CAT-Walk: Inductive Hypergraph Learning via Set Walks

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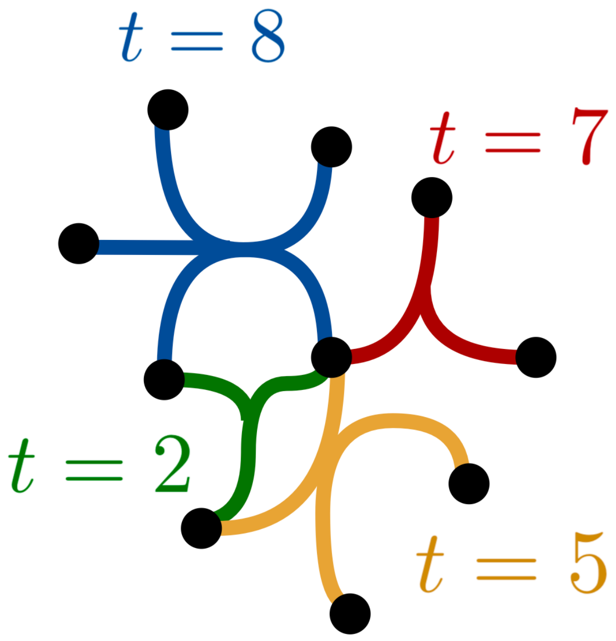
SYSTOPIA

NEURAL INFORMATION PROCESSING SYSTEMS

Temporal Hypergraphs

- ✶ Hypergraphs allow higher-order connections between a group of nodes at the same time!
- ✶ Temporal hypergraphs are powerful paradigms for modeling time-dependent, higher-order interactions in complex systems.



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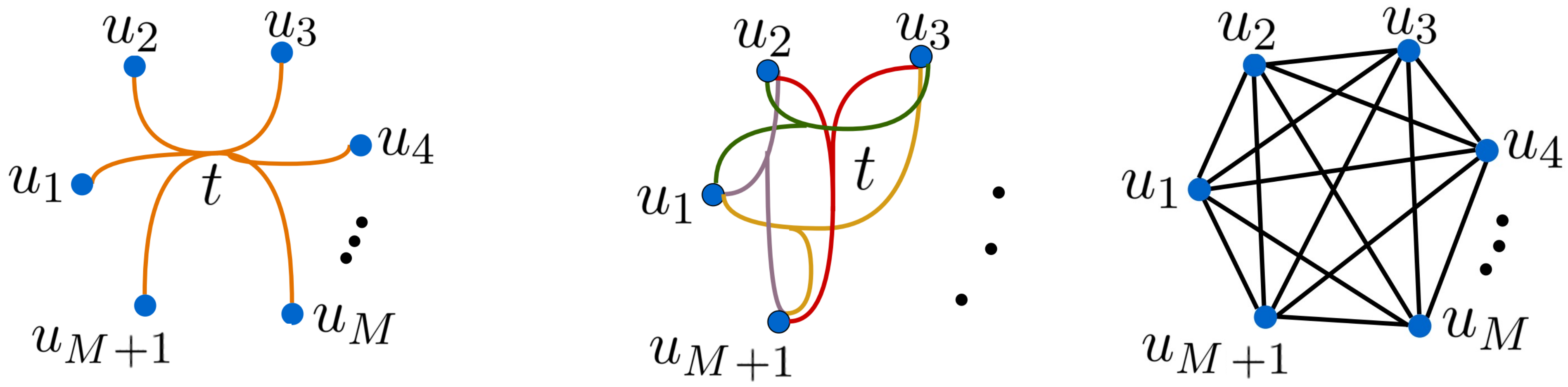
- ✶ Temporal hypergraphs are powerful paradigms for modeling time-dependent, higher-order interactions in complex systems.
- ✶ Existing methods are typically designed only for specific tasks or static hypergraphs.



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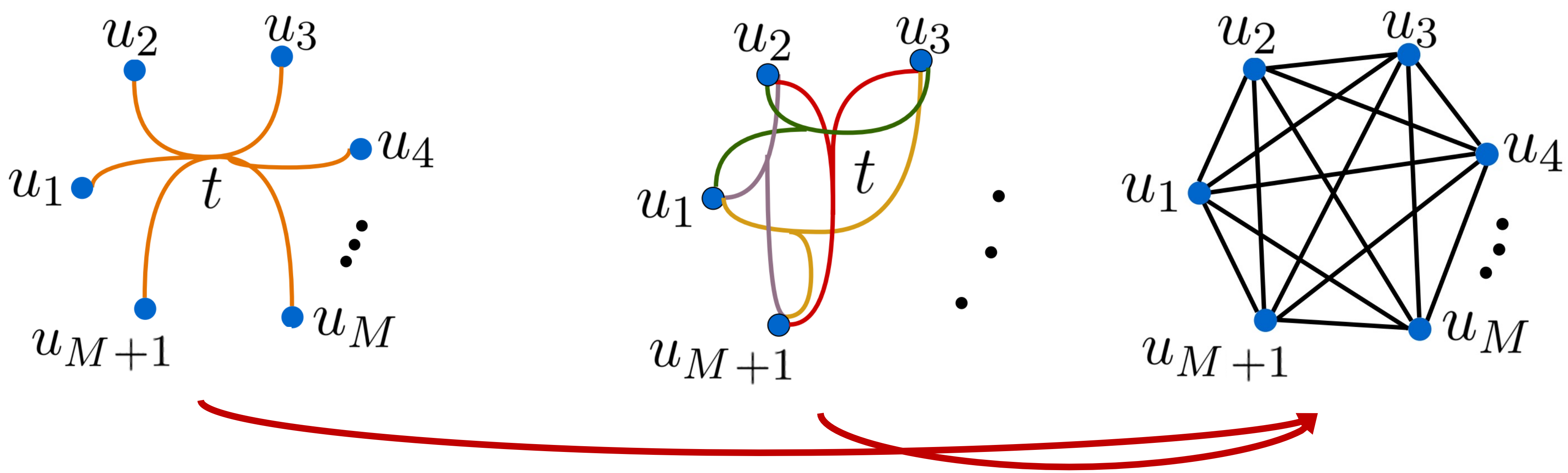
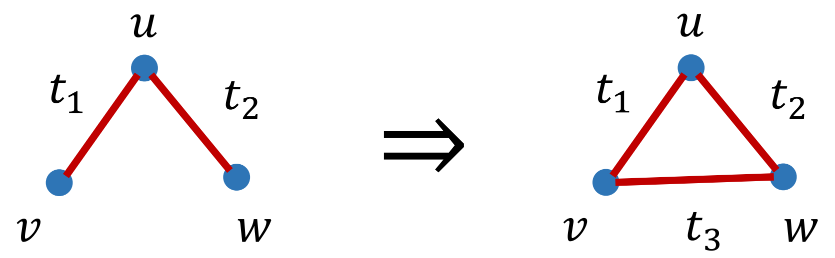


Temporal Hypergraphs

- ✶ Hypergraphs allow higher-order connections between a group of nodes at the same time!
- ✶ Temporal hypergraphs are powerful paradigms for modeling time-dependent, higher-order interactions in complex systems.
- ✶ Existing methods are typically designed only for specific tasks or static hypergraphs.
- ✶ We present CAT-Walk, an inductive hyperedge learning method!

Hypergraph Random Walk

- Underlying laws of the networks:
  - ✶ **Triadic Closure**



[1] Inductive Representation Learning in Temporal Networks via Causal Anonymous Walks. Wang et al., ICLR 2021.

Hypergraph Random Walk

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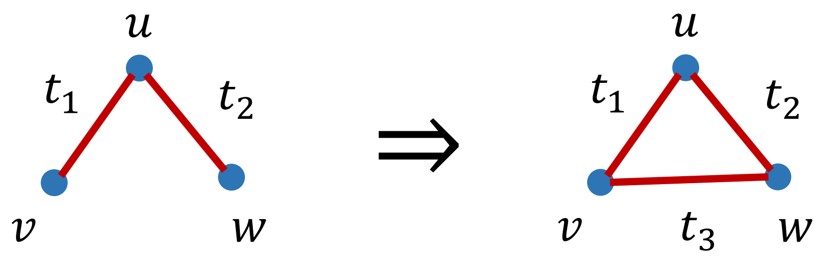
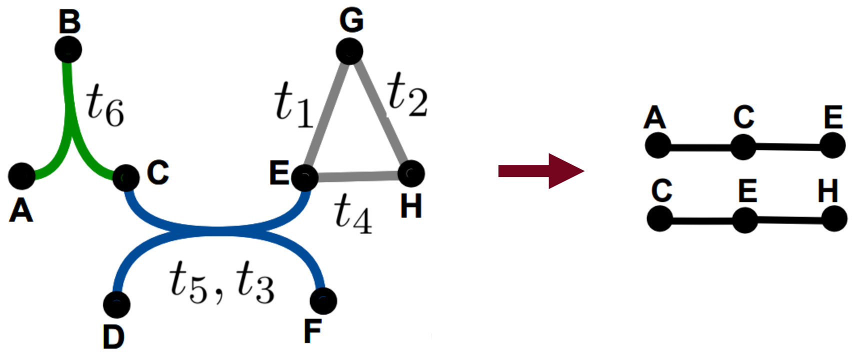
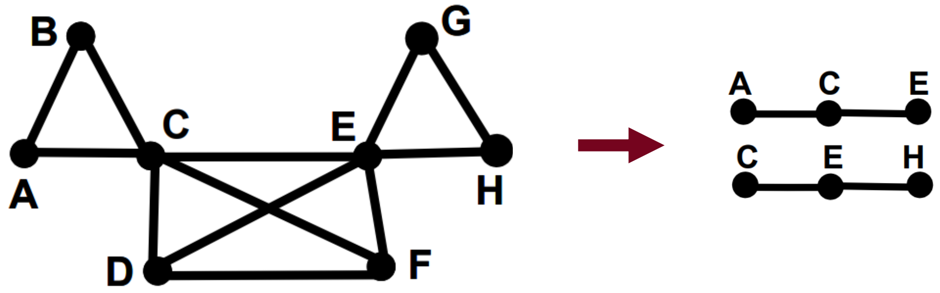


- Existing hypergraph random walks miss information!





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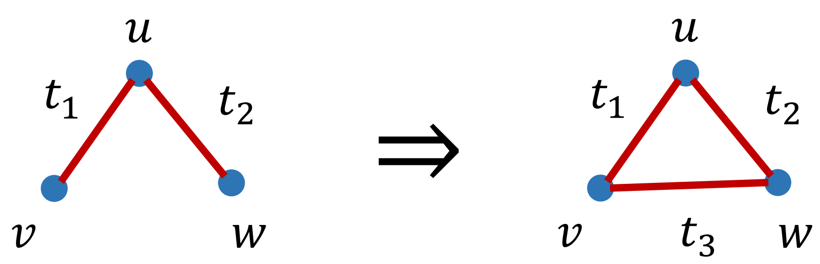
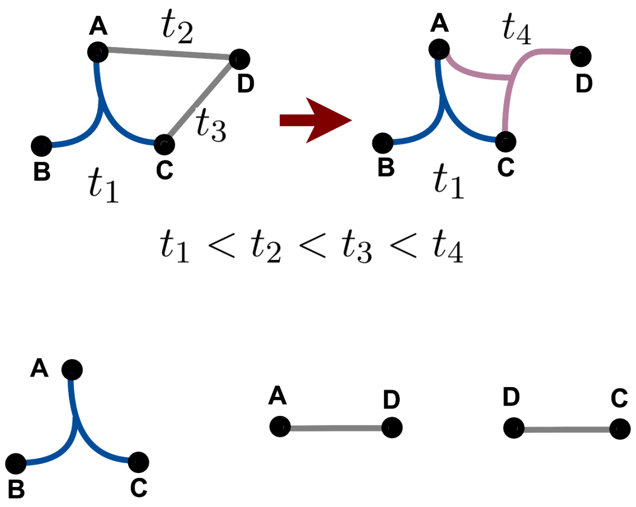
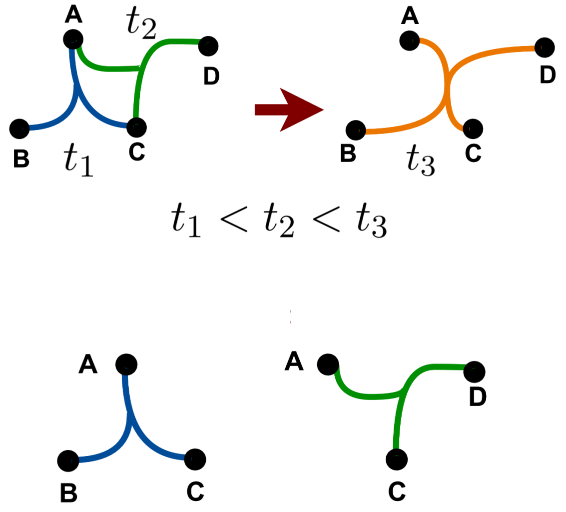
Hypergraph Random Walk

- Underlying laws of the networks:
  - ✶ **Triadic Closure**
  - ✶ **Complex Dynamic Laws in Hypergraph:**





Law Explanation: When a node is pairwise connected to two other nodes that are themselves connected by a three-way connection, it tends to form a three-way connection with them.



Law Explanation: When a node has three-way connection with two other nodes that are themselves connected by a three-way connection, all tend to form a four-way connection with each other.

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SetWalks: Higher-order Random Walk on Hypergraphs

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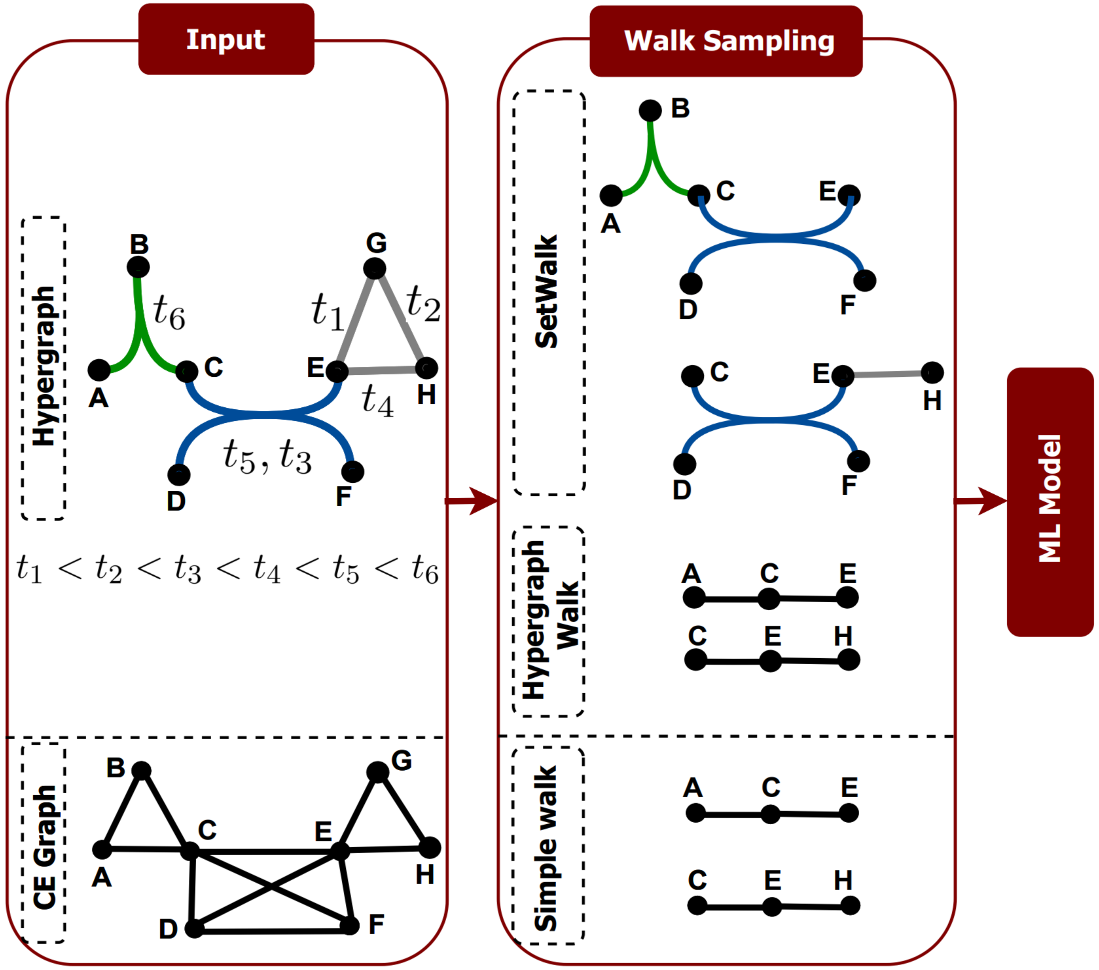
- ✶ Hypergraph random walks are sequences of nodes.
- ✶ SetWalks are sequences of hyperedges!



The advantage of SETWALKS in walk-based hypergraph learning.

Schematic of the CAT-WALK

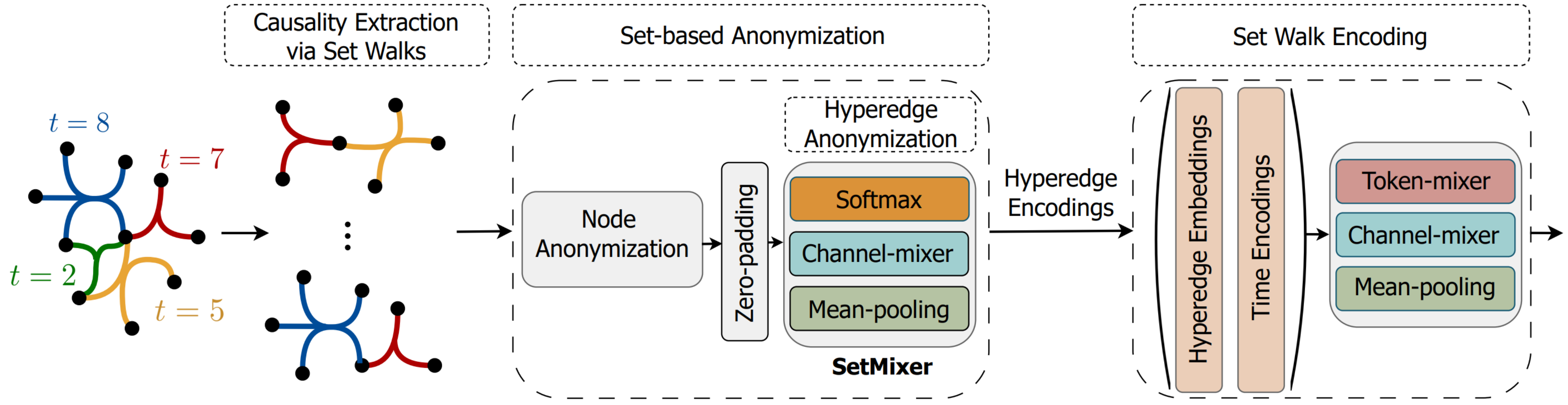


Figure 3: **Schematic of the CAT-WALK.** CAT-WALK consists of three stages: (1) Causality Extraction via Set Walks, (2) Set-based Anonymization , and (3) Set Walk Encoding.

- ✶ We present a novel pooling method that is theoretically proven to be powerful!
- ✶ CAT-Walk allows continuous time hyperedge encoding by using MLP-Mixer instead of sequential encoders like RNN and Transformers!

Experimental Results: Hyperedge Prediction

Table 1: Performance on hyperedge prediction: Mean AUC (%) ± standard deviation. Boldfaced letters shaded blue indicate the best result, while gray shaded boxes indicate results within one standard deviation of the best result. N/A: the method has numerical precision or computational issues.

	Methods	NDC Class	High School	Primary School	Congress Bill	Email Enron	Email Eu	Question Tags	Users-Threads
Inductive	Strongly Inductive								
	CE-GCN	52.31 ± 2.99	60.54 ± 2.06	52.34 ± 2.75	49.18 ± 3.61	63.04 ± 1.80	52.76 ± 2.41	56.10 ± 1.88	57.91 ± 1.56
	CE-EvolveGCN	49.78 ± 3.13	46.12 ± 3.83	58.01 ± 2.56	54.00 ± 1.84	57.31 ± 4.19	44.16 ± 1.27	64.08 ± 2.75	52.00 ± 2.32
	CE-CAW	76.45 ± 0.29	83.73 ± 1.42	80.31 ± 1.46	75.38 ± 1.25	70.81 ± 1.13	72.99 ± 0.20	70.14 ± 1.89	73.12 ± 1.06
	NHP	70.53 ± 4.95	65.29 ± 3.80	70.86 ± 3.42	69.82 ± 2.19	49.71 ± 6.09	65.35 ± 2.07	68.23 ± 3.34	71.83 ± 2.64
	HyperSAGCN	79.05 ± 2.48	88.12 ± 3.01	80.13 ± 1.38	79.51 ± 1.27	73.09 ± 2.60	78.01 ± 1.24	73.66 ± 1.95	73.94 ± 2.57
	CHESHIRE	72.24 ± 2.63	82.54 ± 0.88	77.26 ± 1.01	79.43 ± 1.58	70.03 ± 2.55	69.98 ± 2.71	N/A	76.99 ± 2.82
	CAt-Walk	**98.89 ± 1.82**	**96.03 ± 1.50**	**95.32 ± 0.89**	**93.54 ± 0.56**	**73.45 ± 2.92**	**91.68 ± 2.78**	**88.03 ± 3.38**	**89.84 ± 6.02**
	Weakly Inductive								
	CE-GCN	51.80 ± 3.29	50.33 ± 3.40	52.19 ± 2.54	52.38 ± 2.75	50.81 ± 2.87	49.60 ± 3.96	55.13 ± 2.76	57.06 ± 3.16
	CE-EvolveGCN	55.39 ± 5.16	57.85 ± 3.51	51.50 ± 4.07	55.63 ± 3.41	45.66 ± 2.10	52.44 ± 2.38	61.79 ± 1.63	55.81 ± 2.54
	CE-CAW	77.61 ± 1.05	83.77 ± 1.41	82.98 ± 1.06	79.51 ± 0.94	**80.54 ± 1.02**	73.54 ± 1.19	77.29 ± 0.86	80.79 ± 0.82
	NHP	75.17 ± 2.02	67.25 ± 5.19	71.92 ± 1.83	69.58 ± 4.07	60.38 ± 4.45	67.19 ± 4.33	70.46 ± 3.52	76.44 ± 1.90
	HyperSAGCN	79.45 ± 2.18	88.53 ± 1.26	85.08 ± 1.45	80.12 ± 2.00	78.86 ± 0.63	77.26 ± 2.09	78.15 ± 1.41	75.38 ± 1.43
	CHESHIRE	79.03 ± 1.24	88.40 ± 1.06	83.55 ± 1.27	79.67 ± 0.83	74.53 ± 0.91	77.31 ± 0.95	N/A	81.27 ± 0.85
	CAt-Walk	**99.16 ± 1.08**	**94.68 ± 2.37**	**96.53 ± 1.39**	**98.38 ± 0.21**	64.11 ± 7.96	**91.98 ± 2.41**	**90.28 ± 2.81**	**97.15 ± 1.81**
Transductive	HPRA	70.83 ± 0.01	94.91 ± 0.00	89.86 ± 0.06	79.48 ± 0.03	78.62 ± 0.00	72.51 ± 0.00	83.18 ± 0.00	70.49 ± 0.02
	HPLSF	76.19 ± 0.82	92.14 ± 0.29	88.57 ± 1.09	79.31 ± 0.52	75.73 ± 0.05	75.27 ± 0.31	83.45 ± 0.93	74.38 ± 1.11
	CE-GCN	66.83 ± 3.74	62.99 ± 3.02	59.14 ± 3.87	64.42 ± 3.11	58.06 ± 3.80	64.19 ± 2.79	55.18 ± 5.12	62.78 ± 2.69
	CE-EvolveGCN	67.08 ± 3.51	65.19 ± 2.26	63.15 ± 1.32	69.30 ± 2.27	69.98 ± 5.38	64.36 ± 4.17	72.56 ± 1.72	68.55 ± 2.26
	CE-CAW	76.30 ± 0.84	81.63 ± 0.97	86.53 ± 0.84	76.99 ± 1.02	79.57 ± 0.14	78.19 ± 1.10	81.73 ± 2.48	80.86 ± 0.45
	NHP	82.39 ± 2.81	76.85 ± 3.08	80.04 ± 3.42	80.27 ± 2.53	63.17 ± 3.79	78.90 ± 4.39	79.14 ± 3.36	82.33 ± 1.02
	HyperSAGCN	80.76 ± 2.64	94.98 ± 1.30	90.77 ± 2.05	82.84 ± 1.61	**83.59 ± 0.98**	79.61 ± 2.35	84.07 ± 2.50	79.62 ± 2.04
	CHESHIRE	84.91 ± 1.05	95.11 ± 0.94	91.62 ± 1.18	86.81 ± 1.24	82.27 ± 0.86	86.38 ± 1.23	N/A	82.75 ± 1.99
	CAt-Walk	**98.72 ± 1.38**	**95.30 ± 0.43**	**97.91 ± 3.30**	**88.15 ± 1.46**	80.45 ± 5.30	**96.74 ± 1.28**	**91.63 ± 1.41**	**93.51 ± 1.27**

Experimental Results: Ablation Study

Table 2: Ablation study on CAT-WALK. AUC scores on inductive hyperedge prediction.

Methods	High School	Primary School	Users in Threads	Congress bill	Question Tags U	
1	CAT-WALK	**96.03 ± 1.50**	**95.32 ± 0.89**	**89.84 ± 6.02**	**93.54 ± 0.56**	**97.59 ± 2.21**
2	Replace SETWALK by Random Walk	92.10 ± 2.18	51.56 ± 5.63	53.24 ± 1.73	80.27 ± 0.02	67.74 ± 2.92
3	Remove Time Encoding	95.94 ± 0.19	86.80 ± 6.33	70.58 ± 9.32	92.56 ± 0.49	96.91 ± 1.89
4	Replace SETMIXER by MEAN(.)	94.58 ± 1.22	95.14 ± 4.36	63.59 ± 5.26	91.06 ± 0.24	68.62 ± 1.25
5 6	Replace SETMIXER by Sum-based Universal Approximator for Sets	94.77 ± 0.67	90.86 ± 0.57	60.03 ± 1.16	91.07 ± 0.70	89.76 ± 0.45
7	Replace MLP-MIXER by RNN	92.85 ± 1.53	50.29 ± 4.07	58.11 ± 1.60	54.90 ± 0.50	65.18 ± 1.99
8	Replace MLP-MIXER by Transformer	55.98 ± 0.83	86.64 ± 3.55	60.65 ± 1.56	89.38 ± 1.66	56.16 ± 4.03
9	Fix $\alpha = 0$	74.06 ± 14.9	58.3 ± 18.62	74.41 ± 10.69	93.31 ± 0.13	62.41 ± 4.34

- ✶ Each component is critical for achieving CAT-Walk's superior performance.
- ✶ The greatest contribution comes from SetWalk, MLP-Mixer in walk encoding, α in temporal hyperedge sampling, and SetMixer pooling, respectively.

Experimental Results: Temporal Node Classification

Table 5: Performance on node classification: Mean ACC (%) ± standard deviation. Boldfaced letters shaded blue indicate the best result, while gray shaded boxes indicate results within one standard deviation of the best result.

	Methods	High School	Primary School	Average Performance
Inductive	CE-GCN	76.24 ± 2.99	79.03 ± 3.16	77.63 ± 3.07
	HyperGCN	83.91 ± 3.05	86.17 ± 3.40	85.04 ± 3.23
	HyperSAGCN	84.89 ± 3.80	82.13 ± 3.69	83.51 ± 3.75
	AllDeepSets	85.67 ± 4.17	81.43 ± 6.77	83.55 ± 5.47
	UniGCNII	88.36 ± 3.78	88.27 ± 3.52	88.31 ± 3.63
	AllSetTransformer	**91.19 ± 2.85**	90.00 ± 4.35	90.59 ± 3.60
	ED-HNN	89.23 ± 2.98	90.83 ± 3.02	90.03 ± 3.00
	CAt-Walk	88.99 ± 4.76	**93.28 ± 2.41**	**91.13 ± 3.58**
Transductive	CE-GCN	78.93 ± 3.11	77.46 ± 2.97	78.20 ± 3.04
	HyperGCN	84.90 ± 3.59	85.23 ± 3.06	85.07 ± 3.33
	HyperSAGCN	84.52 ± 3.18	83.27 ± 2.94	83.90 ± 3.06
	AllDeepSets	85.97 ± 4.05	80.20 ± 10.18	83.09 ± 7.12
	UniGCNII	89.16 ± 4.37	90.29 ± 4.01	89.73 ± 4.19
	AllSetTransformer	90.75 ± 3.13	89.80 ± 2.55	90.27 ± 2.84
	ED-HNN	**91.41 ± 2.36**	91.74 ± 2.62	91.56 ± 2.49
	CAt-Walk	90.66 ± 4.96	**93.20 ± 2.45**	**91.93 ± 3.71**

Conclusion

- ✶ We present CAT-Walk, an inductive hypergraph learning method to learn higher-order patterns and to uncover dynamic laws in temporal hypergraphs.

- ✶ CAT-Walk use a novel higher-order random walk, SetWalks, which is provably more expressive than existing random walks. CAT-Walk uses SetWalks to actively extract temporal higher-order motifs from hypergraphs and learn temporal and structural patterns

- ✶ Experimental results show CAT-Walk superior performance in temporal hyperedge prediction tasks and its competitive performance in temporal node classification tasks.

Thank you!

Paper

Code