Weisfeiler and Lemann follow the Arrow of Time: Expressive Power of Message Passing in Temporal Event Graphs

Extended Abstract Track Submissions

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Abstract

An important characteristic of temporal graphs is how the directed arrow of time influences their causal topology, i.e. which nodes can possibly influence each other causally via time-respecting paths. The resulting patterns are often neglected by temporal graph neural networks (TGNNs). To formally analyze the expressive power of TGNNs, we lack a generalization of graph isomorphism to temporal graphs that fully captures their causal topology. Addressing this gap, we introduce consistent event graph isomorphism, which utilizes a time-unfolded representation of time-respecting paths in temporal graphs. We compare this definition with existing notions of temporal graph isomorphisms. We highlight the advantages of our approach and develop a temporal generalization of the Weisfeiler-Leman algorithm to heuristically distinguish non-isomorphic temporal graphs. Building on this foundation, we derive a novel message passing scheme for TGNNs that operates on the event graph representation of temporal graphs. An experimental evaluation with synthetic and real-world temporal graphs shows that our approach performs well in a temporal graph classification experiment.

1 Introduction

Graph neural networks (GNNs) have become a cornerstone of deep learning in relational data. They have recently been generalized to temporal GNNs (TGNNs) that capture patterns in time series data on *temporal graphs*, where edges carry timestamps. Different TGNN architectures have been proposed, each designed to capture different temporal patterns. [1]. An important characteristic of temporal graphs is how the directed *arrow of time* influences their *causal topology*, i.e., which nodes can possibly influence each other causally via time-respecting paths. Hence, considering the the temporal ordering of events is an important prerequisite for causality-aware machine learning in temporal graph data.

Numerous works, e.g. in network science, studied how the temporal ordering of edges in temporal graphs influences connectivity, dynamical processes like spreading or diffusion, node centralities, cluster patterns, or controllability [2–7]. These patterns are often neglected by TGNNs, which can limit their performance in high-resolution time series data on temporal graphs. To formally analyze this issue, in line with works on the expressivity of (static) GNNs [8, 9], we lack a generalization of graph isomorphism to temporal graphs that captures how their *causal topology* is shaped by the arrow of time. Addressing this gap, the contributions of our work are:

- We propose a new temporal generalization of graph isomorphism called *time-respecting path isomorphism*, which focuses on the preservation of time-respecting paths in temporal graphs.
- We show that time-respecting path isomorphism is equivalent to static graph isomorphism on the *augmented event graph*, an auxiliary graph that (i) captures time-respecting paths in a static line graph expansion of the temporal graph, and (ii) is augmented by nodes in the original graph.
- We use our insights to derive a novel message passing scheme for augmented event graphs, which generates representations that allow to distinguish non-isomorphic temporal graphs. We show that this has the same expressive power as the WL test on the augmented event graph.

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2 Related Work

Prior work on temporal graph neural networks (TGNNs) can broadly be divided into snapshot-based models, which operate on sequences of static graphs, and event-based models, which directly process streams of timestamped edges [1]. While powerful architectures have been proposed in both categories (e.g. ROLAND, TGN, TGAT) [10–12], none of these methods explicitly model patterns that are due to how the *arrow of time* influences time-respecting paths in temporal graphs. This limitation has been studied in network science, where the temporal ordering of edges has been shown to affect spreading processes , clustering patterns, centralities and diffiusion. [2–4, 13] In graph learning, related work has explored message passing in higher order de Bruijn graphs or the transformatin to line-graphs together with a graph kernel based on the Weisfeiler-Leman (WL) algorithm. [14–16] On the theoretical side, the expressive power of message passing GNNS is known to be limited by the WL graph isomorphism test [8, 9] and several extensions have been proposed to go beyond this limit using, for example, the k-dimensional WL test [17]. However, the temporal setting is less explored. One of the reasons is that there is no universally agreed-upon definition of temporal graph isomorphism. Existing notions of temporal isomorphism [18–20] either treat snapshots independently or require exact preservation of timestamps, but none of those definitions precisely capture causal reachability.

Complementing this research, our work introduces a time-respecting path isomorphism, which precisely preserves the causal topology. We show its equivalence to static isomorphism on augmented event graphs, which enables a direct extension of WL and message passing to temporal graphs.

3 Preliminaries

A directed, labeled (static) graph $G = (V, E, \ell_V, \ell_E)$ consists of a set V of nodes, a set $E \subseteq V \times V$ of directed edges, a *node labeling* $\ell_V : V \to \mathcal{L}_V$ and an *edge labeling* $\ell_E : E \to \mathcal{L}_E$, with countable sets $\mathcal{L}_V$ and $\mathcal{L}_E$. In unlabeled graphs, we omit ℓ_V or ℓ_E accordingly. For a node v, we denote its incoming neighbors by $N_I(v) = \{u \mid (u, v) \in E\}$ and its outgoing neighbors by $N_O(v) = \{u \mid (v, u) \in E\}$. Finally, we define the set of paths $P(G)$ as the set of all alternating node/edge sequences $(v_0, e_1, v_1, e_2, \ldots, e_k, v_k)$ with $e_i = (v_{i-1}, v_i) \in E$ for $i \in \{1, \ldots, k\}$. Note that we do not distinguish between walks and paths or, equivalently, do not require paths to be simple.

Definition 1 (Graph isomorphism)**.** *For two static graphs $G_1 = (V_1, E_1, \ell_V^1, \ell_E^1)$ and $G_2 = (V_2, E_2, \ell_V^2, \ell_E^2)$, an* isomorphism *is a bijective mapping $\pi : V_1 \to V_2$ with these properties:*

(i) Edge-preserving: $(u, v) \in E_1 \iff (\pi(u), \pi(v)) \in E_2 \quad \forall u, v \in V$
(ii) Node label-preserving: $\ell_V(u) = \ell_V(\pi(u)) \quad \forall u \in V$
(iii) Edge label-preserving: $\ell_E(u, v) = \ell_E(\pi(u), \pi(v)) \quad \forall (u, v) \in E$

We say that the graphs G_1 and G_2 are isomorphic *iff such a mapping π exists.*

Definition 2 (Temporal graph)**.** *We define a (directed) temporal graph as $G^\tau = (V, E^\tau)$, where V is the set of nodes and $E^\tau \subseteq V \times V \times \mathbb{N}$ is the set of timestamped edges, i.e., an edge $(u, v; t) \in E^\tau$ describes an interaction between u and v at time t.*

Definition 3 (Time-respecting path)**.** *A path of length k in a temporal graph $G^\tau = (V, E^\tau)$ is an alternating sequence of nodes and timestamped edges $p = (v_0, e_1, v_1, \ldots, e_k, v_k)$ with $e_i = (v_{i-1}, v_i; t_i) \in E^\tau$ for $i \in \{1, \ldots, k\}$. For a maximum time difference (or waiting time) $\delta \in \mathbb{N}$, we say that p is* time-respecting *if $1 \leq t_i - t_{i-1} \leq \delta$ for $i \in \{1, \ldots, k\}$. We denote the set of time-respecting paths in G^τ as $P^\tau(G^\tau)$.*

The structure of time-respecting paths can be encoded in the temporal event graph, which is a static graph whose nodes are the timestamped edges. Two nodes are connected by an edge if the corresponding timestamped edges form a time-respecting path of length two.

Definition 4 (Temporal event graph)**.** *Let $G^\tau = (V, E^\tau)$ be a temporal graph with waiting time δ. The temporal event graph is given by $G^{\mathcal{E}} = (E^\tau, \mathcal{E})$ with*

$$\mathcal{E} = \{((u, v; t), (v, w; t')) \mid (u, v; t), (v, w; t') \in E^\tau, 1 \leq t' - t \leq \delta\}.$$

Note that the time-respecting paths of length $k \geq 2$ in G^τ correspond to the paths of length $k - 1$ in $G^{\mathcal{E}}$, whereas the time-respecting paths of length 1 in G^τ correspond to the nodes in $G^{\mathcal{E}}$.

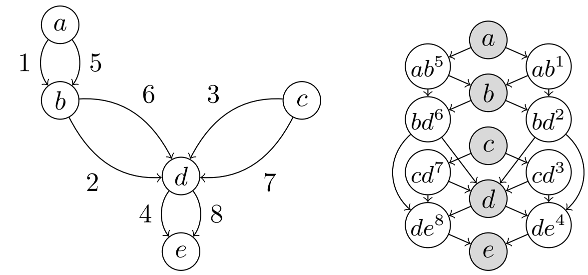

Figure 1: A temporal graph G^τ (left) and the corresponding augmented event graph G^{aug} (right).

4 Isomorphisms in Temporal Graphs

To motivate our temporal generalization of graph isomorphism, we make the following observation.

Observation 1. *Let $\pi\colon V_1 \to V_2$ be a bijective node mapping between two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$. For any edge $e = (u, v) \in E$, we write $\pi(e) = (\pi(u), \pi(v))$. Then π is edge-preserving if and only if it is* path-preserving*, i.e., the following holds for all alternating node/edge sequences $(v_0, e_1, v_1, \ldots, e_{k-1}, v_k)$ with $k \in \mathbb{N}$:*

$$(v_0, e_1, v_1, \ldots, e_{k-1}, v_k) \in P(G_1) \iff (\pi(v_0), \pi(e_1), \pi(v_1), \ldots, \pi(e_{k-1}), \pi(v_k)) \in P(G_2).$$

This is due to the fact that adjacent edges transitively expand into paths. This guarantees that two isomorphic static graphs are topologically equivalent in terms of edges *and* paths. Importantly, this property does not directly translate to time-respecting paths in temporal graphs: two adjacent timestamped edges $(u, v; t)$ and $(v, w; t')$ only form a time-respecting path if $1 \leq t' - t \leq \delta$. Hence, a temporal generalization of graph isomorphism should preserve not only the timestamped edges, but also the *causal topology* in terms of time-respecting paths. Conversely, we are interested in an isomorphism definition that does not force the *values* of timestamps to be preserved, provided that the resulting time-respecting paths in two temporal graphs are identical.

Definition 5 (Time-respecting path isomorphism)**.** *Let $G_1^\tau = (V_1, E_1^\tau)$ and $G_2^\tau = (V_2, E_2^\tau)$ be two temporal graphs. We say that G_1^τ and G_2^τ are* time-respecting path isomorphic *if there is a bijective node mapping $\pi_V : V_1 \to V_2$ and a bijective timestamped edge mapping $\pi_E\colon E_1^\tau \to E_2^\tau$ such that the following holds for all alternating node/edge sequences $(v_0, e_1, v_1, \ldots, e_{k-1}, v_k)$ with $k \in \mathbb{N}$:*

$$\begin{aligned} & (v_0, e_1, v_1, \ldots, e_{k-1}, v_k) \in P^\tau(G_1^\tau) \\ \iff \quad & (\pi_V(v_0), \pi_E(e_1), \pi_V(v_1), \ldots, \pi_E(e_{k-1}), \pi_V(v_k)) \in P^\tau(G_2^\tau). \end{aligned}$$

A drawback of this isomorphism definition is that it appears difficult to test, since the number of time-respecting paths may be exponential in the graph size. Therefore, we derive equivalent notions of temporal graph isomorphism that are easier to test. In order to preserve paths of length 1, which consist of a single timestamped edge $e = (u, v; t)$ and are always time-respecting, we must ensure that $\pi_E(e)$ connects $\pi_V(u)$ to $\pi_V(v)$. We call this property *node consistency*. Node-consistent mappings preserve paths, but not necessarily their time-respecting property. To ensure this, we observe that time-respecting paths of length $k \geq 2$ correspond to paths in the temporal event graph. We can preserve them by requiring π_E to be path-preserving between the temporal event graphs.

This can be simplified further by constructing an *augmented event graph* (see Fig. 1), which encodes the node consistency property in its topology. In this way, we reduce the problem of testing for time-respecting path isomorphism to the problem of testing for static graph isomorphism on the augmented event graphs.

Definition 6 (Augmented event graph)**.** *Let $G^\tau = (V, E^\tau)$ be a temporal graph with event graph $G^{\mathcal{E}} = (E^\tau, \mathcal{E})$. The* augmented event graph *is the static, directed, node-labeled graph $G^{aug} = (V^{aug}, E^{aug}, \ell)$ with*

$$V^{aug} = V \cup E^\tau, \qquad E^{aug} = \mathcal{E} \cup E^{out} \cup E^{in},$$

$$\ell(v) = \begin{cases} 0 & \text{if } v \in V, \\ 1 & \text{if } v \in E^\tau, \end{cases} \qquad \begin{aligned} E^{out} &= \{(u, (u, v; t) \mid (u, v; t) \in E^\tau\}, \\ E^{in} &= \{((u, v; t), v) \mid (u, v; t) \in E^\tau\}. \end{aligned}$$

Theorem 1. *(Proof in Appendix A) Let G_1^τ and G_2^τ be two temporal graphs with corresponding augmented event graphs G_1^{aug} and G_2^{aug}. Then the following statements are equivalent:*

(i) G_1^τ and G_2^τ are time-respecting path isomorphic.
(ii) G_1^{aug} and G_2^{aug} are isomorphic.

5 Message Passing for the Augmented Event Graph

We use the equivalency of time-respecting path isomorphism to static isomorphism on the augmented event graph to derive a message-passing GNN architecture for temporal graphs. Note that the augmented event graph is directed, even if the underlying temporal graph is undirected. Edge directions are crucial because they represent the arrow of time, which is why we use the directed GNN Dir-GNN [21]. It iteratively computes embeddings $f^{(t)}(v)$ for each node v at layer k. This is done by aggregating embeddings of its neighbors at layer $k-1$, using the function $\overrightarrow{f}^{(t)}_{\text{agg}}$ for incoming neighbors and $\overleftarrow{f}^{(t)}_{\text{agg}}$ for outgoing neighbors. A function $f^{(t)}_{\text{com}}$ combines these with the previous embedding of v to a new embedding. The combination and aggregation functions $f^{(t)}_{\text{com}}$, $\overrightarrow{f}^{(t)}_{\text{agg}}$ and $\overleftarrow{f}^{(t)}_{\text{agg}}$ are learnable. The initial node embeddings are obtained by applying an injective encoding function to the node labels. To obtain a final representation of the entire graph, the embeddings $f^{(k)}(v)$ of all nodes v on the final layer k are combined using an injective readout function. Our proposed GNN architecture simply applies Dir-GNNs to the augmented event graph. By using the augmented event graph, this approach is specifically tailored towards detecting time-respecting path isomorphism.

6 Experimental Evaluation

We evaluate our TGNN on synthetic temporal graphs specifically constructed such that all classes share the same time-aggregated static graph, while differing only in their causal topology. This allows us to directly test whether our model captures patterns in time-respecting paths.

Experiment A: Shuffled timestamps. Starting from random graphs, we generate temporal edge sequences and shuffle timestamps of a fraction α of edges. Increasing α destroys more causal dependencies without changing the time-aggregated graph. Our TGNN reliably separates original graphs from their shuffled counterparts, achieving near-perfect accuracy for $\alpha > 0.2$ (Fig. 2, left).

Experiment B: Cluster connectivity. We generate temporal graphs with two densely connected clusters and vary the likelihood of time-respecting paths between clusters using a parameter σ. For $\sigma < 0$ cross-cluster paths are suppressed, while for $\sigma > 0$ they are overrepresented, yet the aggregated graph remains unchanged. We assign graphs with $\sigma = 0$ to one class and graphs with $\sigma \neq 0$ to the other. Our TGNN detects these differences with high accuracy, while accuracy peaks as $|\sigma|$ increases (Fig. 2, middle/right).

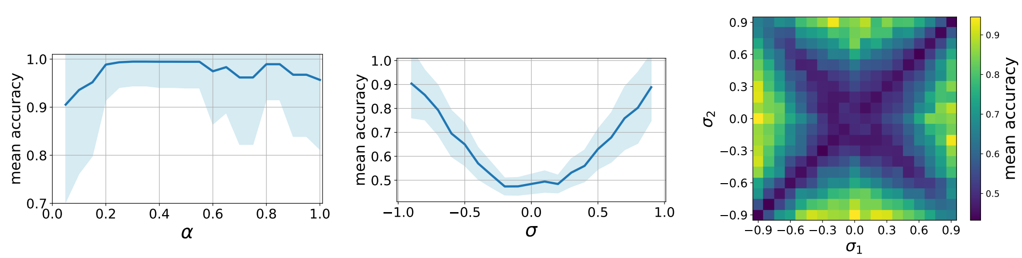

Figure 2: Results of classification experiments A (left) and B (middle). Results are averaged over 100 runs (hull curve shows standard deviation). Right panel: mean classification accuracy for temporal graphs generated with σ_1 vs. σ_2 (for all pairs σ_1, σ_2, 25 runs each).

7 Conclusion

Our work contributes to the theoretical foundation of temporal graph learning, providing a basis for the development and investigation of neural message passing architectures that consider how the arrow of time shapes the causal topology in temporal graphs.

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A Proof of Theorem 1

For the proof we additionally introduce the notion of consistent event graph isomorphism.

Definition 7 (Consistent event graph isomorphism)**.** *Let $G_1^\tau = (V_1, E_1^\tau)$ and $G_2^\tau = (V_2, E_2^\tau)$ be two temporal graphs with corresponding temporal event graphs $G_1^{\mathcal{E}} = (E_1^\tau, \mathcal{E}_1)$ and $G_2^{\mathcal{E}} = (E_2^\tau, \mathcal{E}_2)$. A mapping $\pi_E \colon E_1^\tau \to E_2^\tau$ is a* consistent event graph isomorphism *if and only if*

(i) there exists a mapping $\pi_V \colon V_1 \to V_2$ such that

$$\forall (u, v; t) \in E_1^\tau \quad \exists t' \colon \pi_E(u, v; t) = (\pi_V(u), \pi_V(v); t'), \text{ and}$$

(ii) π_E is a graph isomorphism between $G_1^{\mathcal{E}}$ and $G_2^{\mathcal{E}}$.

In the following we give the proof of an extended version of Theorem 1:

Theorem. *Let $G_1^\tau = (V_1, E_1^\tau)$ and $G_2^\tau = (V_2, G_2^\tau)$ be two temporal graphs with corresponding augmented event graphs $G_1^{aug} = (V_1^{aug}, E_1^{aug}, \ell_1)$ and $G_2^{aug} = (V_2^{aug}, E_2^{aug}, \ell_2)$. Then the following statements are equivalent:*

(i) G_1^τ and G_2^τ are time-respecting path isomorphic.
(ii) G_1^τ and G_2^τ are consistent event graph isomorphic.
(iii) G_1^{aug} and G_2^{aug} are isomorphic.

We begin by showing the equivalence of (i) and (ii):

Proof. Let $\pi_V \colon V_1 \to V_2$ and $\pi_E \colon E_1^\tau \to E_2^\tau$ be a node and edge mapping, respectively. Let $p = (v_0, e_1, v_1, \ldots, e_{k-1}, v_k)$ be an alternating sequence of nodes and timestamped edges in G_1^τ. We denote the corresponding sequence in G_2^τ that is induced by π_V and π_E as $\pi(p) =$

$(\pi_V(v_0), \pi_E(e_1), \pi_V(v_1), \ldots, \pi_E(e_{k-1}), \pi_V(v_k))$. We say that π_V and π_E are *path-preserving* between G_1^τ and G_2^τ if for each sequence p as defined above, p is a path in G_1^τ if and only if $\pi(p)$ is a path in G_2^τ. It is easy to see that π_V and π_E are path-preserving between G_1^τ and G_2^τ if and only if π_E is node-consistent with π_V.

Assume therefore that π_V and π_E are path-preserving between G_1^τ and G_2^τ. We show that π_E is a graph isomorphism between the temporal event graphs $G_1^{\mathcal{E}}$ and $G_2^{\mathcal{E}}$ if and only if it is *time-preserving*, i.e., a path p in G_1^τ is time-respecting iff $\pi(p)$ is time-respecting in G_2^τ. If $k = 1$, this holds trivially because all paths of length 1 are time-respecting. If $k \geq 2$, then p is time-respecting if and only if $(e_1, (e_1, e_2), e_2, \ldots, (e_{k-2}, e_{k-1}), e_{k-1})$ is a path in $G_1^{\mathcal{E}}$. Hence, π_E is time-preserving if and only if it is path-preserving between $G_1^{\mathcal{E}}$ and $G_2^{\mathcal{E}}$. Because the event graphs are unlabeled, this is the case if and only if π_E is a graph isomorphism by def. 1. □

Next, we show the equivalence of (ii) and (iii):

Proof. Let $\pi\colon V_1^{\text{aug}} \to V_2^{\text{aug}}$ be an isomorphism between G_1^{aug} and G_2^{aug}. Because π preserves the node labels, it can be decomposed into bijective mappings $\pi_V\colon V_1 \to V_2$ and $\pi_E\colon E_1^\tau \to E_2^\tau$. Then π_E is an isomorphism between $G_1^{\mathcal{E}}$ and $G_2^{\mathcal{E}}$ because these are subgraphs of G_1^{aug} and G_2^{aug}, respectively. Consider an edge $e = (u, v; t) \in E_1^\tau$. By construction, G_1^{aug} includes the edges $(u, e) \in E_1^{\text{out}}$ and $(e, v) \in E_1^{\text{in}}$. Because π is an isomorphism, it follows that $(\pi_V(u), \pi_E(e)) \in E_2^{\text{out}}$ and $(\pi_E(e), \pi_V(v)) \in E_2^{\text{in}}$. Then it follows by construction of G_2^{aug} that $\pi_E(e) = (\pi_V(u), \pi_V(v); t')$ for some $t' \in \mathbb{N}$.

Conversely, let $\pi_E\colon E_1^\tau \to E_2^\tau$ be a consistent event graph isomorphism between G_1^τ and G_2^τ, and let $\pi_V : V_1 \to V_2$ be the induced node mapping such that

$$\forall (u, v; t) \in E_1^\tau \quad \exists t' \colon \pi_E(u, v; t) = (\pi_V(u), \pi_V(v); t').$$

Then π_E and π_V can be combined into a bijective mapping $\pi\colon V_1^{\text{aug}} \to V_2^{\text{aug}}$. We show that π is an isomorphism between G_1^{aug} and G_2^{aug}. By construction, π preserves the node labels. For every pair of nodes $x, y \in V_1^{\text{aug}}$ and every set of edges $E' \in \{\mathcal{E}, E^{\text{out}}, E^{\text{in}}\}$, we show that

$$(x, y) \in E'_1 \quad \iff \quad (\pi(x), \pi(y)) \in E'_2.$$

For $E' = \mathcal{E}$, this follows from the fact that π_E is an isomorphism between $G_1^{\mathcal{E}}$ and $G_2^{\mathcal{E}}$. We show the case $E' = E^{\text{out}}$ (the case $E' = E^{\text{in}}$ is symmetrical): We have $(u, y) \in E_1^{\text{out}}$ if and only if $y = (x, v; t)$ for some $v \in V_1$ and $t \in \mathbb{N}$. We have $\pi(y) = \pi_E(y) = (\pi_V(x), \pi_V(v); t') = (\pi(x), \pi(v); t')$ for some $t' \in \mathbb{N}$. By definition of E^{out}, we have $(\pi(x), \pi(y)) \in E_2^{\text{out}}$. □