handle new nodes (inductive)

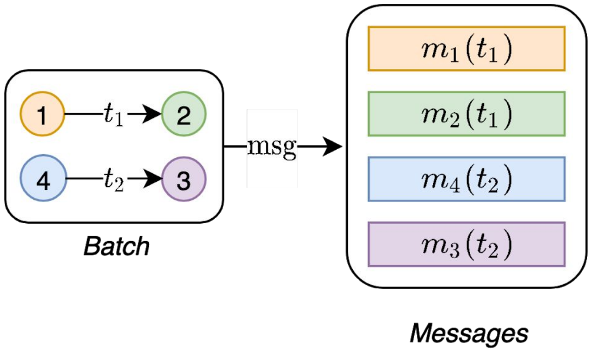


Memory

Observe Modules: Message Function

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

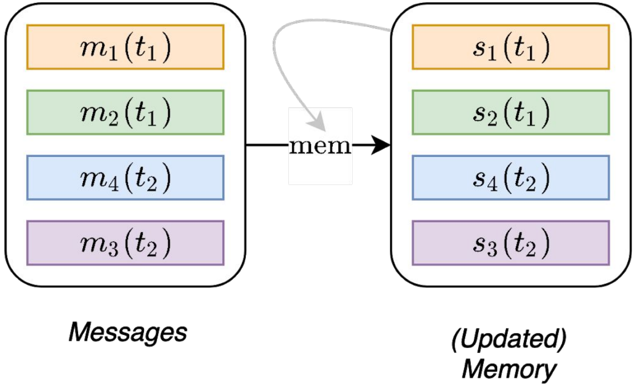
$$\mathbf{m}_i(t) = \operatorname{msg}\left(\mathbf{s}_i(t^-), \mathbf{s}_j(t^-), t, \mathbf{e}_{ij}(t)\right),$$
$$\mathbf{m}_j(t) = \operatorname{msg}\left(\mathbf{s}_j(t^-), \mathbf{s}_i(t^-), t, \mathbf{e}_{ij}(t)\right)$$



Observe Modules: Memory Updater

- **Updates memory** using new messages

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

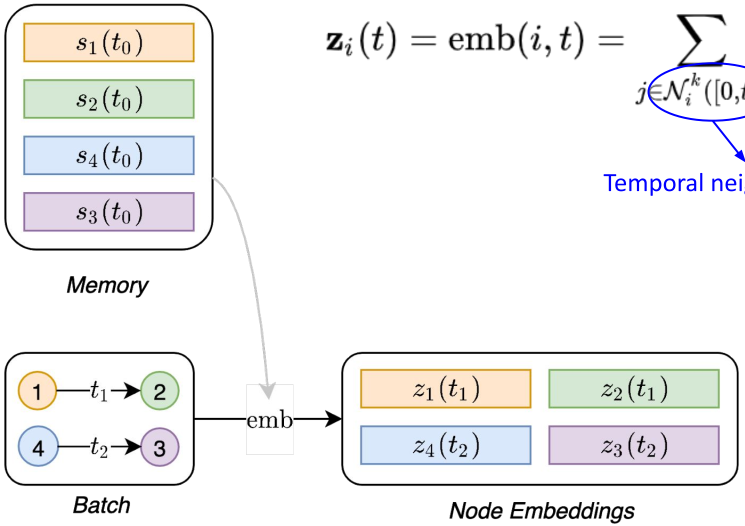


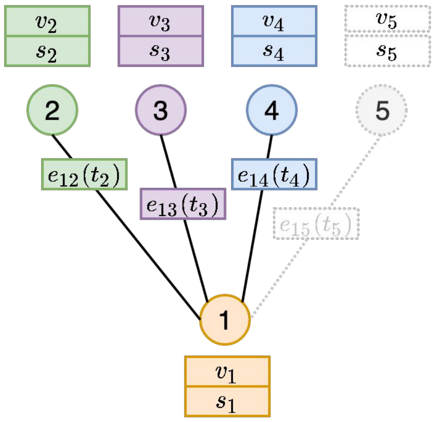
Predict Modules: (Graph) Embedding

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

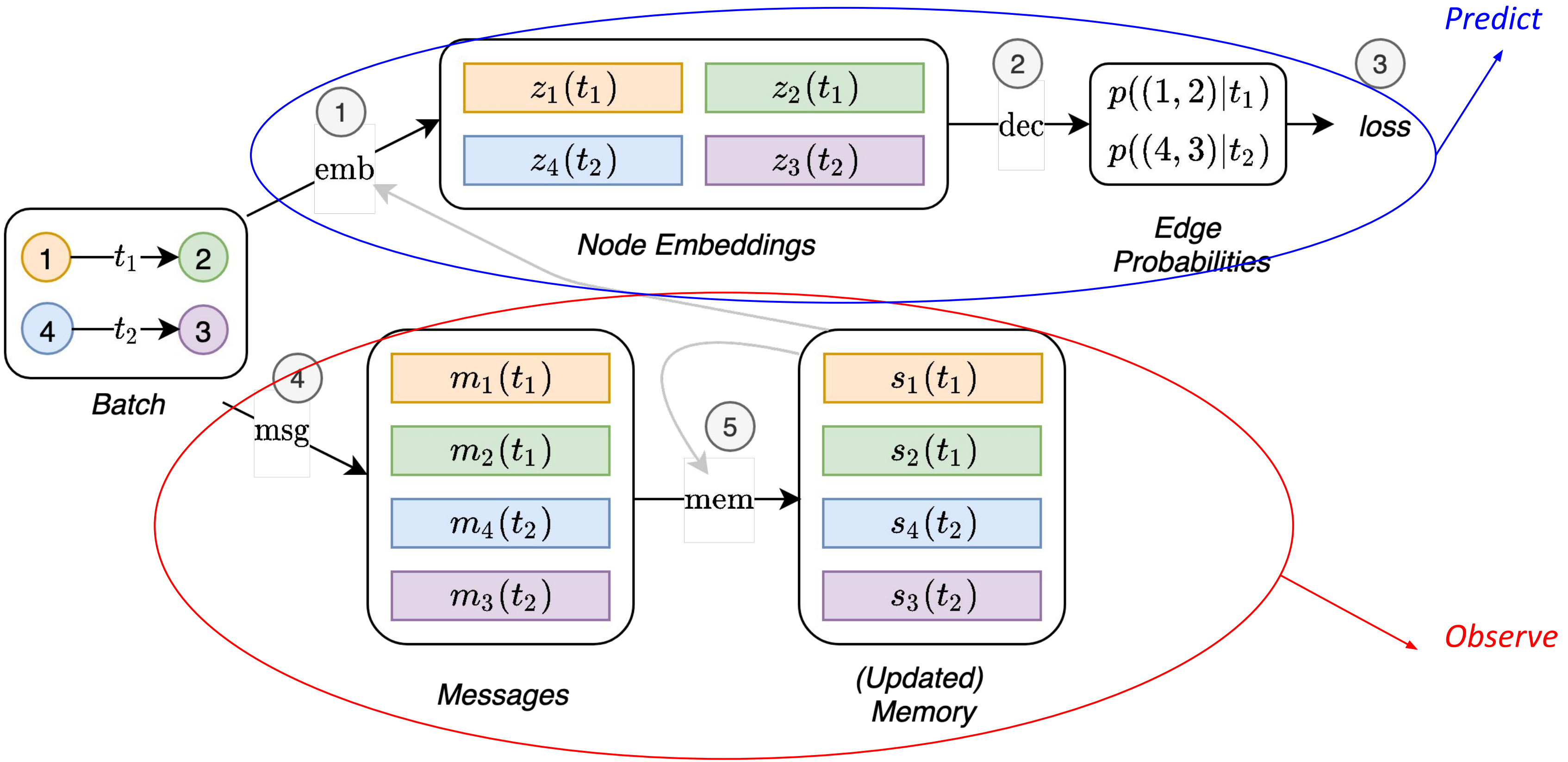
$$\mathbf{z}_i(t) = \mathrm{emb}(i,t) = \sum_{j \in \mathcal{N}_i^k([0,t])} h\left(\mathbf{s}_i(t), \mathbf{s}_j(t), \mathbf{e}_{ij}, \mathbf{v}_i(t), \mathbf{v}_j(t)\right),$$

Temporal neighborhood





TGN: Overview



Learning TGN

- **Problem 1:** CTDGs can be seen as a sequence for each node, but the *sequences are inter-dependent*
    - We cannot use standard BPTT
- **Solution**: Process interactions according to a global chronological order

```
for event, t in events:
  (u, v) = event
  # Predict probability of the next event
  u_embedding = model.predict(u, t)
  v_embedding = model.predict(v, t)
  link_prob   = sigmoid(np.dot(u, v))

  ### Also compute prob. of some negatively
  ### sampled events, and compute CE Loss

  # Observe that ground truth event
  model.observe(event, t)
```

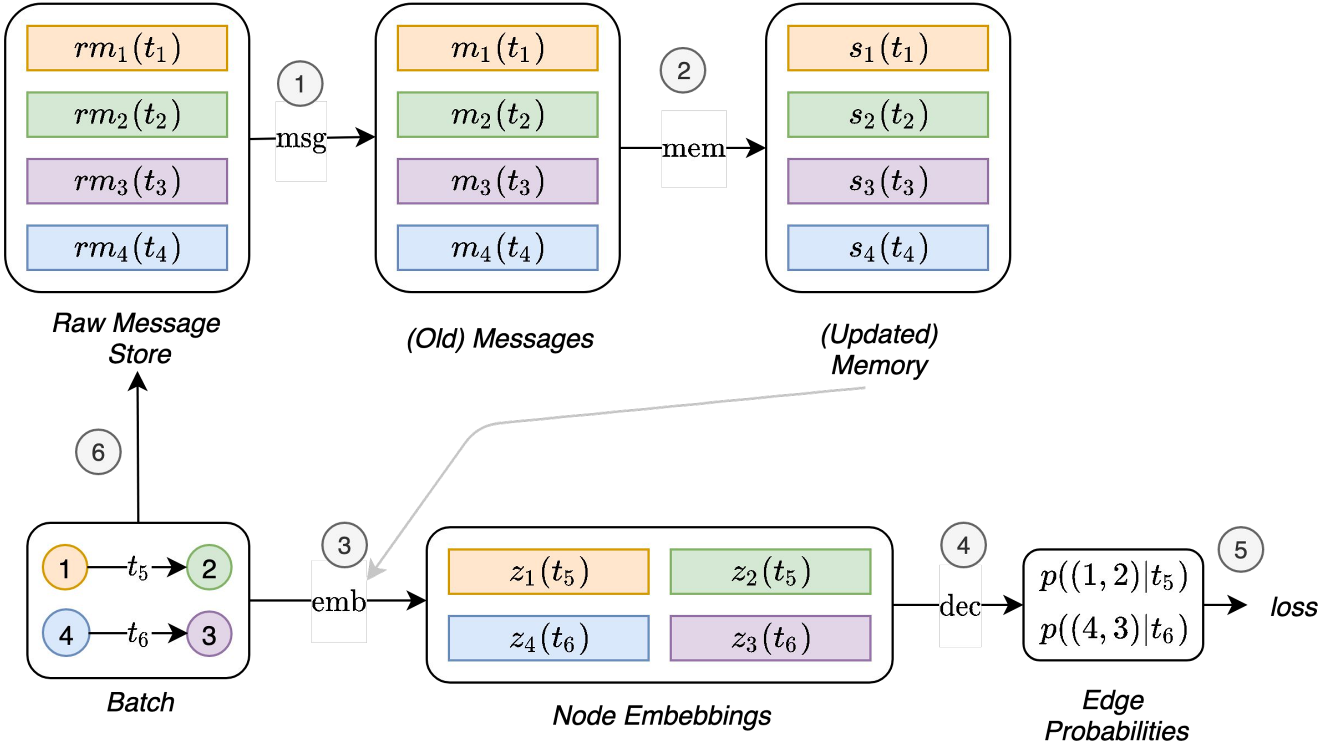
Learning TGN

- **Problem 2**: Memory-related modules do not directly influence the loss and therefore do not receive a gradient
  - The memory must be updated before predicting an interaction
  - However, updating the memory with the same interaction we then predict causes a leakage
- **Trivial Solution**:
  - Update memory with **messages from current batch**, and **predict interactions of next batch**
  - However, nodes in the current batch may be different from nodes in the next batch → Still no gradient

Learning TGN

- **Solution**:
    - Always store most recent message for each node
    - Update memory with **stored messages for each of the nodes involved in the batch (and their neighbors)**

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	94.62 ± 0.5	**93.11** ± 0.4	97.11 ± 0.3	94.36 ± 1.1	**85.20** ± 2.4	**79.83** ± 2.5
TGAT	**95.34** ± 0.1	**93.99** ± 0.3	**98.12** ± 0.2	**96.62** ± 0.3	70.02 ± 0.6	66.35 ± 0.8
DyRep	94.59 ± 0.2	92.05 ± 0.3	**97.98** ± 0.1	95.68 ± 0.2	**83.52** ± 3.0	**78.38** ± 4.0
TGN-attn	**98.46** ± 0.1	**97.81** ± 0.1	**98.70** ± 0.1	**97.55** ± 0.1	**94.52** ± 0.5	**91.37** ± 1.1

Experiments: Dynamic Node Classification

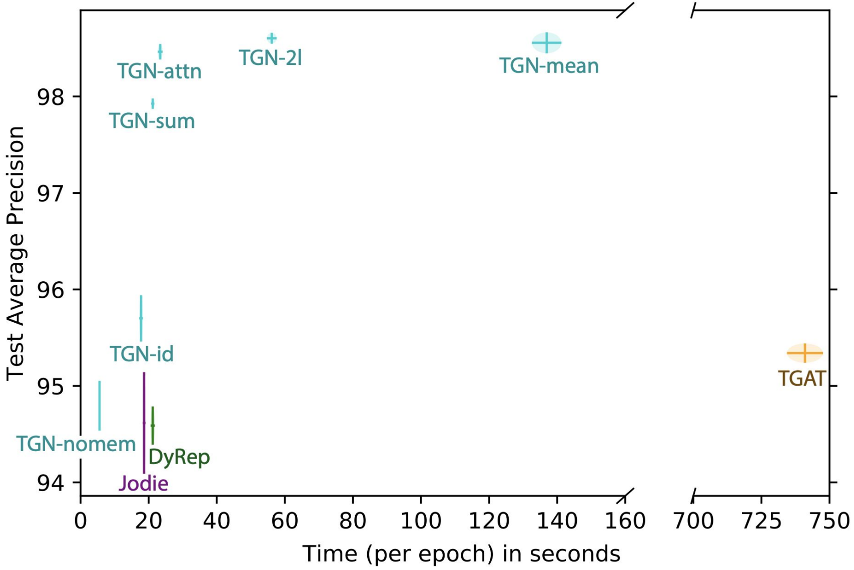
	Wikipedia	Reddit
GAE*	74.85 ± 0.6	58.39 ± 0.5
VAGE*	73.67 ± 0.8	57.98 ± 0.6
GAT*	82.34 ± 0.8	$\mathbf{64.52} \pm 0.5$
GraphSAGE*	82.42 ± 0.7	61.24 ± 0.6
CTDNE	75.89 ± 0.5	59.43 ± 0.6
JODIE	$\mathbf{84.84} \pm 1.2$	61.83 ± 2.7
TGAT	83.69 ± 0.7	$\mathbf{65.56} \pm 0.7$
DyRep	$\mathbf{84.59} \pm 2.2$	62.91 ± 2.4
TGN-attn	$\mathbf{87.81} \pm 0.3$	$\mathbf{67.06} \pm 0.9$

Ablation Study

(Future edge prediction)

	Mem.	Mem. Updater	Embedding	Mess. Agg.	Mess. Func.
Jodie	node	RNN	time	—†	id
TGAT	—	—	attn (2l, 20n)*	—	—
DyRep	node	RNN	id	—‡	attn‖
TGN-attn	node	GRU	attn (1l, 10n)	last	id
TGN-2l	node	GRU	attn (2l, 10n)	last	id
TGN-no-mem	—	—	attn (1l, 10n)	—	—
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

- **Faster** and **more accurate** than other approaches
- **Memory** (*TGN-att* vs *TGN-no-mem*) leads to a **vast improvement** in performance
- **Embedding** module is also extremely **important** (*TGN-attn* vs *TGN-id*) and **graph attention performs best**
- Using the memory makes it enough to have 1 graph attention layer



Future Work

- **Benchmark datasets** for dynamic graphs (see OGB)
- **Time in ML**: Improve how we use timestamp information in ML
- **Method Extensions:** *Global* (graph-wise) *memory*, *continuous models* (eg. neural ODEs) to model the memory evolution
- **Training Algorithm**: Coming up with an even *more efficient training algorithm* for dynamic graphs
- **Scalability**: Propose methods which scale better (possibly combining with literature on graph sampling, but not trivial)
- **Applications**: Recommender Systems, biology (molecular pathways, cancer evolution), finance (transaction networks) 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?

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