Dynamic Graph Representation Learning

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Outline

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Paper References

Model Name	**Paper**	**Code**
DyRep	DyRep: Learning Representations over Dynamic Graphs (ICLR'19)	unofficial code
DySAT	DySAT: Deep Neural Representation Learning on Dynamic Graphs via Self-Attention Networks (WSDM'20)	on Github
DyGNN	Streaming Graph Neural Networks (SIGIR'20)	(not yet ready)
TGAT	Inductive Representation Learning on Temporal Graphs (ICLR'20)	on Github

- Based on discrete screenshot:
  - DynamicGEM (DynGEM: Deep Embedding Method for Dynamic Graphs, IJCAI'17): adopted *Net2WiderNet* and *Net2DeeperNet* approaches ($G^t = (V^t, E^t), t \in \{1, 2, \ldots, T\}$) (code on Github)
  - DynamicTriad (Dynamic Network Embedding by Modeling Triadic Closure Process, AAAI'18): based on Triadic closure process etc. ($G^t = (V, E^t, W^t), t \in \{1, 2, \ldots, T\}$) (code on Github)

Other Papers II

- Based on continuous interaction:
  - HTNE (Embedding Temporal Network via Neighborhood Formation, KDD'18): using Hawkes process to model neighborhood formation (event). ($G = (V, E, A)$)
  - CTDNE (Continuous-Time Dynamic Network Embeddings, WWW'18): using Temporal Random Walk to select edges. ($G = (V, E_T, T)$) (code on Github)
  - NetWalk (NetWalk: A Flexible Deep Embedding Approach for Anomaly Detection in Dynamic Networks, KDD'18): encoding network streams. ($G(t) = (V(t), E(t))$)

Dynamic Graph Embedding

Problem: Learning dynamic node representations.

Challenges:

- Time-varying graph structures: links and node can emerge and disappear, communities are changing all the time.
  - requires the node representations capture both **structural proximity** (as in static cases) and their **temporal evolution**.
  - Time intervals of events are uneven.
- Causes of the change: can come from different aspects, e.g. in co-authorship network, research community & career stage perspectives.
  - requires modeling multi-faceted variations.

Static graphs are often defined as:

$$\mathcal{G} = (\mathcal{V}, \mathcal{E})$$

However, there isn't an unified way of defining the dynamic graphs.

Reference: Attention Is All You Need (NeurIPS'17)

An **attention mechanism** has a set of keys and a set of values; it receives a sets of queries.

- (key, value) are paired up, one key matched to one value.
- queries compared to keys, seek for the corresponding values. (e.g. dictionary)

Does not require an exact match; estimate the strength of the query-key match (e.g., cosine similarity)

Assumption: more similar keys provide more reliable values.

Idea:

1. Compute the similarities between each query and **all** of the keys.
2. Compute a **weighted** average of the corresponding values, as the result.

Normally we use dot-product attention, say,

$$\text{Att}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V\,.$$

When the key, the value, the query are exactly the same, $\mathbf{K} = \mathbf{Q} = \mathbf{V}$, the attention is "**self-attention**".

In practice we want more **flexible** self-attention.

We want different dimensions of a vector to have different importance when calculating the attention.

For example, we can apply the linear transformation

$$\mathbf{K} = \mathbf{X}\mathbf{W}_{\mathbf{K}}\,, \qquad \mathbf{Q} = \mathbf{X}\mathbf{W}_{\mathbf{Q}}\,, \qquad \mathbf{V} = \mathbf{X}\mathbf{W}_{\mathbf{V}}\,,$$

to the key, query and value of a self-attention mechanism.

Free parameters $\mathbf{W}_{\mathbf{K}}, \mathbf{W}_{\mathbf{Q}}, \mathbf{W}_{\mathbf{V}}$ bring a lot of randomness to the attention mechanism. Normally, we want to simultaneously try multiple sets of weights. That makes a "**multi-head self-attention**".

Given h sets of weights (which constitute h heads), we write

$$\mathbf{K}_1 = \mathbf{X}\mathbf{W}_{\mathbf{K}_1}, \qquad \mathbf{Q}_1 = \mathbf{X}\mathbf{W}_{\mathbf{Q}_1}, \qquad \mathbf{V}_1 = \mathbf{X}\mathbf{W}_{\mathbf{V_1}},$$

$$\mathbf{K}_2 = \mathbf{X}\mathbf{W}_{\mathbf{K}_2}, \qquad \mathbf{Q}_2 = \mathbf{X}\mathbf{W}_{\mathbf{Q}_2}, \qquad \mathbf{V}_2 = \mathbf{X}\mathbf{W}_{\mathbf{V_2}},$$

$$\vdots$$

$$\mathbf{K}_h = \mathbf{X}\mathbf{W}_{\mathbf{K}_h}, \qquad \mathbf{Q}_h = \mathbf{X}\mathbf{W}_{\mathbf{Q}_h}, \qquad \mathbf{V}_h = \mathbf{X}\mathbf{W}_{\mathbf{V_h}},$$

and we obtain h sets of results. h is called the "**head number**", and each set of result comes from a **head**.

Using the h results together, we can improve the reliability of the self-attention mechanism (e.g., by taking an average).

The Works in Details

Overview of the Models

Model	time steps	directed	relation types
DyRep	Continuous	No	Homogeneous (*)
DySAT	Discrete	No	Homogeneous
DyGNN	Discrete	Yes	Homogeneous
TGAT	Continuous	Yes	Homogeneous

Two kinds of events: (1) association (2) communication.

$$\mathcal{G}^t = (\mathcal{V}, \mathcal{E}^t)$$

is the denotation of **undirected** graph $\mathcal{G}$ at time $t \in [t_0, T]$. An event (u, v, t, k) has u, k being the involved nodes, $t \in R^+$ be the time and $k = \{0, 1\}$ be the event type (0 for association, 1 for communication). The stream of event-observations are (evolution of graph):

$$\mathcal{O} = \{(u, v, t, k)_p\}_{p=1}^{P}$$

Embedding of node v at time t is denoted as $\mathbf{z}^v(t) \in \mathbb{R}^d$. $\mathbf{z}^v(\bar{t})$ represents the *most recently updated embedding* of node v just before t.

Idea: learn functions to compute node embeddings.

Examples of the two kinds of events:

- association: being academic friends
- communication: meeting at a conference

DyRep: the function modeling an event

Given an event $p = (u, v, t, k)$, the conditional intensity function $\lambda_k^{u,v}$ is defined as:

$$\lambda_k^{u,v}(t) = f_k\big(g_k^{u,v}(\bar{t})\big)$$

where $\bar{t}$ signifies the time point just before current event, and

$$g_k^{u,v}(\bar{t}) = \boldsymbol{\omega}_k^T[\mathbf{z}^u(\bar{t}); \mathbf{z}^v(\bar{t})]$$

is a function of node representations learned through GNN.

$$f_k(x) = \psi_k \log(1 + \exp(x/\psi_k))$$

$\psi_k > 0$ is scalar time-scale parameter to learn, corresponding to the rate of events. $\boldsymbol{\omega}_k$ is also a parameter to learn.

DyRep: $f_k(x)$

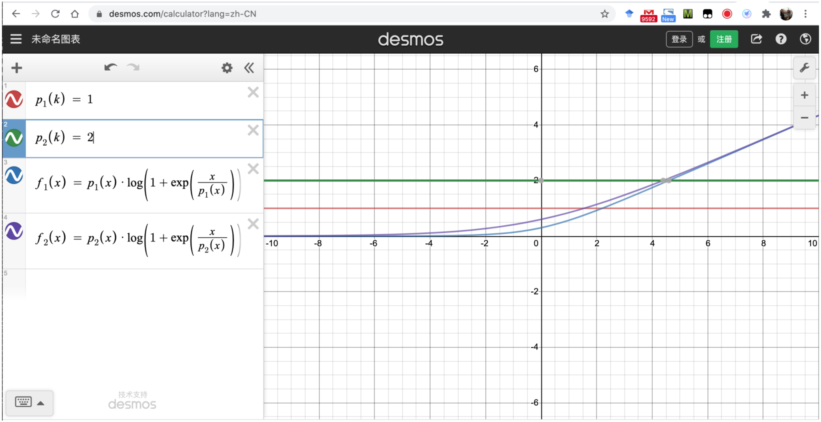


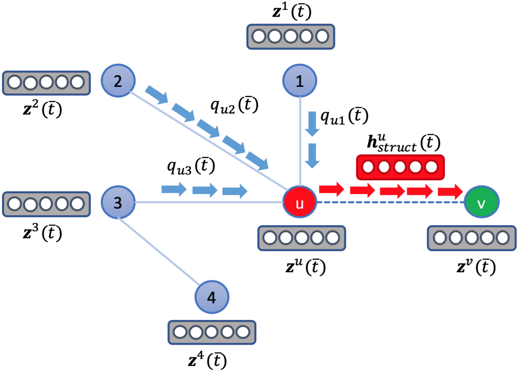
Figure: The plot of $f_k(x)$-x.

DyRep: the GNN-like component

$$\mathbf{z}^v(t_p) = \sigma\Big(\underbrace{\mathbf{W}^{struct}\mathbf{h}^u_{struct}(\bar{t}_p)}_{\text{Localized Embedding Propagation}} + \underbrace{\mathbf{W}^{rec}\mathbf{z}^v(\bar{t}^v_p)}_{\text{Self-Propagation}} + \underbrace{\mathbf{W}^t(t_p - \bar{t}^v_p)}_{\text{Exogenous Drive}} \Big)$$

where $\mathbf{h}^u_{struct}(\bar{t}_p) \in \mathbb{R}^d$ is obtained from aggregating node u's neighbors, $\mathbf{W}^{struct}, \mathbf{W}^{rec} \in \mathbb{R}^{d\times d}$, $\mathbf{W}^t \in \mathbb{R}^d$.

It also inherits the GAT-style multi-head attention.



Temporal Point Process Self-Attention:

$h^u_{struct}(\bar{t}) = \max(\{\sigma(q_{ui}(\bar{t}) * h^i(\bar{t}))\})$

$h^i(\bar{t}) = W^h z^i(\bar{t}) + b^h$

where $i \in N_u(\bar{t})$ is the node in neighborhood of node u.

$$q_{ui}(\bar{t}) = \frac{\exp(S_{ui}(\bar{t}))}{\sum_{i' \in N_u(\bar{t})} \exp(S_{ui'}(\bar{t}))}$$

Figure: DyRep computes the temporally evolving attention based on events. q is an attention coefficient function, parameterized by $\mathcal{S}$, which is computed using the intensity of events between connected nodes.

DyRep: learning algorithm

Algorithm 1 Update Algorithm for $\mathcal{S}$ and $\mathbf{A}$

Input: Event record $o = (u, v, t, k)$, Event Intensity $\lambda_k^{u,v}(t)$ computed in (1), most recently updated $\mathbf{A}(\bar{t})$ and $\mathcal{S}(\bar{t})$. **Output:** $\mathbf{A}(t)$ and $\mathcal{S}(t)$

1. Update $\mathbf{A}$: $\mathbf{A}(t) = \mathbf{A}(\bar{t})$
if $k = 0$ **then** $\mathbf{A}_{uv}(t) = \mathbf{A}_{vu}(t) = 1$ ←{*Association event*}

2. Update $\mathcal{S}$: $\mathcal{S}(t) = \mathcal{S}(\bar{t})$
if $k = 1$ and $\mathbf{A}_{uv}(t) = 0$ **return** $\mathcal{S}(t)$, $\mathbf{A}(t)$ ←{*Communication event, no Association exists*}
for $j \in \{u, v\}$ **do**
  $b = \frac{1}{|\mathcal{N}_j(t)|}$ where $|\mathcal{N}_j(t)|$ is the size of $\mathcal{N}_j(t) = \{i : \mathbf{A}_{ij}(t) = 1\}$
  $\mathbf{y} \leftarrow \mathcal{S}_j(t)$
  if $k = 1$ and $\mathbf{A}_{uv}(t) = 1$ **then** { ←{*Communication event, Association exists*}}
    $\mathbf{y}_i = b + \lambda_k^{ji}(t)$ where i is the other node involved in the event. ←{λ *computed in Eq. 2*}
  else if $k = 0$ and $\mathbf{A}_{uv}(t) = 0$ **then** { ←{*Association event*}}
    $b' = \frac{1}{|\mathcal{N}_j(\bar{t})|}$ where $|\mathcal{N}_j(\bar{t})|$ is the size of $\mathcal{N}_j(\bar{t}) = \{i : \mathbf{A}_{ij}(\bar{t}) = 1\}$
    $x = b' - b$
    $\mathbf{y}_i = b + \lambda_k^{ji}(t)$ where i is the other node involved in the event ←{λ *computed in Eq. 2*}
    $\mathbf{y}_w = \mathbf{y}_w - x; \quad \forall w \neq i, \ \mathbf{y}_w \neq 0$
  end if
  Normalize $\mathbf{y}$ and set $\mathcal{S}_j(t) \leftarrow \mathbf{y}$
end for
return $\mathcal{S}(t)$, $\mathbf{A}(t)$

DyRep: how to learn

This model obtains two set of parameters to be updated:

- $\mathbf{A}(t) \in \mathbb{R}^{n\times n}$, the adjacency matrix of $\mathcal{G}_t$. $\mathbf{A}_{uv}(t) \in \{0,1\}$. Updated only in association events.
- $\mathcal{S}(t) \in \mathbb{R}^{n\times n}$, the stochastic matrix, denoting the likelihood of communication between each pair of nodes. $\mathcal{S}_{uv}(t) \in [0,1]$. Updated according to $\lambda_k^{u,v}(t)$.

$$L = -\sum_{p=1}^{P} \log\left(\lambda_p(t) + \int_0^T \Lambda(\tau)d\tau\right)$$

where $\lambda_p(t) = \lambda_{k_p}^{u_p,v_p}(t)$, and to represent the total survival probability for un-happened events we use: [1]

$$\Lambda(\tau) = \sum_{u=1}^{n}\sum_{v=1}^{n}\sum_{k\in\{0,1\}} \lambda_k^{u,v}(\tau)$$

[1] In practice, mini-batches are applied (see their Appendix).

DyRep experiments focus on the dynamic feature of the model.

- **Dynamic Link Prediction:** given v, k, t fixed, which is the most likely u?

$$f_k^{u,v}(t) = \lambda_k^{u,v}(t) \exp\left(\int_{\bar{t}}^{t} \lambda(s) ds \right)$$

  is the conditional density used to find the most likely node, where $\bar{t}$ is the time of the most recent event on u or v.

- **Event Time Prediction:** what is the next time point when a particular type of event occur?

$$\hat{t} = \int_t^{\infty} t f_k^{u,v}(t) dt$$

DySAT: Problem Definition

A dynamic graph $\mathbb{G}$ is defined as a series of observed static graph snapshots:

$$\mathbb{G} = \{\mathcal{G}^1, \mathcal{G}^2, \ldots, \mathcal{G}^T\}$$

where each snapshot $\mathcal{G}^t$ is defined as:

$$\mathcal{G}^t = (\mathcal{V}, \mathcal{E}^t)$$

it is a **weighted undirected** graph with a shared node set $\mathcal{V}$. The corresponding weighted adjacency matrix at time t is $\mathcal{A}^t$.

Idea: to learn $\mathbf{e}_v^t \in \mathbb{R}^d$, the node representations, preserving (1) the local graph structures centered at v, (2) its temporal evolutionary behaviors at time t (e.g. link connection and removal)

DySAT: Self-attention

Self-attention mechanism used in DySAT:

- Structural:
  - At each $\mathcal{G}^t$ $(t = 1, 2, \ldots, T)$
  - Exactly the same as what a standard GAT does (link)

$$\mathbf{z}_v = \sigma\Big(\sum_{u \in \mathcal{N}_v} \boldsymbol{\alpha}_{uv} \mathbf{W}^s \mathbf{x}_u\Big)$$

  where $\mathbf{W}^s$ is shared by all nodes, attention weight $\boldsymbol{\alpha}_{uv}$ is computed upon $\mathbf{W}^s \mathbf{x}_u$.

- Temporal:
  - Over the sequence $\mathbb{G} = \{\mathcal{G}^1, \mathcal{G}^2, \ldots, \mathcal{G}^T\}$

$$\mathbf{Z}_v = \boldsymbol{\beta}_v(\mathbf{X}_v \mathbf{W}_v)$$

  this time, attention weight $\boldsymbol{\beta}_v \in \mathbb{R}^{T \times T}$ is computed upon $\mathbf{X}_v \mathbf{W}_q$, $\mathbf{X}_v \mathbf{W}_k$ and $\mathbf{M} \in \mathbb{R}^{T \times T}$.

We define $\mathbf{M} \in \mathbb{R}^{T \times T}$ as: [2]

$$M_{ij} = \begin{cases} 0 & i \leq j \\ -\infty & \text{otherwise} \end{cases}$$

The linear projection matrices to generate queries, keys, and values: $\mathbf{W}_k, \mathbf{W}_q, \mathbf{W}_v \in \mathbb{R}^{D' \times F'}$. $\boldsymbol{\beta}_v \in \mathbb{R}^{T \times T}$ is computed as:

$$\beta_v^{ij} = \frac{\exp(e_v^{ij})}{\sum_{k=1}^{T} \exp e_v^{ik}}$$

where $e_v^{ij} \in \mathbb{R}$ is computed as:

$$e_v^{ij} = \left(\frac{((\mathbf{X}_v \mathbf{W}_q)(\mathbf{X}_v \mathbf{W}_k)^T)_{ij}}{\sqrt{F'}} + M_{ij} \right)$$

[2] $\mathbf{M}$ forces the model to attend to previous time steps only.

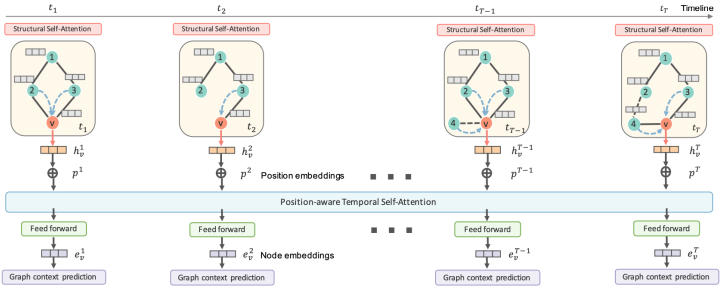


Figure: Multi-Faceted Graph Evolution is modeled by applying multiple attention heads to both structural and temporal attention.

DySAT: objective function

Designed for: preserving the local structure around a node across multiple time steps.

$$L = \sum_{t=1}^{T} \sum_{v \in \mathcal{V}} \Bigg(\sum_{u \in \mathcal{N}_{walk}^{t}(v)} - \log \sigma \langle \mathbf{e}_u^t, \mathbf{e}_v^t \rangle - w_n \sum_{u' \in P_n^t(v)} \log(1 - \sigma \langle \mathbf{e}_{u'}^t, \mathbf{e}_v^t \rangle) \Bigg)$$

Intuition: binary cross-entropy loss at each time step, with negative sampling, to encourage close [3] nodes to have similar representations.

[3] Close nodes are co-occurring in fixed-length random walks.

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The experiments are focusing on link prediction.

- Single and multiple step link-prediction performances
- Link-prediction involving unseen nodes and links
- Ablation studies on the attention layers

Significantly outperforms the SOTA models, and found that within the range of $(1, 16)$, the more attention heads, the better. More findings are in their paper.

DyGNN: Problem Definition

A dynamic graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is **directed** in this case, and it involves N nodes:

$$\mathcal{V} = \{v_1, v_2, \ldots, v_N\}$$

and a directed edge e could be represented as (v_s, v_g, t), meaning an edge linked from v_s to v_g at time t.

This time, "right before time t " is denoted as $t-$.

Idea: to learn an embedding, dynamic is achieved by the Update and Propagation components working together.

DyGNN: the components

There are two major components of the model:

- **Update Component:** based on the long-short term memory (LSTM) unit.
- **Propagation Component:** very similar with a standard GAT layer's propagation, except some details e.g. the selection of activation function, and:
  - ignoring the very-old neighbors (long-time no interaction) that hasn't interacted for an interval of $\Delta > \tau$.

DyGNN Overall Structure

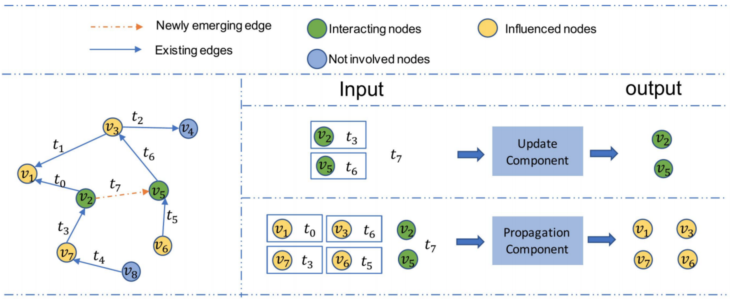

Figure: What happened in DyGNN when a new interaction happened at t_7 from v_2 to v_5. v_1, v_3, v_6, v_7, the direct neighbors, are the influenced nodes. For more details please refer to their paper.

DyGNN: Learning

The DyGNN model itself serves as an encoder that gives $\mathbf{u}_v(t)$ as the node v's embedding at time t.

Losses are different depending on different downstream tasks in the decoder.

- Link Prediction: negative log-sigmoid of the source & target inner product; negative-sampling used.
- Node Classification: cross-entropy loss at the last layer (unit $= 2$).

TGAT: Problem Definition

On a dynamic graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ (can be **directed** or **undirected**), all interactions ($e \in \mathcal{E}$) have time associated with them.
We seek to learn a continuous functional mapping $\Phi : T \rightarrow \mathbb{R}^{d_T}$ to encode time, where time domain $T = [0, t_{max}]$ (t_{max} is determined by the observed data).

Idea: learn time-aware embedding, using functional time encoding and the temporal graph attention layer (TGAT layer).

- TGAT layer: a local aggregation operator that takes (1) the temporal neighborhood with their hidden representations (or features) and (2) timestamps as input, and the output is the time-aware representation.

For node v_0 at time t, we define its neighborhood as:

$$\mathcal{N}(v_0; t) = \{v_1, v_2, \ldots, v_N\}$$

where, for each $v_i \in \mathcal{N}(v_0; t)$, the interaction between v_0 and v_i took place at $t_i < t$.

TGAT Architecture

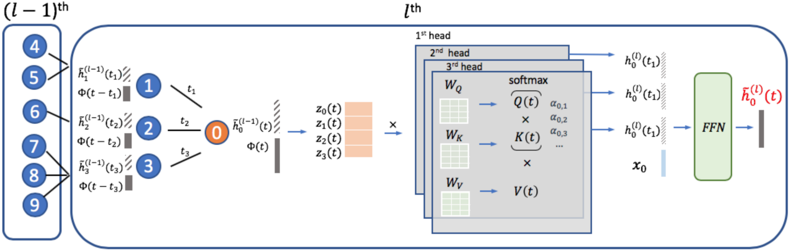

Figure: The architect of the l^{th} TGAT layer with $k = 3$ attention heads for node v_0 at time t. Output is $\tilde{\mathbf{h}}_i^{(l)}(t)$ where $i = 0$ is the node index. Feature vectors $\tilde{\mathbf{h}}_i^{(l-1)}(t)$ and $\mathbf{\Phi}(t - t_i)$ are simply concatenated, as the layer's input. $\mathbf{\Phi}(t - t_i) \in \mathbb{R}^{d_T}$ takes the place of positional encoding in a standard transformer layer (ref). The remaining parts (masked multi-head self attention etc.) are almost the same as GAT.

TGAT: More Details on Φ

It seems that there's a glitch in their paper writing (if you follow their description of Φ_d, the output dimension will be $2d$ instead of d), the Φ_d implemented in the code is:

$$\Phi_d(t) = [cos(\omega_1 t + \theta_1), cos(\omega_2 t + \theta_2), \ldots, cos(\omega_d t + \theta_d)] \in \mathbb{R}^d$$

where both $\boldsymbol{\omega} = [\omega_1, \ldots, \omega_d]$ and $\boldsymbol{\theta} = [\theta_1, \ldots, \theta_d]$ are parameters to be trained.

In fact, we should consider $\boldsymbol{\Phi}(t_i)$ instead of $\boldsymbol{\Phi}(t - t_i)$ $(i = 1, 2, \ldots, N)$. However, we are only interested in the timespan:

$$|t_i - t_j| = |(t - t_i) - (t - t_j)|$$

so it doesn't matter which way we use it.

Two kinds of tasks:

- **Transductive task:** node classification & link prediction on **observed** nodes.
- **Inductive task:** node classification & link prediction involving **unseen** nodes.

It outperforms all SOTA models under all tasks.

Conclusion

1. No agreement at all on how to model dynamic graph.
2. Multi-head self-attention mechanism is very frequently applied.
3. To model a continuous time stream, people usually define a *continuous function* and learn its parameters.
4. etc.