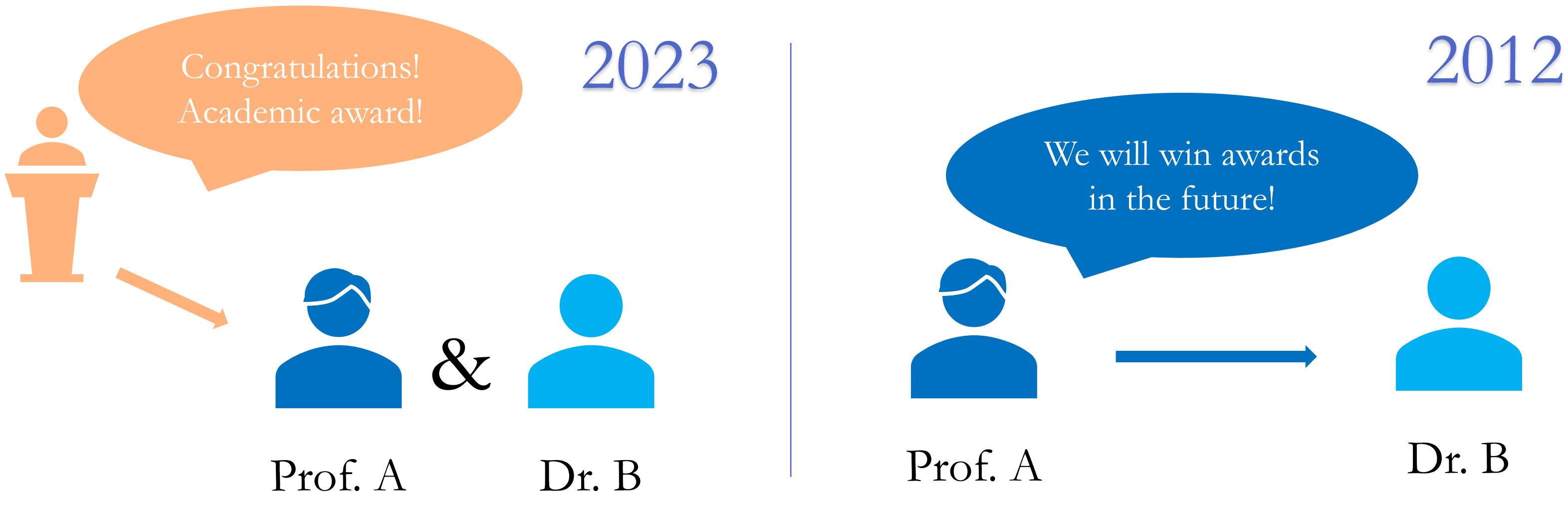
Deep Temporal Graph Clustering

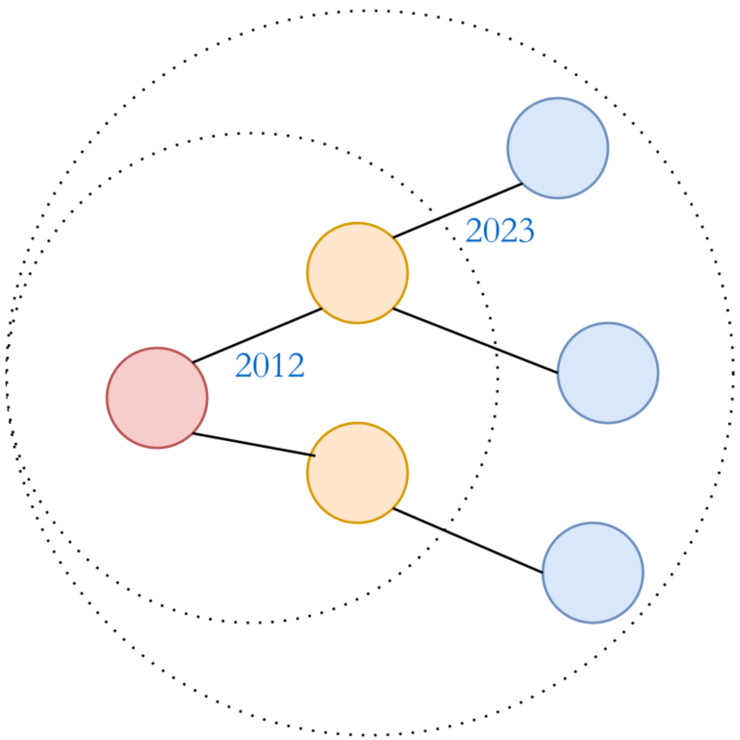
Meng Liu[1] **Yue Liu**[1] **Ke Liang**[1] **Wenxuan Tu**[1]
Siwei Wang[2] **Sihang Zhou**[1] **Xinwang Liu**[1*]

Presenters: Meng Liu and Ke Liang

Contact: mengliuedu@163.com

Importance of Time



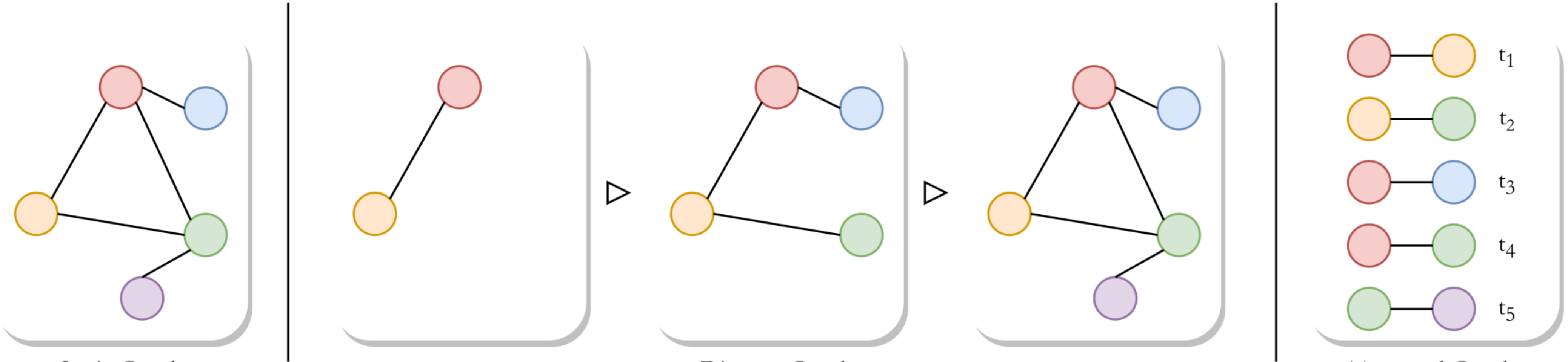


Message Propagation

- In the real world, the past cannot predict the future.
- However, the classic message propagation mechanism of graph neural networks may cause this problem, that is, knowledge leakage.
- In this case, time information is particularly important.

Classification of Graphs

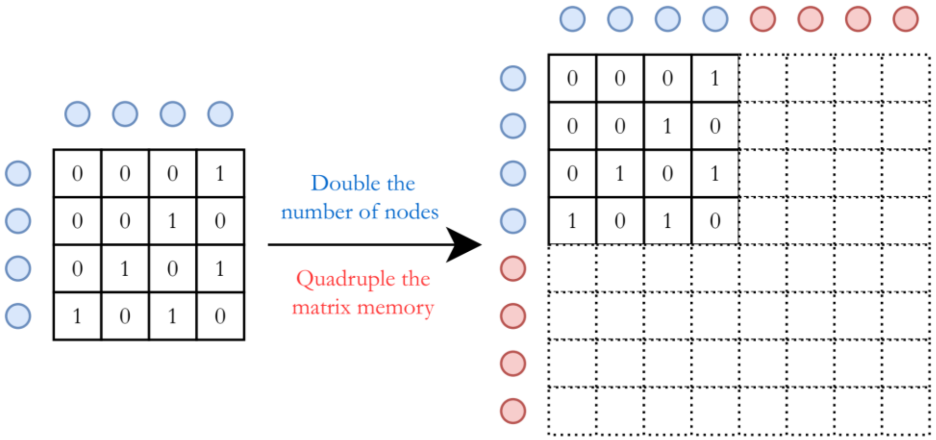
- Graph data can be divided into Static Graph and Dynamic Graph according to whether it contains dynamic information.
- Dynamic graphs can be subdivided into Discrete Graph (Discrete-Time Dynamic Graph, DTDG) and Temporal Graph (Continuous-Time Dynamic Graph, CTDG).

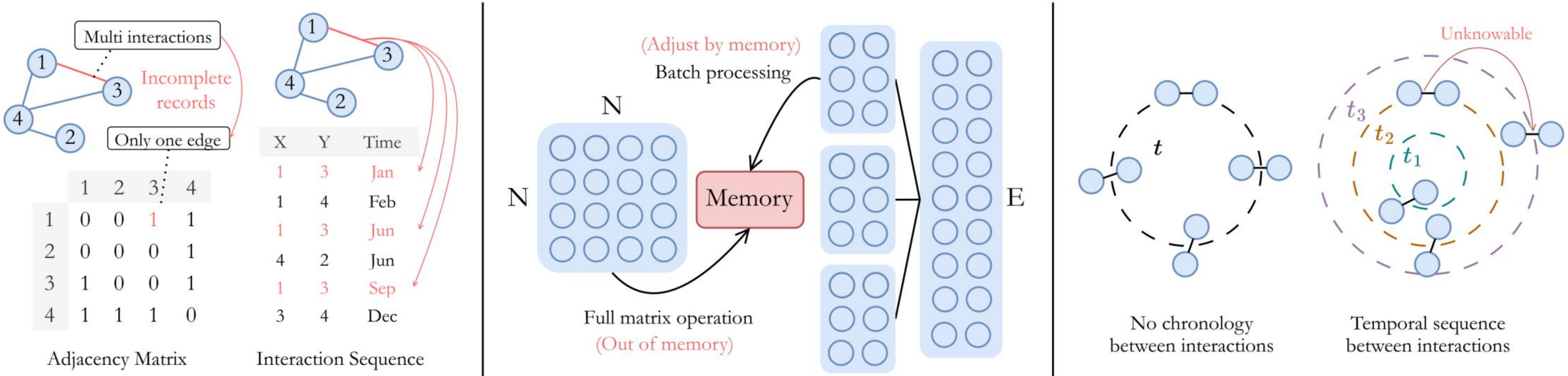


Static Graph   Discrete Graph   Temporal Graph

Static Graphs and Temporal Graphs

- Compared with static graphs based on adjacency matrix, temporal graphs adopt interaction sequence and batch processing patterns, which are more flexible and more detailed.

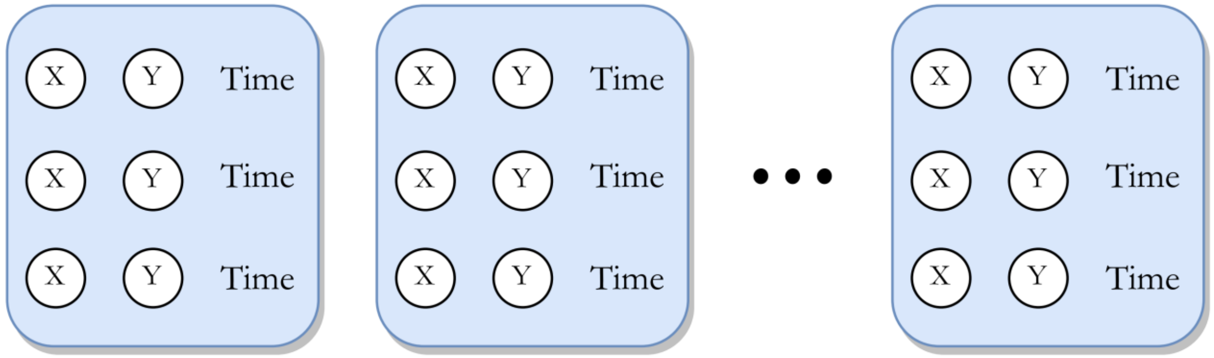




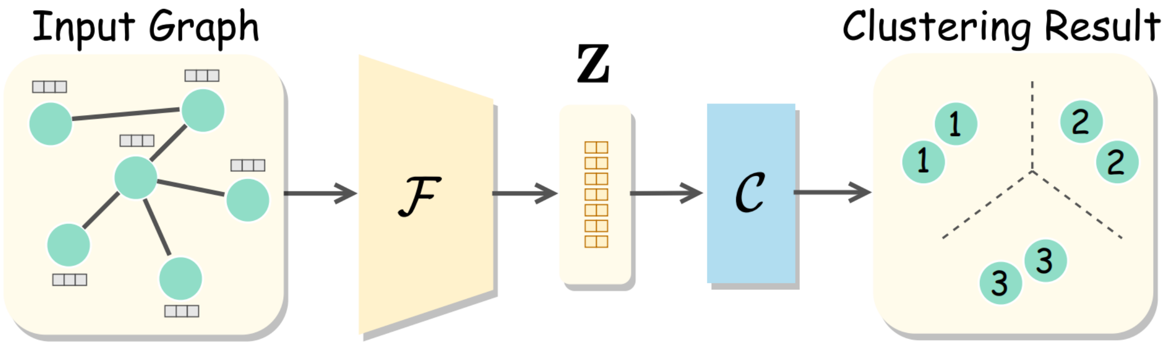
(a) Adjacency matrix and interaction sequence. (b) Full matrix operation and batch processing. (c) Strict chronological order in temporal graphs.

Challenge 1: Inapplicable Clustering Techniques

- Temporal Graph clustering changes from the adjacency matrix to the interaction sequence form, which brings a richer data storage structure and a more convenient batch training pattern, but it also brings new challenges.



Interaction Sequence-Based Batch Processing



- Without the data form of adjacency matrix, many classic static graph clustering techniques are no longer applicable. After breaking away from the adjacency matrix, it becomes more difficult to obtain high-order structural information.

TGC Framework

- We improve existing classical clustering techniques by adding them to temporal graph learning methods.
- We select HTNE as the baseline method, but it can also be migrated to any other methods.

Node-Level Distribution

$$q_{(x,k,t)} = \frac{(1+||\boldsymbol{z}_x^0 - \boldsymbol{z}_{c_k}^t||^2/v)^{-\frac{v+1}{2}}}{\sum_{c_j \in C}(1+||\boldsymbol{z}_x^0 - \boldsymbol{z}_{c_j}^t||^2/v)^{-\frac{v+1}{2}}}$$

$$p_{(x,k,t)} = \frac{q_{(x,k,t)}^2 / \sum_{i \in V} q_{(i,k,t)}}{\sum_{c_j \in C}(q_{(x,j,t)}^2 / \sum_{i \in V} q_{(i,j,t)})}$$

$$L_{node} = \sum_{c_k \in C} p_{(x,k,t)} \log \frac{p_{(x,k,t)}}{q'_{(x,k,t)}}$$

Batch-Level Reconstruction

$$L_{batch} = |1 - \cos(\boldsymbol{z}_x^t, \boldsymbol{z}_y^t)| + |1 - \cos(\boldsymbol{z}_x^t, \boldsymbol{z}_h^t)| + |0 - \cos(\boldsymbol{z}_x^t, \boldsymbol{z}_n^t)|$$

Loss Function

$$L_{clu} = L_{node} + L_{batch}$$

$$L = \sum^E (L_{tem} + L_{clu})$$

Complexity Discussion

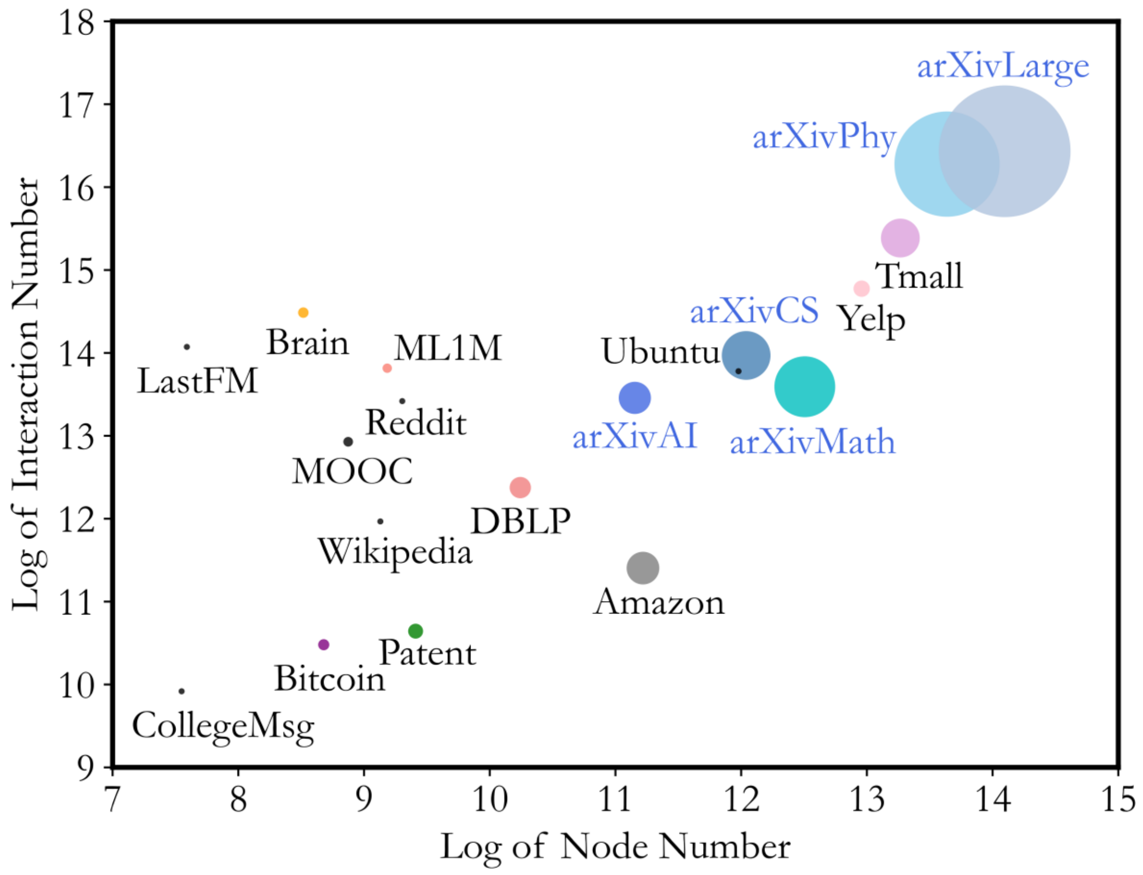
- The core complexity of the static graph method is N^2, and the complexity of temporal method is $|E|$.
- In most cases, $N^2 > |E|$, because N^2 approximates a fully connected graph.
- In a few cases, $N^2 < |E|$, which means the edge information is lost or omitted.

Table 1: Dataset statistics.

Datasets	Nodes	Interactions	Edges	Complexity	Timestamps	K	Degree	MinI	MaxI
DBLP	28,085	236,894	162,441	$N^2 \gg E$	27	10	16.87	1	955
Brain	5,000	1,955,488	1,751,910	$N^2 > E$	12	10	782	484	1,456
Patent	12,214	41,916	41,915	$N^2 \gg E$	891	6	6.86	1	789
School	327	188,508	5,802	$N^2 < E$	7,375	9	1153	7	4,647
arXivAI	69,854	699,206	699,198	$N^2 \gg E$	27	5	20.02	1	11,594
arXivCS	169,343	1,166,243	1,166,237	$N^2 \gg E$	29	40	13.77	1	13,161

Challenge 2: Dataset mismatch

Dataset	Nodes	Interactions	Class	Labels	Timestamps
CollegeMsg	1,899	20,296	N/A	N/A	193
LastFM	1,980	1,293,103	N/A	N/A	30
Wikipedia	9,228	157,474	N/A	N/A	30
Reddit	10,985	672,447	N/A	N/A	30
Ubuntu	159,316	964,437	N/A	N/A	2,613
MOOC	7,144	411,749	N/A	N/A	-
Bitcoin	5,881	35,592	21	5,858	27,487
ML1M	9,746	1,000,209	5	3,706	25,212
Amazon	74,526	89,689	5	72,098	5,804
Yelp	424,450	2,610,143	5	15,154	153
Tmall	577,314	4,807,545	10	104,410	186
Brain	5,000	1,955,488	10	5,000	12
Patent	12,214	41,916	6	12,214	891
DBLP	28,085	236,894	10	28,085	27
arXivAI	69,854	699,206	5	69,854	27
arXivCS	169,343	1,166,243	40	169,343	29
arXivMath	270,013	799,745	31	270,013	31
arXivPhy	837,212	11,733,619	53	837,212	41
arXivLarge	1,324,064	13,701,428	172	1,324,064	41



Scales of Different Datasets

Experimental Results

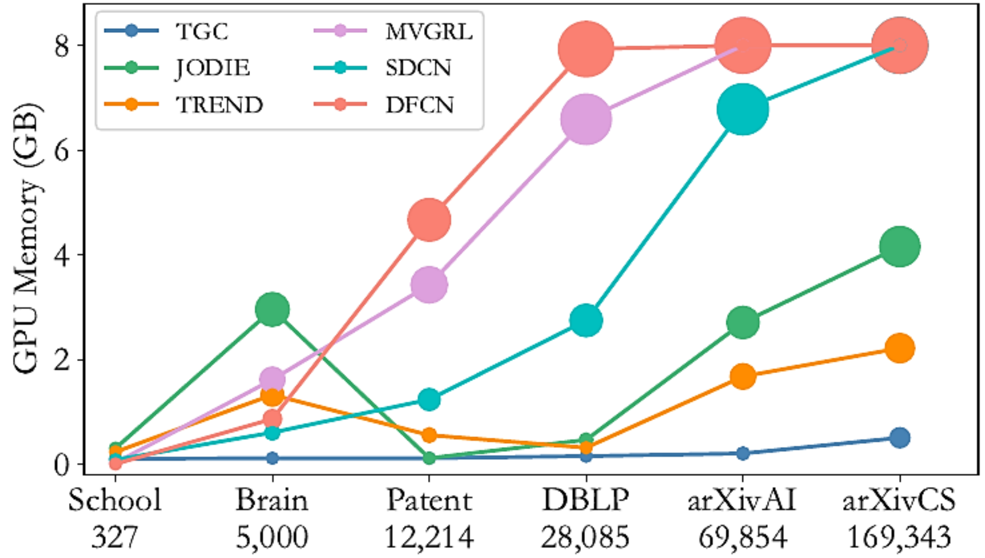
Table 2: Node clustering results in common datasets. We bold the best results and underline the second best results. If a method face the out-of-memory problem, we record as OOM.

Data	Metric	deepwalk	AE	node2vec	GAE	MVGRL	AGE	DAEGC	SDCN	SDCNQ	DFCN	HTNE	TGAT	JODIE	TGN	TREND	TGC
DBLP	ACC	45.07	42.16	46.31	39.31	28.95	OOM	OOM	46.69	40.47	41.97	45.74	36.76	20.79	19.78	46.82	**48.75**
	NMI	31.46	36.71	34.87	29.75	22.03	OOM	OOM	35.07	31.86	36.94	35.95	28.98	1.70	9.82	36.56	**37.08**
	ARI	17.89	22.54	20.40	17.17	13.73	OOM	OOM	**23.74**	19.80	21.46	22.13	17.64	1.64	5.46	22.83	22.86
	F1	38.56	37.84	43.35	35.04	24.79	OOM	OOM	40.31	35.18	35.97	43.98	34.22	13.23	10.66	44.54	**45.03**
Brain	ACC	41.28	43.48	43.92	31.22	15.76	38.48	42.52	42.62	43.42	**47.46**	43.20	41.43	19.14	17.40	39.83	44.30
	NMI	49.09	50.49	45.96	32.23	21.15	39.64	49.86	46.61	47.40	48.53	50.33	48.72	10.50	8.04	45.64	**50.68**
	ARI	28.40	29.78	26.08	14.97	9.77	28.82	27.47	27.93	27.69	28.58	29.26	23.64	5.00	4.56	22.82	**30.03**
	F1	42.54	43.26	46.61	34.11	13.56	36.47	43.24	41.42	37.27	**50.45**	43.85	41.13	11.12	13.49	33.67	44.42
Patent	ACC	38.69	30.81	40.36	39.65	31.13	43.28	46.64	37.28	32.76	39.23	45.07	38.26	30.82	38.77	38.72	**50.36**
	NMI	22.71	8.76	24.84	17.73	10.19	20.72	21.28	13.17	9.11	15.42	20.77	19.74	9.55	8.24	14.44	**25.04**
	ARI	10.32	7.43	18.95	13.61	10.26	**19.23**	16.74	10.12	7.84	12.24	10.69	13.31	7.46	6.01	13.45	18.81
	F1	31.48	26.65	34.97	30.95	18.06	35.45	32.83	31.38	28.27	30.32	28.85	26.97	20.83	21.40	28.41	**38.69**
School	ACC	90.60	30.88	91.56	85.62	32.37	84.71	34.25	48.32	33.94	49.85	99.38	80.54	19.88	31.71	94.18	**99.69**
	NMI	91.72	21.42	92.63	89.41	31.23	81.51	29.53	53.35	25.79	43.37	98.73	73.25	9.26	19.45	89.55	**99.36**
	ARI	89.66	12.04	90.25	83.09	25.00	70.24	15.38	33.81	15.82	28.31	98.70	80.04	2.85	32.12	87.50	**99.33**
	F1	92.63	31.00	91.74	82.64	24.41	84.80	31.39	45.62	33.25	47.05	99.34	79.56	13.02	29.50	94.18	**99.69**

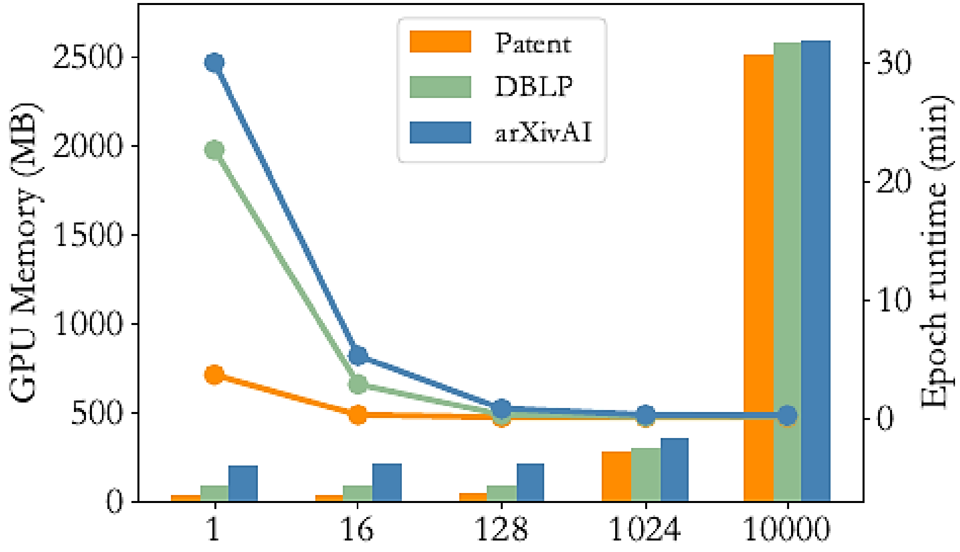
Experimental Results

Table 3: Node clustering results in large-scale datasets. We bold the best results and underline the second best results. If a method face the out-of-memory problem, we record as OOM.

Data	Metric	deepwalk	AE	node2vec	GAE	MVGRL	AGE	DAEGC	SDCN	SDCNQ	DFCN	HTNE	TGAT	JODIE	TGN	TREND	TGC
arXivAI	ACC	60.91	23.85	65.01	38.72	OOM	OOM	OOM	44.44	37.62	OOM	65.66	48.69	30.71	31.25	29.82	**73.59**
	NMI	34.34	10.20	36.18	32.54	OOM	OOM	OOM	21.63	20.73	OOM	39.24	32.12	2.91	24.74	1.28	**42.46**
	ARI	36.08	14.00	40.35	32.98	OOM	OOM	OOM	23.43	21.29	OOM	43.73	30.34	5.35	11.91	1.12	**48.98**
	F1	49.47	19.20	53.66	16.97	OOM	OOM	OOM	33.96	31.62	OOM	52.86	43.62	23.24	21.93	19.22	**57.86**
arXivCS	ACC	34.42	24.20	27.39	OOM	OOM	OOM	OOM	29.78	27.05	OOM	25.57	20.53	11.27	20.10	8.94	**39.95**
	NMI	40.86	14.03	41.18	OOM	OOM	OOM	OOM	13.27	11.57	OOM	40.83	38.64	5.12	16.21	5.57	**43.89**
	ARI	24.65	11.80	19.14	OOM	OOM	OOM	OOM	14.32	12.02	OOM	16.51	15.54	5.31	18.63	3.49	**36.06**
	F1	20.39	12.33	21.41	OOM	OOM	OOM	OOM	14.08	13.28	OOM	19.56	13.23	4.85	22.67	4.02	**25.46**



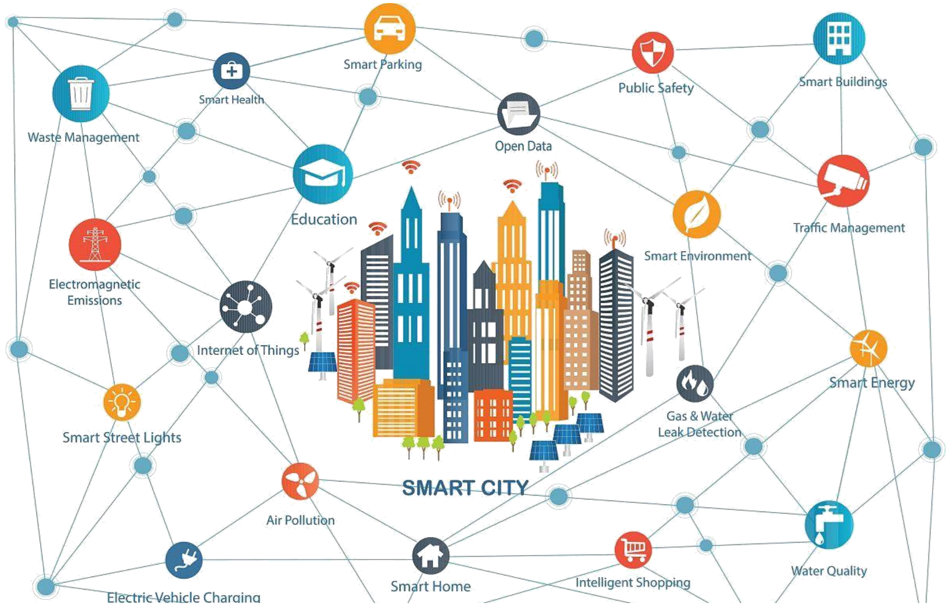
GPU Memory with Different Dataset Scales

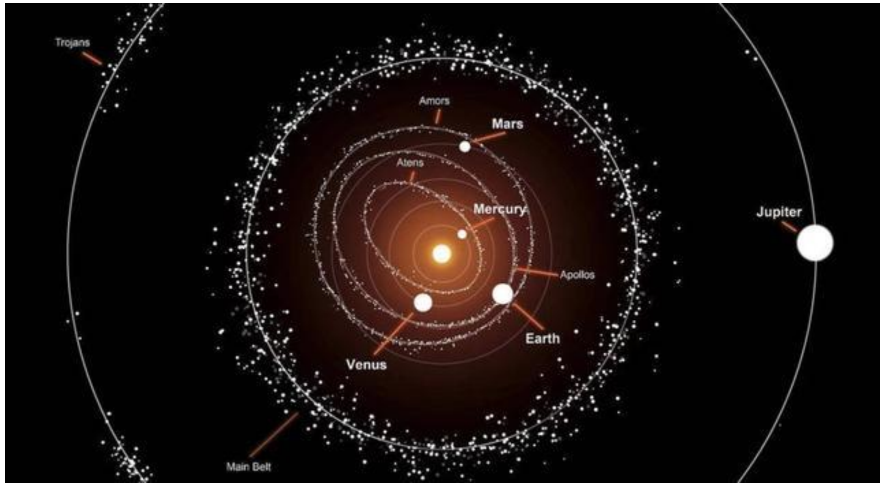


GPU Memory and Epoch Time

Summary

- Temporal graph clustering provides new possibilities.
- Inapplicable clustering techniques and mismatched datasets are two major challenges.
- Temporal graph clustering can find a balance between time and space requirements.
- Dynamic real-world data is the foundation of temporal graph clustering.





Open Source

- Data4TGC

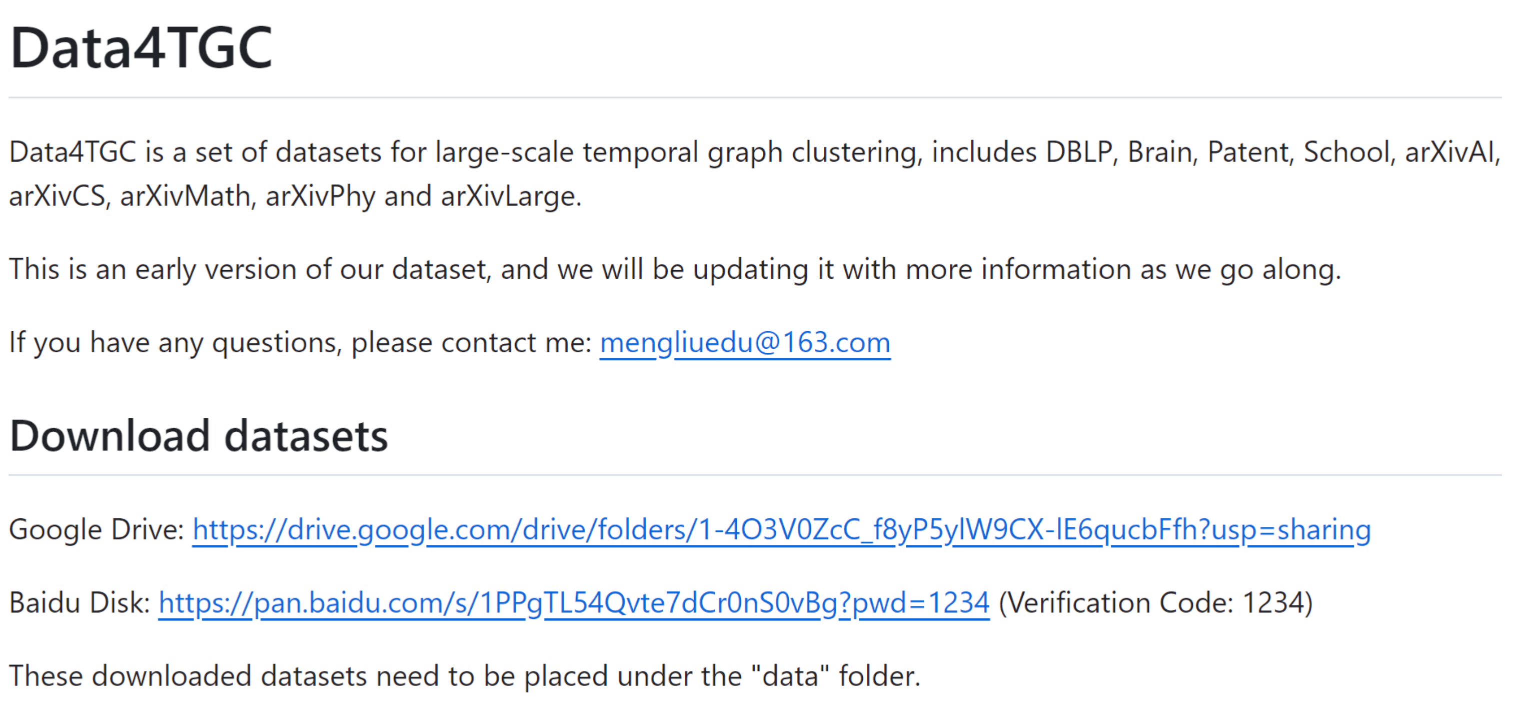
  https://github.com/MGitHubL/Data4TGC

- Deep Temporal Graph Clustering

  https://github.com/MGitHubL/Deep-Temporal-Graph-Clustering

- Awesome Knowledge Graph Reasoning

  https://github.com/LIANGKE23/Awesome-Knowledge-Graph-Reasoning



Data4TGC

Data4TGC is a set of datasets for large-scale temporal graph clustering, includes DBLP, Brain, Patent, School, arXivAI, arXivCS, arXivMath, arXivPhy and arXivLarge.

This is an early version of our dataset, and we will be updating it with more information as we go along.

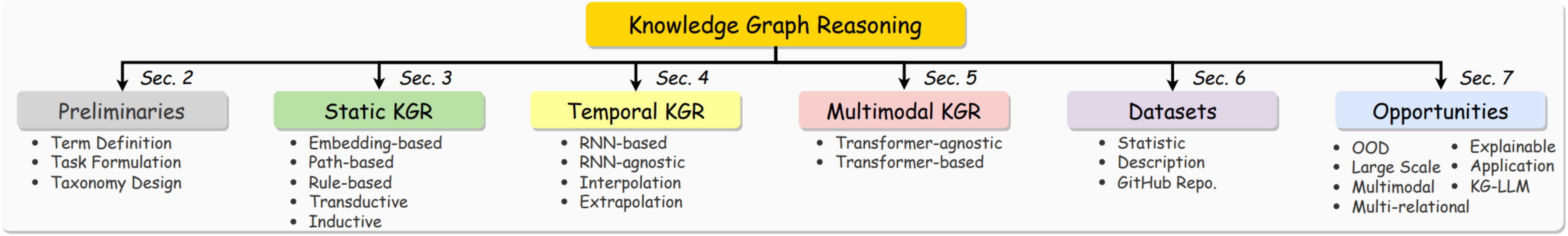
If you have any questions, please contact me: mengliuedu@163.com

Download datasets

Google Drive: https://drive.google.com/drive/folders/1-4O3V0ZcC_f8yP5ylW9CX-lE6qucbFfh?usp=sharing

Baidu Disk: https://pan.baidu.com/s/1PPgTL54Qvte7dCr0nS0vBg?pwd=1234 (Verification Code: 1234)

These downloaded datasets need to be placed under the "data" folder.



Thanks!

Presenter: Meng Liu and Ke Liang

Contact: mengliuedu@163.com