CausalSKyHop: Knowledge-Aware Causal Explanation of Dynamic GNNs via Higher-Order Semantic Reasoning

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Background & Motivation

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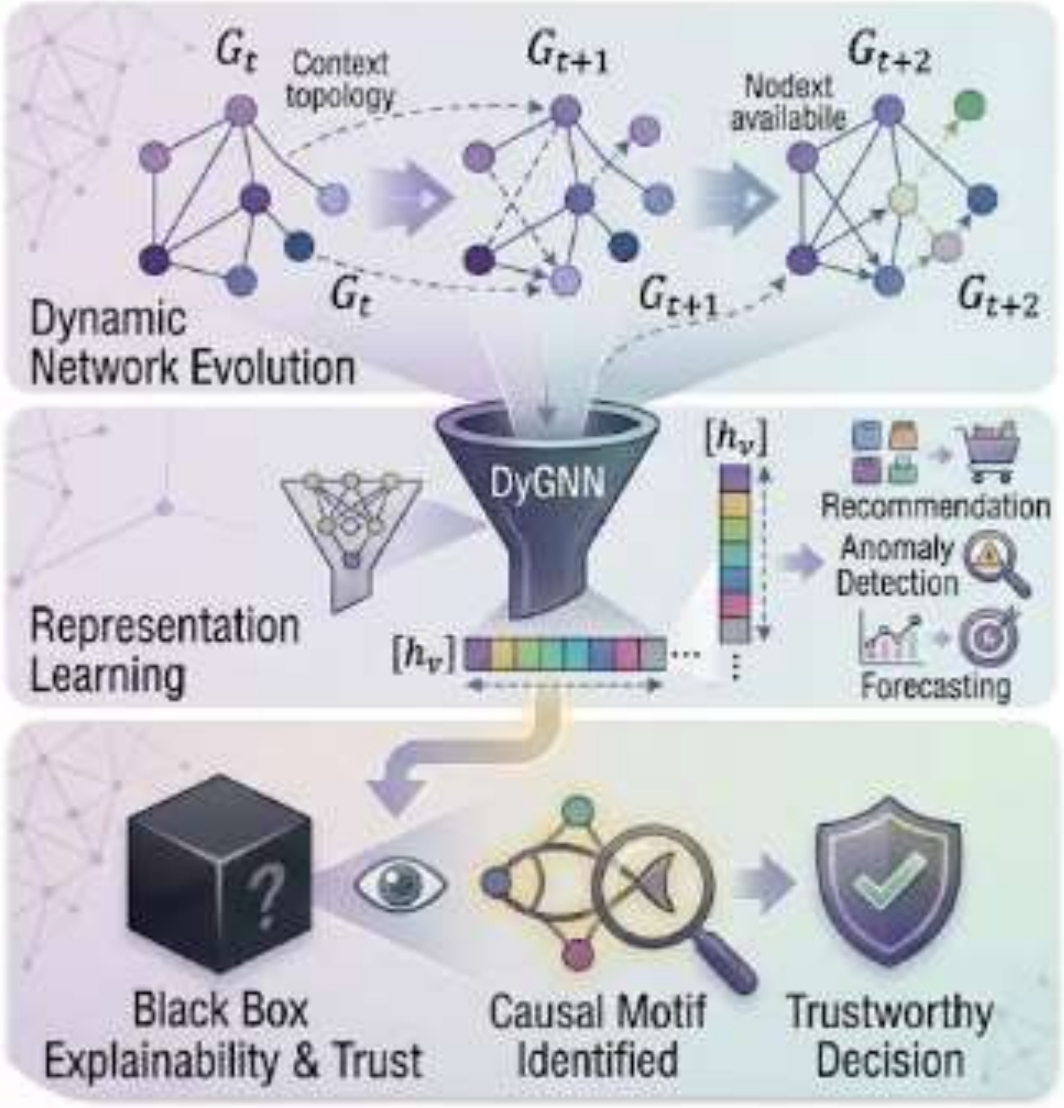
Background



Semantic-Rich Dynamic Web Graphs

- Evolving graph structures with **rich semantic contexts**
- Dynamic changes in **topology and interactions**
- Widely used in recommendation and anomaly detection

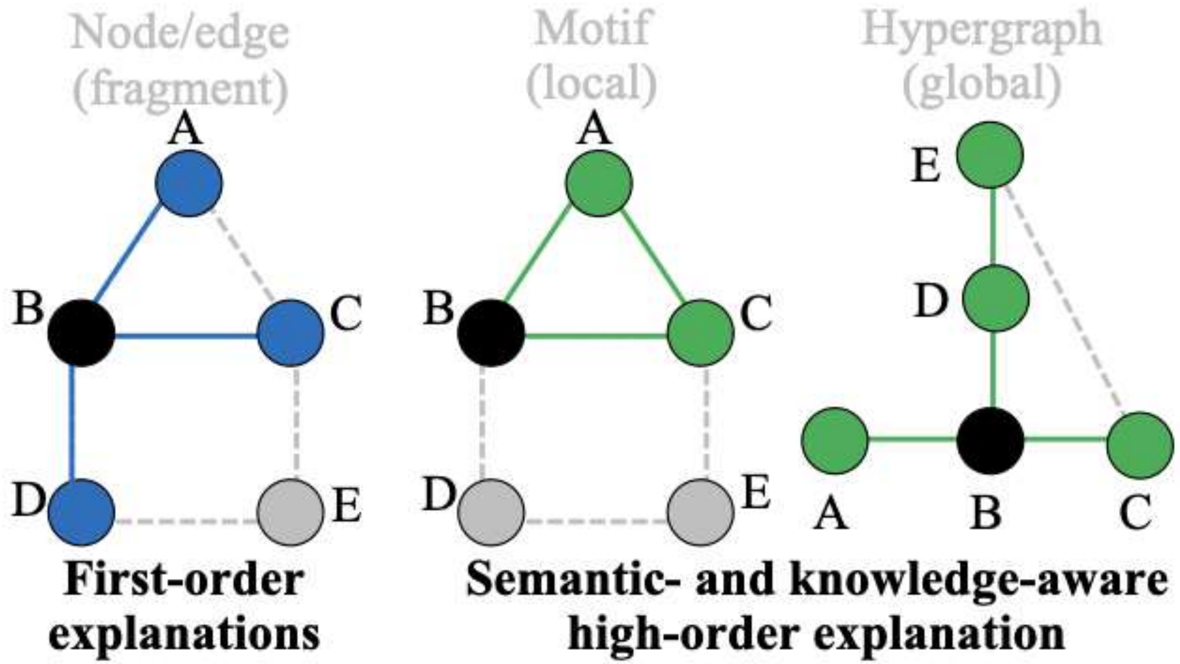
DyGNNs for Dynamic Graph Modeling

- Capturing **structural and temporal** dependencies
- Learning highly **expressive representations**
- Enabling diverse graph intelligence applications

Towards Trustworthy Dynamic Graph Learning

- High predictive capability, yet inherently **black-box**
- Limited transparency hinders **trustworthy decisions**
- **Faithful explanations** are as crucial as accurate predictions

Motivation



Existing DyGNN Explanation Methods:

- Mainly focus on pairwise **node-edge interactions**
- Limited capability in capturing **higher-order semantic structures**

Challenges in Dynamic Graph Explanation:

- Temporal graph evolution introduces **complex semantic dependencies**
- Learned representations are often entangled with **spurious correlations**
- Stable and faithful explanation pathways remain difficult to identify

Motivation for this Research:

There is an urgent need for an explanation framework that jointly models **temporal evolution**, **higher-order semantics**, and **causal mechanisms** for trustworthy dynamic graph learning.

key Contributions of the Paper

- CausalSKyHop Framework:

A **causal-aware framework** for dynamic graph explanation, disentangling **causal and spurious factors** in evolving graphs

- Higher-Order Semantic Modeling:

Capturing complex structures like **motifs and hypergraphs** for a richer understanding

- Causal–Spurious Disentanglement:

Separates **causal signals** from **spurious correlations**, enabling more **faithful explanations**

- Extensive Experiments:

Consistent improvements in **explanation fidelity and robustness** across multiple dynamic graph benchmarks

CausalSkyHop Framework

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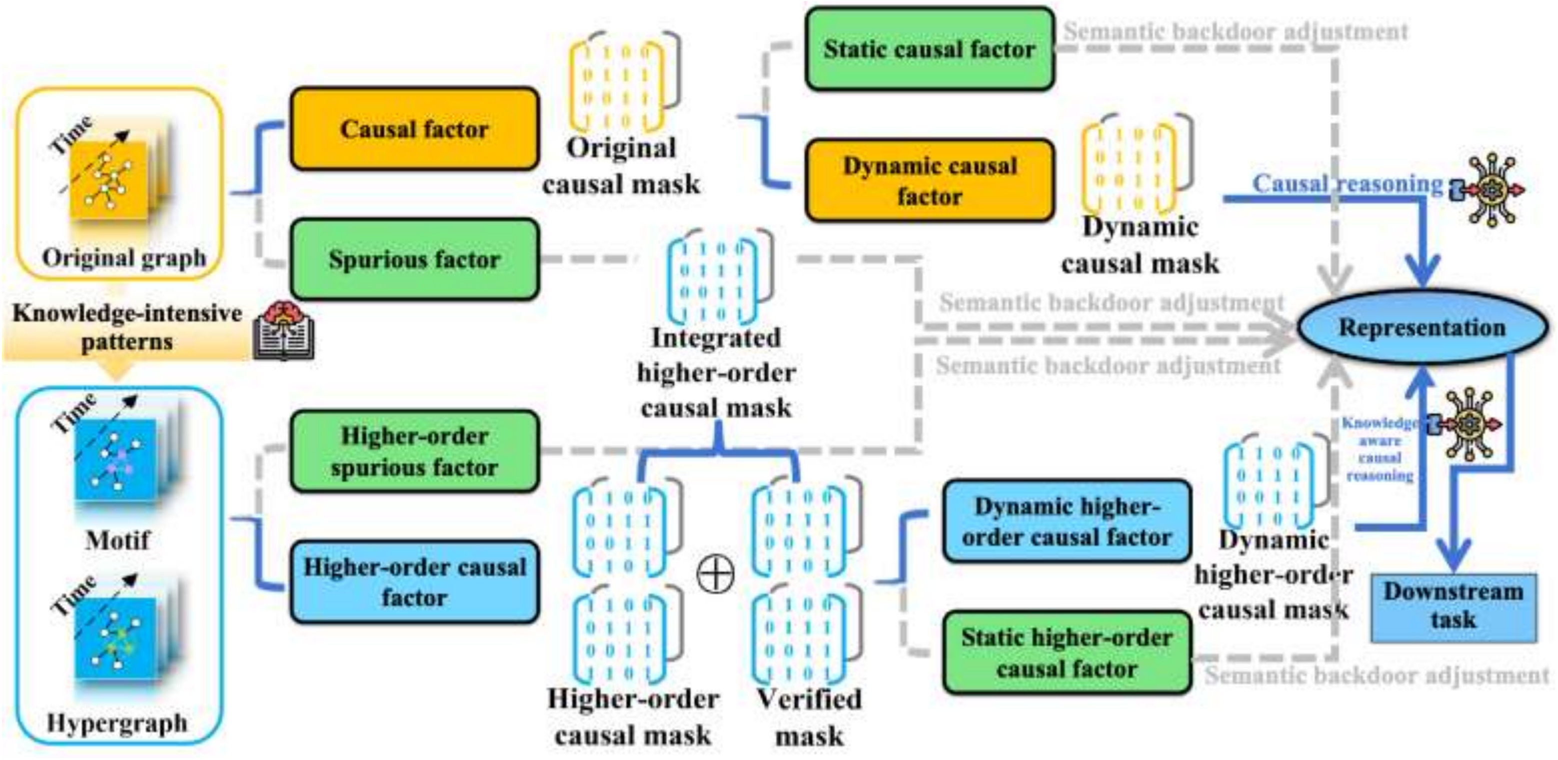
Overview of the CausalSkyHop Framework



Core Mechanism: Employs semantic backdoor adjustment to isolate genuine causal relationships from spurious ones

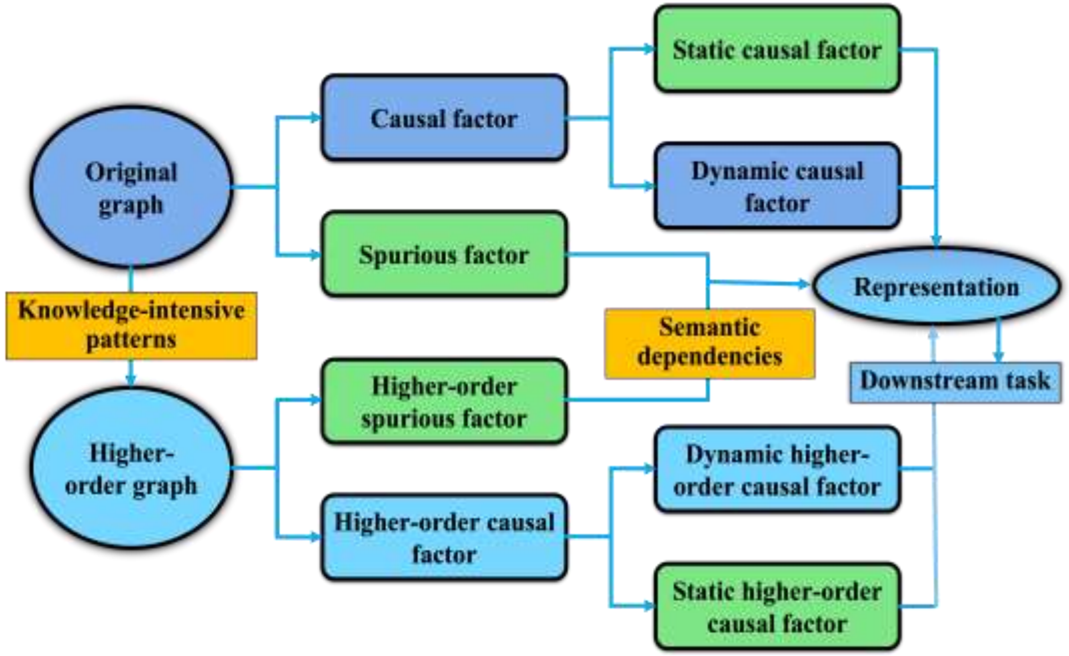
Core Objective:

A semantic- and knowledge-aware framework that explains DyGNNs by uncovering causal higher-order patterns in evolving knowledge structures

Key Components:

- **Higher-Order Structural Causal Model (HOSCM):** Captures multi-node knowledge-intensive patterns via causal reasoning
- **Temporal Reasoning Module:** Separates persistent knowledge from evolving semantic contexts

Higher-Order Structural Causal Model (HOSCM)



HOSCM Variables Definition :

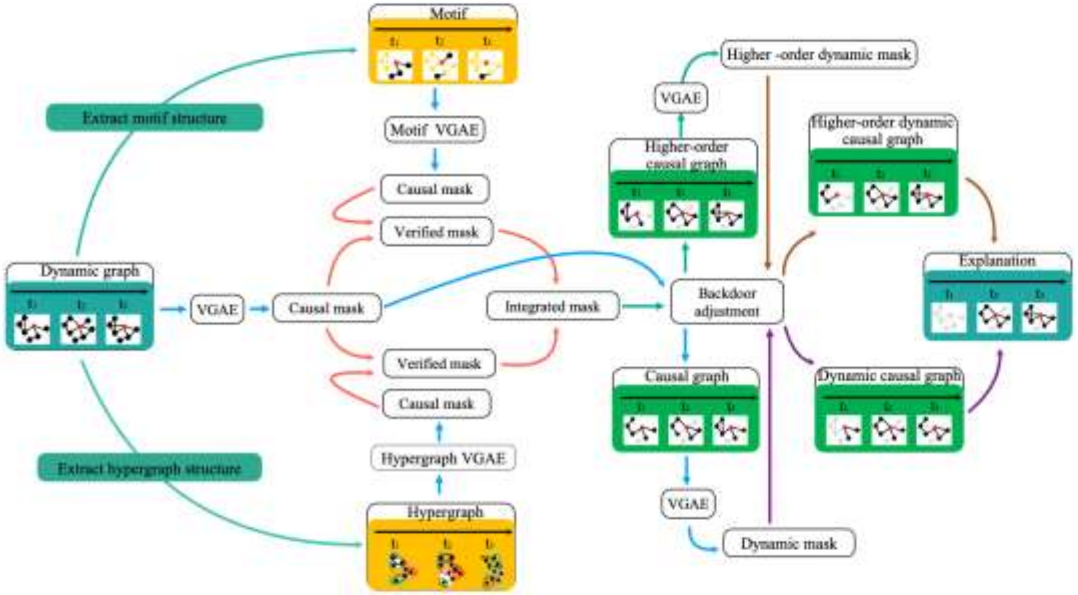
- **Graphs:** Original graph (G), Higher-order graph (HG)
- **Factors:** Causal (C, HC), Spurious (S, HS), Dynamic (DC, DHC), Static (SC, SHC)
- **Outputs:** Learned representation (R), Downstream task (Y)

Four Critical Backdoor Paths:

- **Path 1 (Spurious):** $C \leftarrow G \rightarrow S \rightarrow R \rightarrow Y$
- **Path 2 (HO Spurious):** $HC \leftarrow HG \rightarrow HS \rightarrow R \rightarrow Y$
- **Path 3 (Static):** $DC \leftarrow C \rightarrow SC \rightarrow R \rightarrow Y$
- **Path 4 (HO Static):** $DHC \leftarrow HC \rightarrow SHC \rightarrow R \rightarrow Y$

Semantic Backdoor Adjustment : Uses a knowledge-infused masking strategy to suppress non-causal components (S, HS, SC, SHC), effectively blocking the interference pathways

Disentangling Semantic Causal Relations



Causal Mask Generation

Generate initial mask via knowledge-enhanced VGAE:

$$\mathrm{M}_t^C = f_v(\mathrm{X}_{1:t}, \mathrm{A}_{1:t}; \vartheta_C)$$

Multi-Level Mask Fusion

- **Verify:** Filter noise via cross-validation:

$$\mathbf{M}_t^{\text{struct\_verified}} = \mathbf{M}_t^C \odot \mathbf{M}_{\text{struct}_t}^C$$

- **Fuse:** Adaptive weighting based on semantic importance:

$$\mathbf{M}_t^{HC} = w_1 \cdot \mathbf{M}_t^{\text{motif\_verified}} + w_2 \cdot \mathbf{M}_t^{\text{hyper\_verified}}$$

Dynamic Disentanglement

Isolate evolving dynamic patterns from static knowledge:

$$\mathbf{M}_t^{DHC} = f_v\left(\mathbf{X}_{1:t}, \mathbf{A}_{1:t}^C \odot \mathbf{M}_{1:t}^{HC}; \theta_{DHC}\right)$$

Knowledge-Grounded Optimization

Semantic Decoupling (Contrastive Learning)

Distinguishes causal relationships from spurious noise:

$$\mathcal{L}_c = \frac{1}{T}\sum_{t=1}^{T} \log \frac{\exp(s(e_t, e_t^C, e_t^{HC})/\tau))}{\exp(s(e_t, e_t^C, e_t^{HC})/\tau) + Z_t^C + Z_t^{HC})}$$

Temporal Semantic Consistency

Ensures dynamic relationships maintain temporal continuity:

$$\mathcal{L}_d = \frac{1}{T-1}\sum_{t=2}^{T} d\left(f_a\left(G_{1:(t-1)}^{DC}\right), H_t^{DC}\right)$$

Higher-Order Structural Consistency

Ensures semantic coherence and integration across diverse structural perspectives (motifs and hypergraphs):

$$\mathcal{L}_{high} = \frac{1}{T}\sum_{t=1}^{T}\left(\mathcal{L}_t^{verify} + \beta \cdot \mathcal{L}_t^{balance}\right)$$

Experiments & Results

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Main Results

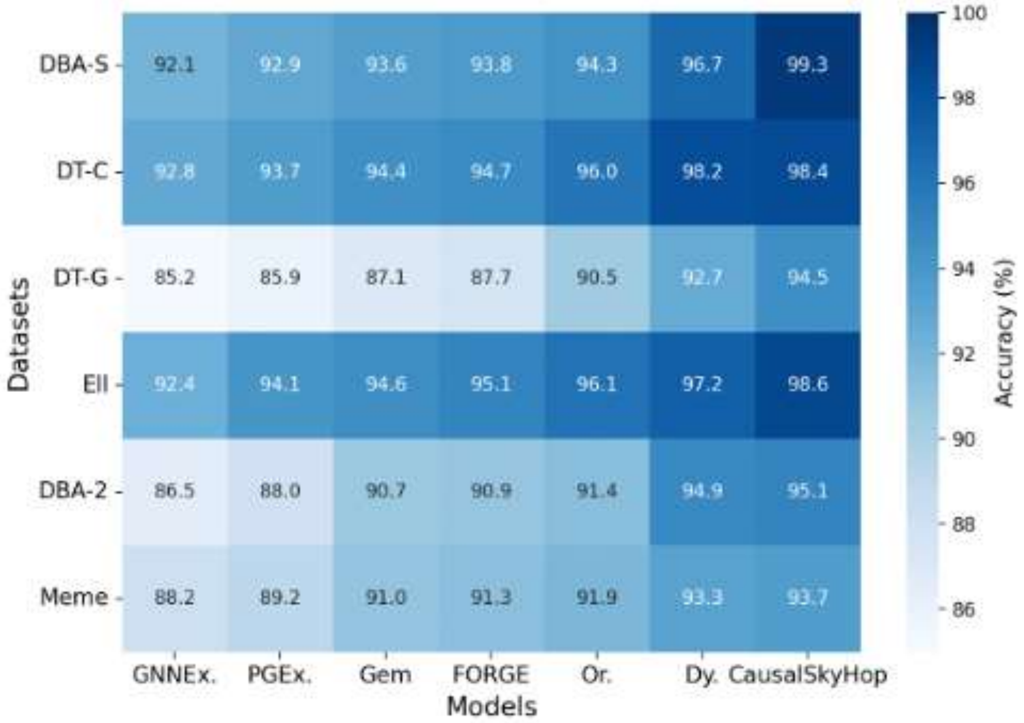
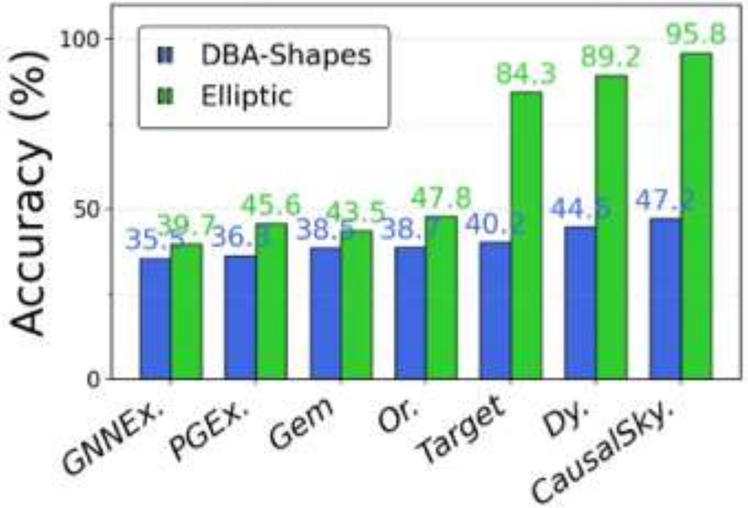


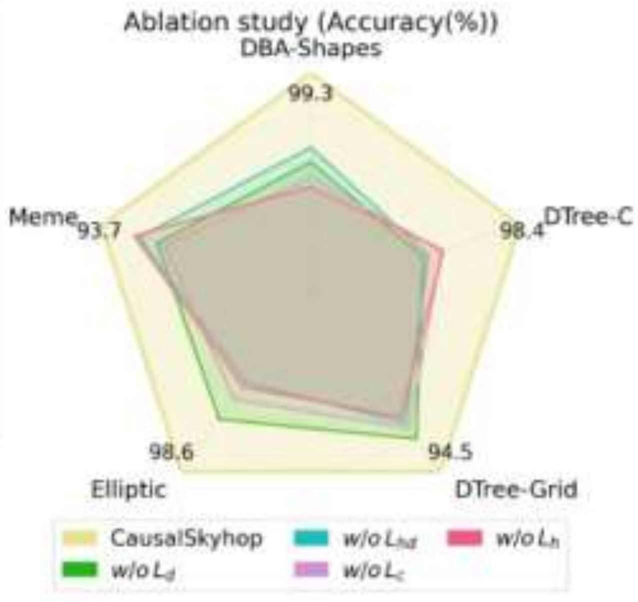
Figure 4: Comparative performance analysis of explainable DyGNN methods across multiple benchmarks. The heatmap visualization highlights the consistent superiority of CausalSkyHop in terms of explanation fidelity across all evaluated datasets. The color intensity corresponds to performance metrics, with darker shades indicating higher scores.

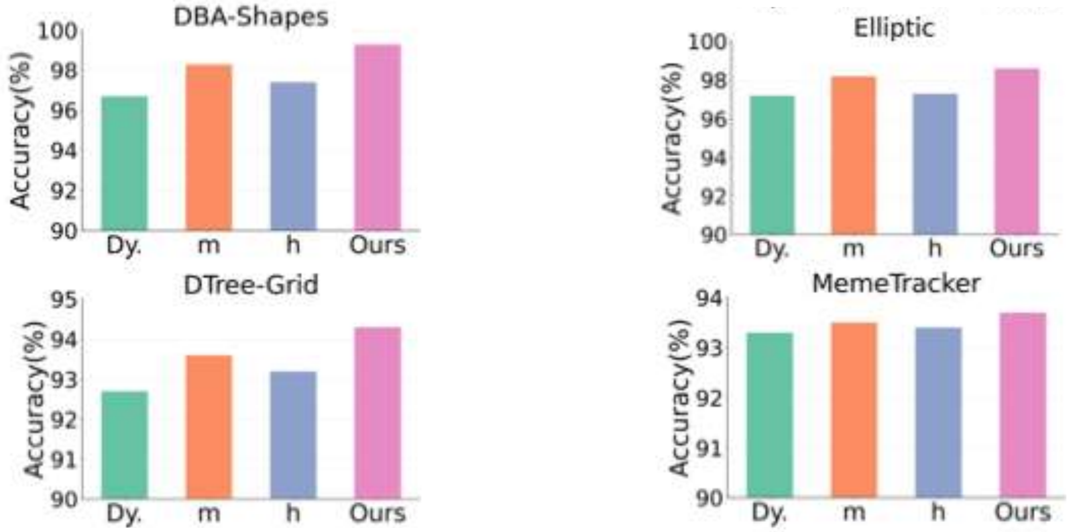


Explanation Fidelity (Heatmap): Significant improvements in explanation accuracy and faithfulness

Prediction Accuracy (Bar Chart): Maintains or boosts downstream task performance

Ablation studies

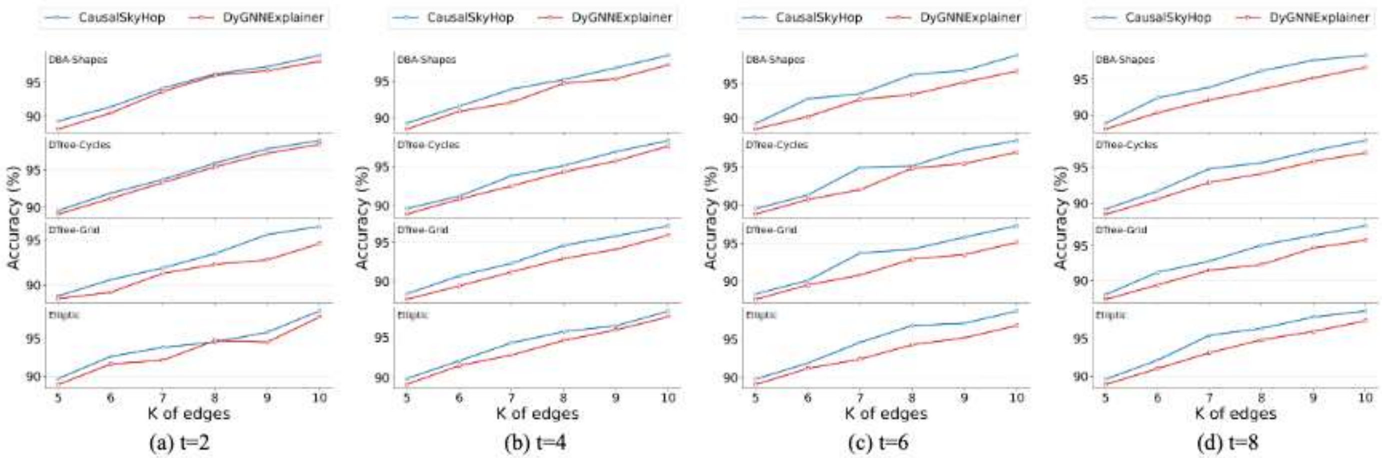




Optimization Losses (Radar Chart): Confirms the effectiveness of the joint objective, especially **contrastive semantic decoupling**

Higher-Order Structures (Bar Chart): Demonstrates the necessity of incorporating **motifs and hypergraphs** for stable causal reasoning

Interpretability & Sparsity



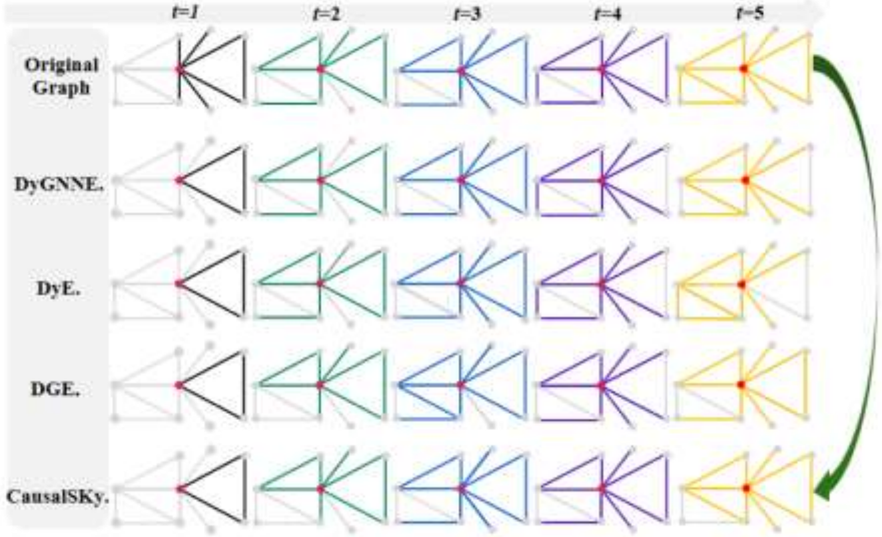


Figure 3: Interpretability analysis of CausalSKyHop versus baselines. Our method produces more sparse and semantically coherent explanations by leveraging higher-order structures (motifs and hypergraphs), effectively isolating causal pathways from spurious correlations.

Advantage in Sparsity(Line Chart): Achieves comparable or better accuracy using **fewer, more focused edges**

Qualitative Interpretability(Case Study): Consistently identifies the complete, semantically meaningful **'fish' motif** across all time steps

Conclusion & Future work

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Summary

- **Framework Design:** Introduced **CausalSKyHop** to explore higher-order semantic causal relations in dynamic graphs.
- **Mechanism:** Provided a mechanism to decouple structural semantics (motifs and hypergraphs) from spurious correlations via temporal and structural constraints.
- **Empirical Findings:** Experimental evaluations demonstrate consistent improvements in both prediction accuracy and explanation fidelity across benchmarks.

Future Work

- **Efficiency:** Improve the computational efficiency of higher-order structure extraction for larger-scale continuous dynamic networks.
- **Generalization:** Extend the framework to handle more complex temporal shifts and unseen node types in open-world scenarios.

Thanks!