

Temporal GNN

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Graph Neural Networks and Applications

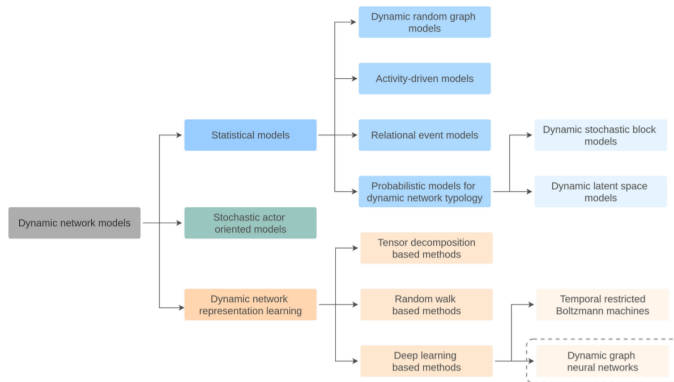


- 1 Categorization
- 2 Temporal Graph Embeddings
- 3 Temporal & Spatial Aggregation and Attention

Taxonomy of Temporal Models

Foundations and modeling of dynamic networks using dynamic graph neural networks

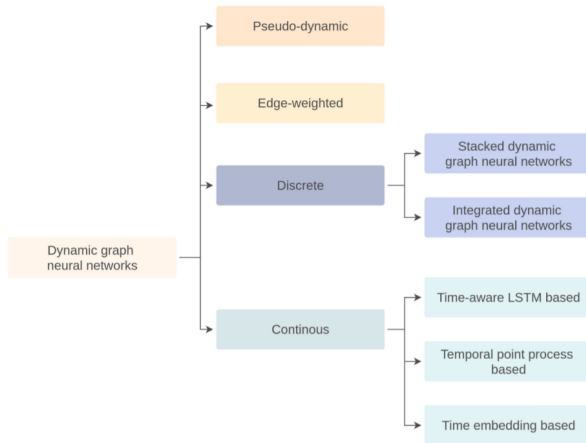
- Statistical, Representation Learning, Stochastic Agent-based



from Musial et al., 2021

Foundations and modeling of dynamic networks using dynamic graph neural networks

- Network type, and Discrete or Continuous models



Simple Models

TemporalNode2vec: Temporal Node Embedding in Temporal Networks

- 1 Compute PPMI (Positive Pointwise Mutual Information) over temporal window ω
- 2 Factorize PPMI with regularization tricks and temporal consistency

$$PPMI_t(v_1, v_2) = \max \left(0, \log \left(\theta \frac{|v_1, v_2|_t^w \cdot |V|}{|v_1|_t \cdot |v_2|_t} \right) \right)$$
$$\forall (v_1, v_2 \neq v_1, t) \in V^2 \times \llbracket 1, T \rrbracket$$

$$L = L_{St} + \tau L_{Sm} + \lambda L_{LR}$$
$$= \sum_{t=1}^T \|PPMI_t - U_t U_t^T\|_F^2 + \tau \sum_{t=2}^T \|U_t - U_{t-1}\|_F^2 + \lambda \sum_{t=1}^T \|U_t\|_F^2$$

from Bedart et al., 2019

Node Embedding over Temporal Graphs

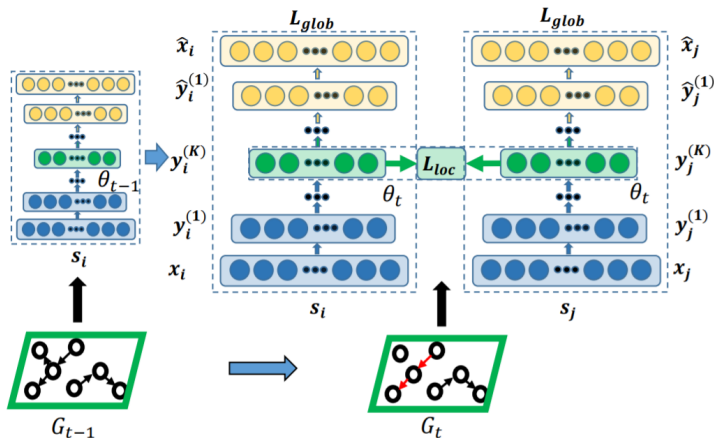
- 1 Recurrent snapshot model
- 2 Initialization by node2vec
- 3 Q_t as static embeddings rotated by R_t

$$f_{t+1}(v) = \sigma(Af_t(v) + BR_tQ_tv) \\ - \sum_t \sum_{v_t \in V_t} \log \Pr(N(v_t)|Q_tv_t)$$

$$\sum_t \|R_{t+1}Q_{t+1} - Q_t\| + \lambda \|R_{t+1}^T R_{t+1} - I\| \\ R_{t+1} = \operatorname{argmin}_{R \text{ s.t. } R^T R = I} \|RQ_{t+1} - Q_t\|$$

DynGEM: Deep Embedding Method for Dynamic Graphs

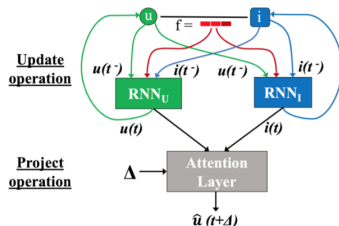
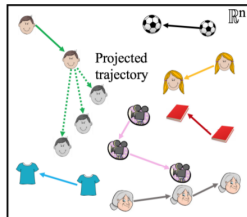
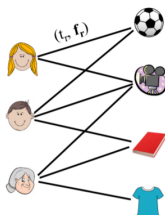
- 1 Extension of SDNE graph autoencoders
- 2 Retraining with parameters from previous snapshots



Recommender Systems

Predicting Dynamic Embedding Trajectory in Temporal Interaction Networks

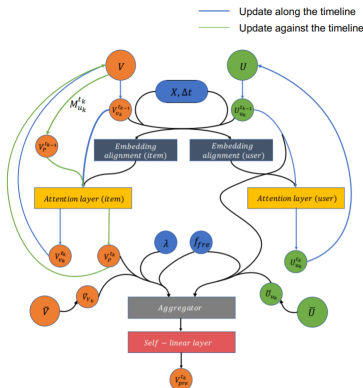
- 1 JODIE adapts user positions along sessions adapting current recommendations
- 2 RNN updates for user and item embeddings, while predicting user position for next point.



from Leskovec et al., 2019

Highly Liquid Temporal Interaction Graph Embeddings

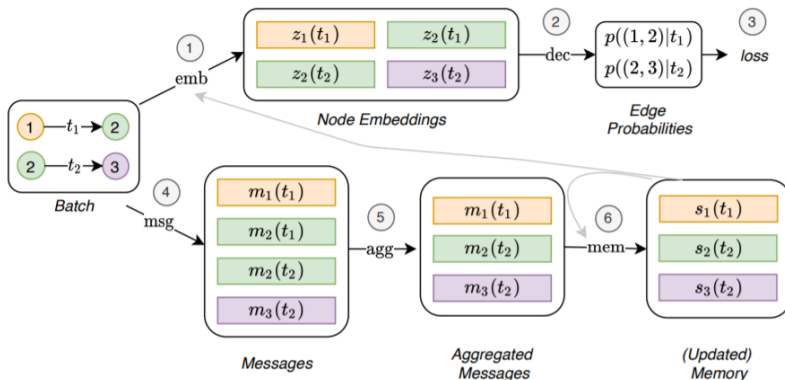
- 1 Used-based and frequency-based windows for priority of updates
- 2 Dynamic and static embeddings, frequent previous nodes window, time decay and frequency factors.



General Framework

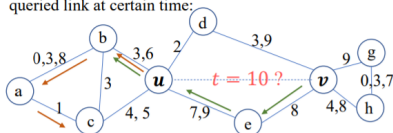
Temporal graph networks for deep learning on dynamic graphs

- 1 Universal framework for temporal graph processing
- 2 Embedding incorporates memory updates

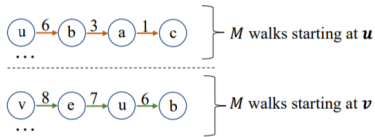


Inductive Representation Learning in Temporal Networks via Causal Anonymous Walks

A **temporal graph** with timestamped links and a queried link at certain time:

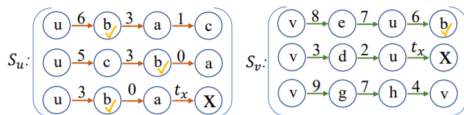


Backtrack m -step random walks over time before $t=10$:



Causality Extraction

Example: three 3-step walks (t_x, X are the default timestamp and the default node when no historical links can be found)



Count number of b 's in different positions:

$$(0, 2, 1, 0)^T \quad (0, 0, 0, 1)^T$$

$$I_{CAW}(b; S_u, S_v) = \{g(b; S_u), g(b; S_v)\} \text{ (Relative node identity)}$$

Anonymize $u \xrightarrow{6} b \xrightarrow{3} a \xrightarrow{1} c$:

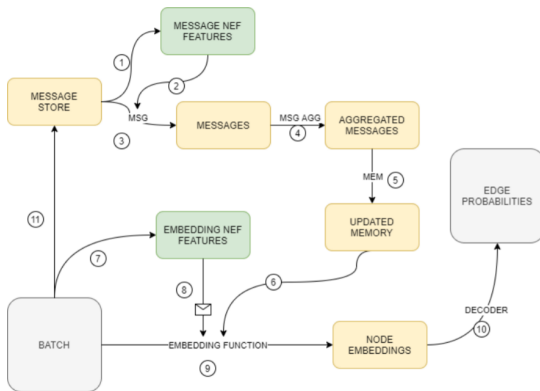
$$I_{CAW}(u) \xrightarrow{6} I_{CAW}(b) \xrightarrow{3} I_{CAW}(a) \xrightarrow{1} I_{CAW}(c)$$

Set-based Anonymization

from Li et al., 2021

Temporal Graph Network Embedding with Causal Anonymous Walks Representations

- 1 Efficient integration of CAW for LP and TGN for NC
- 2 Temporal Network Embedding benchmarking

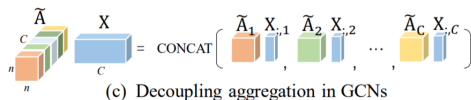
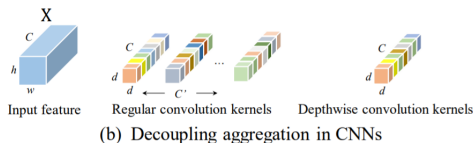
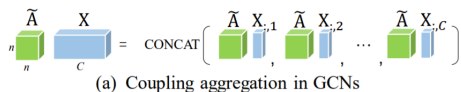


from Babaev et al., 2021

Decomposition-based Models

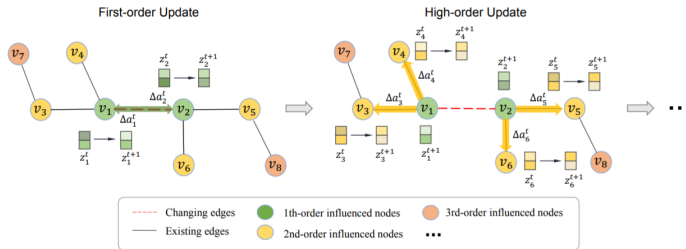
Decoupling GCN with DropGraph Module for Skeleton-Based Action Recognition

- Decoupling aggregation patterns may help decomposing dynamic and static patterns



DyGCN: Dynamic Graph Embedding with Graph Convolutional Network

- 1 Iteratively propagate updates from temporal changes
- 2 Use historic and update decomposition in model training



from Ai et al., 2021

DyGCN: Dynamic Graph Embedding with Graph Convolutional Network

Algorithm 1 DyGCN

Input: $\mathcal{G}^t = \{\mathcal{V}^t, \mathcal{E}^t\}$, $\mathcal{G}^{t+1} = \{\mathcal{V}^{t+1}, \mathcal{E}^{t+1}\}$: the graph at time t and $t + 1$;

$Z_t = \{z_v^t, v \in \mathcal{V}^t\}$: the node embeddings at time t ;

$\{W_0, W_1, W_2, \dots, W_K\}$: the transformation matrices.

Output: $Z^{t+1} = \{z_v^{t+1}, v \in \mathcal{V}^t\}$, the node embeddings at time $t + 1$.

1: // The update of first-order influenced nodes

2: **for** $v \in \mathcal{V}_1^t$ **do**

3: $\Delta a_v^t = \sum_{u \in \mathcal{N}^{t+1}(v) \cup v} z_u^t - \sum_{u \in \mathcal{N}^t(v) \cup v} z_u^t$;

4: $z_v^{t+1} = \sigma(W_0 z_v^t + W_1 \Delta a_v^t)$;

5: **end for**

6: // The update of high-order influenced nodes

7: **for** $k \in [2, \dots, K]$ **do**

8: **for** $v \in \mathcal{V}_k^t$ **do**

9: $\Delta a_v^t = \sum_{u \in \mathcal{N}^{t+1}(v) \cup v} (z_u^{t+1} - z_u^t)$;

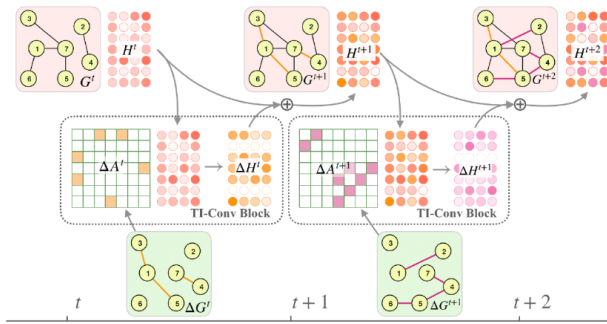
10: $z_v^{t+1} = \sigma(W_0 z_v^t + W_k \Delta a_v^t)$.

11: **end for**

12: **end for**

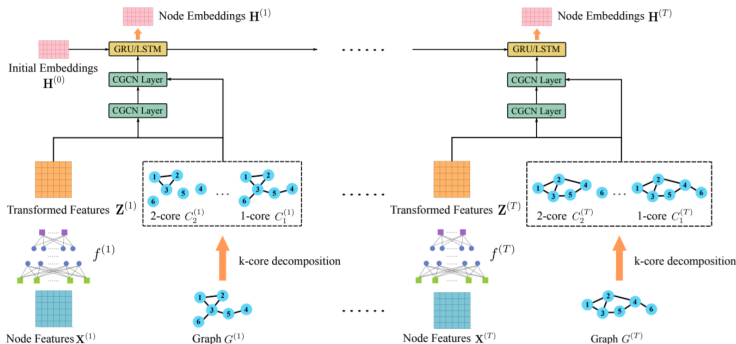
TI-GCN: A Dynamic Network Embedding Method with Time Interval Information

- 1 Pink backgrounds are network snapshots
- 2 Green are the changed networks
- 3 Orange lines mean edges appear during t and $t + 1$, purple ones means edges appear during $t + 1$ and $t + 2$



K-Core based Temporal Graph Convolutional Network for Dynamic Graphs

- 1 Preserving local proximity and global similarity
- 2 Feature transformation and feature aggregation for temporal case

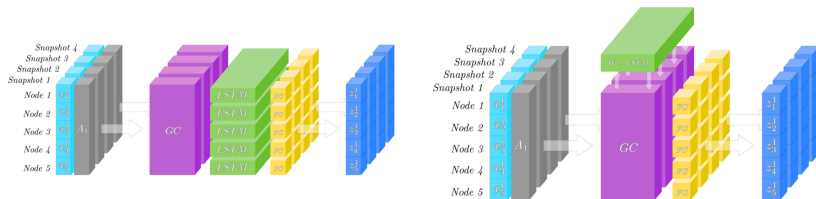


from Song et al., 2020

Combinations of GCN and LSTM

Dynamic Graph Convolutional Networks

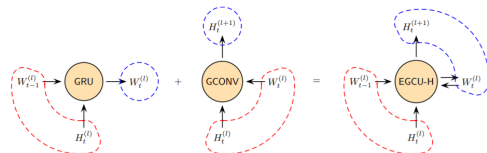
- 1 Combine Long Short-Term Memory networks and Graph Convolutional Networks to learn long short-term dependencies together with graph structure.



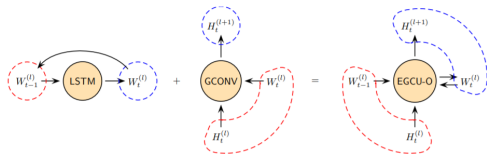
from Manzo et al., 2020

EvolveGCN: Evolving Graph Convolutional Networks for Dynamic Graphs

- 1 Left is a recurrent architecture; Middle is the graph convolution unit; Right is the evolving graph convolution unit.
- 2 Red region denotes information input to the unit and blue region denotes output information.



(a) EvolveGCN-H, where the GCN parameters are hidden states of a recurrent architecture that takes node embeddings as input.

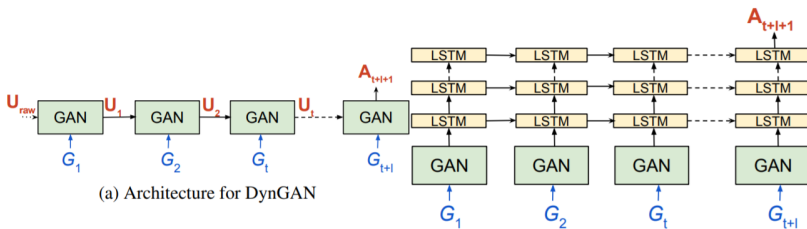


(b) EvolveGCN-O, where the GCN parameters are input/outputs of a recurrent architecture.

Generative Models

DynGAN: Generative Adversarial Networks for Dynamic Network Embedding

- 1 GAN instead of temporal VGAE
- 2 Stacked LSTMs



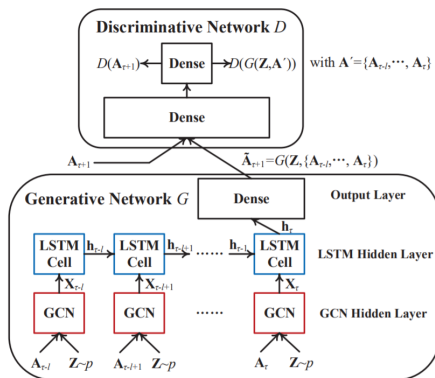
(a) Architecture for DynGAN

(b) Architecture for DynGAN-LSTM

from Ramakrishnan et al., 2019

GCN-GAN: A Non-linear Temporal Link Prediction Model for Weighted Dynamic Networks

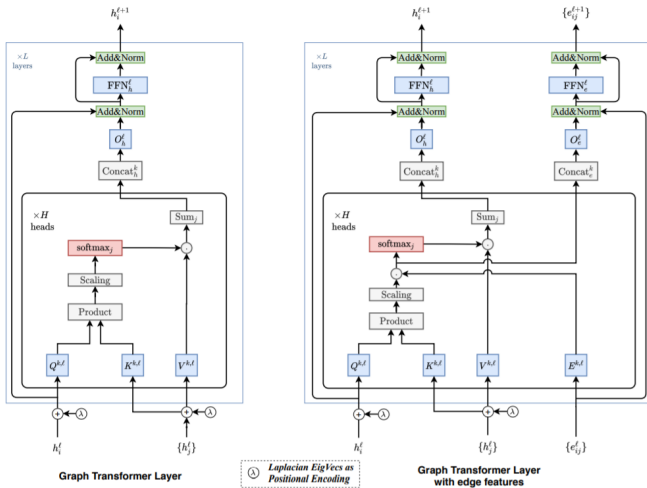
- 1 GCN-GAN temporal link prediction model
- 2 Generator is GCN stacked with LSTM and output FC
- 3 Discriminator is FC feedforward network.



from Yang et al., 2019

Attention-based Models

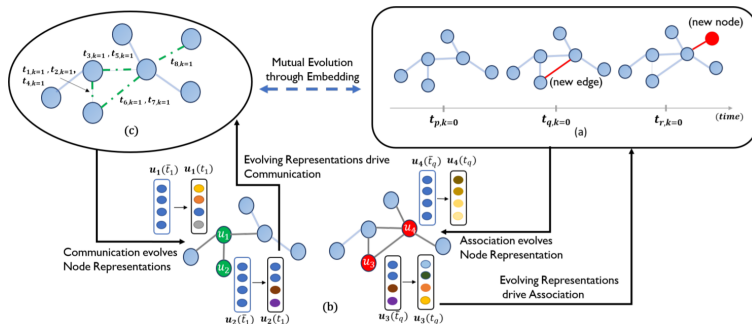
A Generalization of Transformer Networks to Graphs



from Bresson et al., 2020

DyREP: Learning representations over dynamic graphs

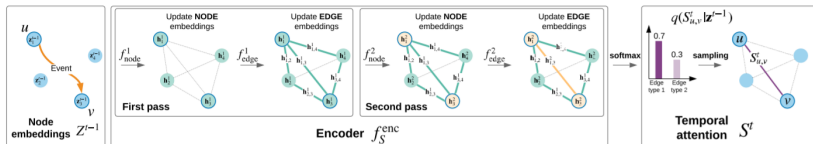
- 1 Deep temporal point process
- 2 Temporal-attentive representation network



from Zha et al., 2019

Learning Temporal Attention in Dynamic Graphs with Bilinear Interactions

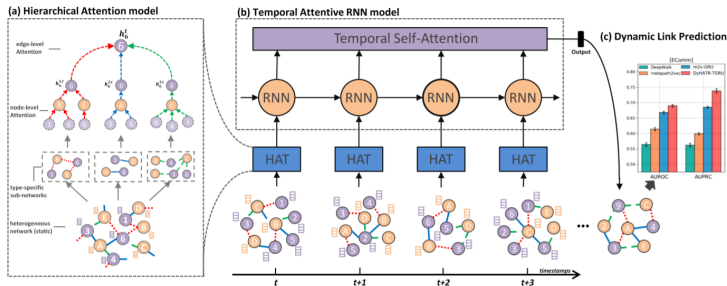
- 1 Temporal attention drives between-node feature propagation
- 2 Bilinear transformation layer for pairs of node features instead of concatenation



from Taylor et al., 2020

Modeling Dynamic Heterogeneous Network for Link Prediction using Hierarchical Attention with Temporal RNN

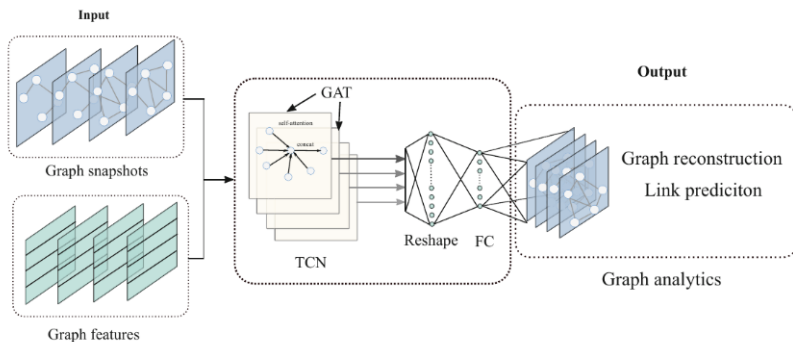
- 1 Hierarchical Attention model
- 2 Temporal Attentive RNN model
- 3 Dynamic Link Prediction



from Lin et al., 2020

TemporalGAT: Attention-Based Dynamic Graph Representation Learning

- 1 Decomposition into Snapshots with Spatial Attention
- 2 Temporal Convolutions for Dynamics



from Li et al., 2020

- Skardinga, J., Gabrys, B. and Musial, K., 2021. Foundations and modelling of dynamic networks using dynamic graph neural networks: A survey. IEEE Access.
- Haddad, M., Bothorel, C., Lenca, P. and Bedart, D., 2019, December. Temporalnode2vec: temporal node embedding in temporal networks. In International Conference on Complex Networks and Their Applications (pp. 891-902). Springer, Cham.
- Singer, U., Guy, I. and Radinsky, K., 2019. Node embedding over temporal graphs. arXiv preprint arXiv:1903.08889.
- https://github.com/benedekrozemberczki/pytorch_geometric_temporal
- <https://github.com/HSE-DynGraph-Research-team/DynGraphModelling>

- Goyal, P., Kamra, N., He, X. and Liu, Y., 2018. Dyngem: Deep embedding method for dynamic graphs. arXiv preprint arXiv:1805.11273.
- Huang, S., Bao, Z., Li, G., Zhou, Y. and Culpepper, J.S., 2020, April. Temporal network representation learning via historical neighborhoods aggregation. In 2020 IEEE 36th International Conference on Data Engineering (ICDE) (pp. 1117-1128). IEEE.
- Kumar, S., Zhang, X. and Leskovec, J., 2019, July. Predicting dynamic embedding trajectory in temporal interaction networks. In Proceedings of the 25th ACM SIGKDD (pp. 1269-1278).
- Chen, H., Xiong, Y., Zhu, Y. and Yu, P.S., 2021, April. Highly Liquid Temporal Interaction Graph Embeddings. In Proceedings of the Web Conference 2021 (pp. 1639-1648).
- Zhang, Z., Bu, J., Ester, M., Zhang, J., Yao, C., Li, Z. and Wang, C., 2020, April. Learning temporal interaction graph embedding via coupled memory networks. In Proceedings of The Web Conference 2020 (pp. 3049-3055).

- Ma, Y., Guo, Z., Ren, Z., Tang, J. and Yin, D., 2020, July. Streaming graph neural networks. In Proceedings of the 43rd International ACM SIGIR Conference (pp. 719-728).
- Cui, Z., Li, Z., Wu, S., Zhang, X., Liu, Q., Wang, L. and Ai, M., 2021. DyGCN: Dynamic Graph Embedding with Graph Convolutional Network. arXiv preprint arXiv:2104.02962.
- Mahdavi, S., Khoshraftar, S. and An, A., 2019. Dynamic joint variational graph autoencoders. arXiv preprint arXiv:1910.01963.
- Du, L., Wang, Y., Song, G., Lu, Z. and Wang, J., 2018, July. Dynamic Network Embedding: An Extended Approach for Skip-gram based Network Embedding. In IJCAI (Vol. 2018, pp. 2086-2092).
- Liu, J., Xu, C., Yin, C., Wu, W. and Song, Y., 2020. K-core based temporal graph convolutional network for dynamic graphs. IEEE Transactions on Knowledge and Data Engineering.

- Cheng, K., Zhang, Y., Cao, C., Shi, L., Cheng, J. and Lu, H., 2020. Decoupling gcn with dropgraph module for skeleton-based action recognition. In Computer Vision–ECCV 2020: 16th European Conference, Glasgow, UK. (pp. 536-553). Springer International Publishing.
- Lu, Y., Wang, X., Shi, C., Yu, P.S. and Ye, Y., 2019, November. Temporal network embedding with micro-and macro-dynamics. In Proceedings of the 28th ACM CIKM (pp. 469-478).
- Nguyen, G.H., Lee, J.B., Rossi, R.A., Ahmed, N.K., Koh, E. and Kim, S., 2018, April. Continuous-time dynamic network embeddings. In Companion Proceedings of the The Web Conference 2018 (pp. 969-976).
- Bonner, S., Brennan, J., Kureshi, I., Theodoropoulos, G., McGough, A.S. and Obara, B., 2018, December. Temporal graph offset reconstruction: Towards temporally robust graph representation learning. In 2018 IEEE International Conference on Big Data (Big Data) (pp. 3737-3746). IEEE.

- Bonner, S., Atapour-Abarghouei, A., Jackson, P.T., Brennan, J., Kureshi, I., Theodoropoulos, G., McGough, A.S. and Obara, B., 2019, December. Temporal neighbourhood aggregation: Predicting future links in temporal graphs via recurrent variational graph convolutions. In 2019 IEEE International Conference on Big Data (Big Data) (pp. 5336-5345). IEEE.
- Knyazev, B., Augusta, C. and Taylor, G.W., 2019. Learning temporal attention in dynamic graphs with bilinear interactions. arXiv preprint arXiv:1909.10367.
- Trivedi, R., Farajtabar, M., Biswal, P. and Zha, H., 2019, May. Dyrep: Learning representations over dynamic graphs. In International conference on learning representations.
- Sankar, A., Wu, Y., Gou, L., Zhang, W. and Yang, H., 2018. Dynamic graph representation learning via self-attention networks. arXiv preprint arXiv:1812.09430.

- Venkatakrisnan, S.B., Alizadeh, M. and Viswanath, P., 2018. Graph2seq: Scalable learning dynamics for graphs. arXiv preprint arXiv:1802.04948.
- Lei, K., Qin, M., Bai, B., Zhang, G. and Yang, M., 2019, April. Gcn-gan: A non-linear temporal link prediction model for weighted dynamic networks. In IEEE INFOCOM 2019-IEEE Conference on Computer Communications (pp. 388-396). IEEE.
- Maheshwari, A., Goyal, A., Hanawal, M.K. and Ramakrishnan, G., 2019. DynGAN: Generative Adversarial Networks for Dynamic Network Embedding. In Graph Representation Learning Workshop at NeurIPS.
- Chen, J., Xu, X., Wu, Y. and Zheng, H., 2018. Gc-lstm: Graph convolution embedded lstm for dynamic link prediction. arXiv preprint arXiv:1812.04206.
- Li, Y., Yu, R., Shahabi, C. and Liu, Y., 2017. Diffusion convolutional recurrent neural network: Data-driven traffic forecasting. arXiv preprint arXiv:1707.01926.

References

- Li, J., Han, Z., Cheng, H., Su, J., Wang, P., Zhang, J. and Pan, L., 2019, July. Predicting path failure in time-evolving graphs. In Proceedings of the 25th ACM SIGKDD (pp. 1279-1289).
- Taheri, A., Gimpel, K. and Berger-Wolf, T., 2019, May. Learning to represent the evolution of dynamic graphs with recurrent models. In Companion Proceedings of The 2019 World Wide Web Conference (pp. 301-307).
- Liu, Z., Huang, C., Yu, Y. and Dong, J., 2021, April. Motif-Preserving Dynamic Attributed Network Embedding. In Proceedings of the Web Conference 2021 (pp. 1629-1638).
- Chen, J., Zhang, J., Xu, X., Fu, C., Zhang, D., Zhang, Q. and Xuan, Q., 2019. E-lstm-d: A deep learning framework for dynamic network link prediction. IEEE Transactions on Systems, Man, and Cybernetics: Systems.
- Xue, H., Yang, L., Jiang, W., Wei, Y., Hu, Y. and Lin, Y., 2020. Modeling dynamic heterogeneous network for link prediction using hierarchical attention with temporal rnn. arXiv preprint

- Fathy, A. and Li, K., 2020. Temporalgat: Attention-based dynamic graph representation learning. *Advances in Knowledge Discovery and Data Mining*, 12084, p.413.
- Dwivedi, V.P. and Bresson, X., 2020. A generalization of transformer networks to graphs. *arXiv preprint arXiv:2012.09699*.
- Xu, D., Ruan, C., Korpeoglu, E., Kumar, S. and Achan, K., 2020. Inductive representation learning on temporal graphs. *arXiv preprint arXiv:2002.07962*.
- Seo, Y., Defferrard, M., Vandergheynst, P. and Bresson, X., 2018, December. Structured sequence modeling with graph convolutional recurrent networks. In *International Conference on Neural Information Processing* (pp. 362-373). Springer, Cham.

- Xiang, Y., Xiong, Y. and Zhu, Y., 2020, December. TI-GCN: A Dynamic Network Embedding Method with Time Interval Information. In 2020 IEEE International Conference on Big Data (Big Data) (pp. 838-847). IEEE.
- Pareja, A., Domeniconi, G., Chen, J., Ma, T., Suzumura, T., Kanezashi, H., Kaler, T., Schardl, T. and Leiserson, C., 2020, April. Evolvegc: Evolving graph convolutional networks for dynamic graphs. In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 34, No. 04, pp. 5363-5370).
- Wang, X., Lyu, D., Li, M., Xia, Y., Yang, Q., Wang, X., Wang, X., Cui, P., Yang, Y., Sun, B. and Guo, Z., 2021, June. APAN: Asynchronous Propagation Attention Network for Real-time Temporal Graph Embedding. In Proceedings of the 2021 International Conference on Management of Data (pp. 2628-2638).
- Rossi, E., Chamberlain, B., Frasca, F., Eynard, D., Monti, F. and Bronstein, M., 2020. Temporal graph networks for deep learning on dynamic graphs. arXiv preprint arXiv:2006.10637.

- Wang, Y., Chang, Y.Y., Liu, Y., Leskovec, J. and Li, P., 2021. Inductive Representation Learning in Temporal Networks via Causal Anonymous Walks. arXiv preprint arXiv:2101.05974.
- Makarov, I., Savchenko, A., Korovko, A., Sherstyuk, L., Severin, N., Kiselev, D., Mikheev, A. and Babaev, D., 2021. Temporal Graph Network Embedding with Causal Anonymous Walks Representations. arXiv preprint arXiv:2108.08754.