Reproducibility Study of "Explaining Temporal Graph Models Through an Explorer-Navigator Framework"

Anonymous authors
Paper under double-blind review

Abstract

This paper seeks to reproduce and extend the results of the paper "Explaining Temporal Graph Models Through an Explorer-Navigator Framework" by Xia et al. (2023). The main contribution of the original authors is a novel explainer for temporal graph networks, the Temporal GNN Explainer (T-GNNExplainer), which finds a subset of preceding events that "explain" a prediction made by a temporal graph model. The explorer is tested on two temporal graph models that are trained on two real-world and two synthetic datasets. The explorer is evaluated using a newly proposed metric for explanatory graph models. The authors compare the performance of their explorer to three baseline explainer methods, either adapted from a GNN explainer or developed by the authors. The authors claim that T-GNNExplainer achieves superior performance compared to the baselines when evaluated with their proposed metric. This work reproduces the original experiments by using the code (with minor adjustments), model specifications, and hyperparameters provided by the original authors. To evaluate the robustness of these claims, the method was extended to one new dataset (MOOC). Results show that the T-GNNExplainer performs best on some, but not all metrics as reported in the original findings. We conclude that the main lines of this paper hold up even though all results are less pronounced than claimed. Additional analysis in the graph structure of the data is performed and results suggest that there is a positive relationship between the intial subgraph node density and explainer performance. Results show that the T-GNNExplainer does not perform similarly across different T-GNN models, precise dataset specifications are needed to obtain high performance, and there are simpler, less computationally costly explainer methods (like PBONE) that could offer competitive results.

1 Introduction

Dynamic graph-structured data can be seen as sequences of events between nodes that happen over time, and exist in many applications such as social networks (Pereira et al., 2018)(Gelardi et al., 2021). Temporal Graph Neural Networks (T-GNNs) learn representations of these structures and make predictions on future events (Xia et al., 2023). The rationale for how graph models arrive at these predictions is difficult to interpret (Luo et al., 2020), and this lack of human-intelligible explanations means these powerful tools lack the transparency crucial in establishing fairness, safety, and trust in their output (Doshi-Velez & Kim, 2017). The opacity of graph models could hinder the possibility to ensuring ethical outcomes if potential biases or discrimination arise from their predictions, especially in high-stakes domains like healthcare (Burrell, 2016).

Graph explainers identify important subgraphs of nodes and events that were instrumental in a model's prediction for a target event (Luo et al., 2020). Most methods for explaining these predictions exist for Graph Neural Networks (GNNs), which focus on static graphs (GNNExplainer (Ying et al., 2019), PGExplainer (Luo et al., 2020) and Sub- graphX (Yuan et al., 2020)). These methods cannot be directly applied to explaining T-GNNs, since the time-varying structures of dynamic graphs are not captured by these explainers (He et al., 2022).

The authors of this paper propose the T-GNNExplainer, which provides an instance-level search-based model-agnostic post-hoc explanation for predictions made by temporal graph models. "**Instance-level**" means an explanation is provided only for one prediction instead of at a global level, "search based" means the method explores subsets of possible solutions, "**model-agnostic**" means the explainer should be able to explain any temporal graph model, and "**post-hoc**" means the explanation is based on the output of the model without direct access to the actual steps that occurred during model training.

This paper is structured as follows: In **Section 2**, we explain the scope of reproducibility, summarizing the authors' main claims and the experiments we ran to verify their claims. In **Section 3**, we provide the reader with a summary of the model proposed in the original paper and the experimental methodology used to run the experiments. In **Section 4** we describe all the datasets and in **Section 5** we explained our use of the hyperparameters. In **Section 6** we described the experimental setup and code, where we explain the novel dataset and the computational requirements. **Section 7** provides the replicated results, comparison to the original results, and results that extend beyond the original paper. We end with a discussion in **Section 8**. Beyond the references we have also have an appendix, A to F, that provides an in-depth explanation of the model, further information on the specifics of the experimental setup for those looking to implement this reproducibility study, hyperparameters, further metrics and results, and suggestions for further research.

2 Scope of Reproducibility

The main contribution of the authors is a novel explainer for T-GNNs. They claim superior performance of their explainer by evaluating performance in comparison to other baselines explainers, evaluating the efficiency of their method, and the conciseness of the output compared to the other explainers.

The first metric they use to evaluate performance is called the Area under the Fidelity-Sparsity Curve (AUFSC). It is composed of two metrics (fidelity and sparsity), each of which is used to evaluate graph explainer models (Amara et al., 2022)(Agarwal et al., 2023)(Liu et al., 2021). The curve expresses the relationship between the fidelity (i.e. how accurately the T-GNN makes a similar prediction when it takes as input only the nodes it selects as explanatory) and sparsity (i.e. how few nodes are used to give the explanation). The area under the curve is a measure of the commutative fidelity over a set of sparsity threshold intervals. High fidelity and high sparsity result in a higher AUFSC which indicates better performance. The second metric, Best Fidelity, simply measures the highest fidelity achieved by an explainer without the sparsity limitation, averaged over all test data. The metrics are explained in further detail in Section 3.3.

The main claims that are investigated in the current paper are:

1. Compared to the other baselines, T-GNNExplainer surpasses performance in the **AUFSC** and **Best Fid** metrics by up to ~50%.

2. The T-GNNExplainer is model agnostic in regards to the underlying predictor model.

The aim of this paper is to verify the original authors' main claim by reproducing their main findings, and testing the robustness of this claim by extending their results to a new and different kind of dataset. We perform further analysis on the explanatory graphs and the interaction between the T-GNNExplainer and the underlying model. Further goals of the paper are to increase accessibility and reproducibility of this work by providing supplementary instructions for running the code and in-depth explanations for understanding the methodology.

There are other claims made in the paper in regards to the conciseness of the generated graph and the navigators efficiency. We do not investigate these claims due to computation and time cost.

3 Methodology

The code is publicly available in a zip file of supplementary materials on the OpenReview page for this paper. The data is not included in the zip file, but the top-level ReadMe in the code provides instructions

for downloading the data. There is some inconsistency between the nomenclature used in the paper and the corresponding terminology in the code. For the purpose of this work, we follow the terminology used in the paper.

3.1 Notation

The notation used in the paper is as follows: $\mathcal{G} = (\mathcal{N}, \mathcal{S})$ is a temporal graph. $\mathcal{N}$ is a list of the nodes, and $\mathcal{S} = \{e_1, e_2, \dots\}$ sequence of timestamped events. Each event $e_i = \{n_{u_i}, n_{v_i}, t_i, \text{att}_i\}$ has a timestamp t_i and occurs from node n_{u_i} to node n_{v_i} with the attribute att_i, which is a list of indefinite even length filled with feature values. $\mathcal{G}^k$ is the graph at timestamp k and $\mathcal{R}^k$ is the subset of events in graph $\mathcal{G}^k$ found by the explainer. N_r is a hyperparameter controlling the amount of nodes that the explanatory subgraph is allowed to have.

The function $f(\cdot)$ represents a trained temporal graph model. $f(\mathcal{G}^k)[e_k]$ is the probability prediction of the event e_k that occurs when the graph $\mathcal{G}^k$ is input into the network. The output is a logit value. Y_k is a value of either 0 or 1 that classifies the prediction of the network for whether or not an event occurs at the time step k.

3.2 Model description

For a detailed and intuitive explanation of how the explorer-navigator framework works, and the equations included above, please see the Appendix B.

3.2.1 T-GNN Explainer

A temporal graph network predicts whether a target event e_k will occur or not (Rossi et al., 2020)(Xu et al., 2020). The purpose of the T-GNNExplainer is to find a set of preceding events that explain why the model made this prediction, henceforth referred to as the "explanatory subgraph".

The explainer module is made up of two parts, the navigator and the explorer, that work together to "prune" events from a graph of candidate events, resulting in a graph of only the most relevant events that lead to the prediction of the target event.

The navigator is inspired by the "explanation network for node classification" from the parameterized explainer proposed by Luo et al. (2020). The navigator $h_\theta(e_j, e_k)$ implemented in this paper is a two-layer neural network that learns a correlation or "importance" between two events e_j (the candidate) and e_k (the target).

The navigator $h_\theta(e_j, e_k)$ finds the least important event in relation to the target/predicted event e_k:

$$e^* = \underset{e_j \in \mathcal{N}^i / \mathcal{C}(\mathcal{N}^i)}{\arg\min} \; h_\theta(e_j, e_k) \tag{1}$$

Instead of generating and searching a tree of all possible subgraphs, the explorer uses the navigator to create subgraphs that are relevant to its search. The explorer uses a modified Monte Carlo Tree Search to explore possible relevant subgraphs that could be good explanations for $\mathcal{G}^k$. Instead of exploring all possible subgraphs, the explorer uses the navigator to select which subgraphs to explore by "removing" the least important events related to the target event.

The search path is selected using the following formula:

$$e^* = \underset{e_j \in \mathcal{C}(\mathcal{N}^i)}{\arg\max} \left(\frac{c(\mathcal{N}^i, e_j)}{n(\mathcal{N}^i, e_j)} + \lambda \frac{\sqrt{\sum_{e_l \in \mathcal{C}(\mathcal{N}^i)} n(\mathcal{N}^i, e_l)}}{1 + n(\mathcal{N}^i, e_j)} \right) \tag{2}$$

Child nodes are selected and expanded until we reach a leaf node. Once we have reached this leaf node, a reward is calculated through the negative cross-entropy loss based on the work of Farnia & Tse (2017):

$$\min_{\mathcal{R}^k} - \sum_{c=0,1} \mathbb{1}(Y_k = c) \log P(Y_{new} = c|\mathcal{R}^k) \tag{3}$$

The loss looks at how much the probability of a prediction (Y_k) of the original graph ($\mathcal{G}_k$) changes when the input is limited to a specific subgraph ($\mathcal{R}^k$). If the probability changes a lot, then that subgraph is not a good explanation for the prediction made on event e_k by the original graph. The output of the loss function is used as the "reward" for back-propagation. The back-propagation step itself keeps track of two values: the cumulative reward value for each node $c(\mathcal{N}^i, e_j)$, and how many times the node has received a reward $c(\mathcal{N}^i, e_j)$.

3.2.2 Selecting the explanatory subgraph

The explorer-navigator process is repeated through several rounds or "rollouts" to explore different possible subgraphs from root to leaf. The best explanation for the prediction e_k is the subgraph that has the highest cumulative reward and has the simplest explanation according to the sparsity threshold ($|\mathcal{R}^k| \leq N_r$ in equation 8).

3.3 Evaluation

The two metrics used to evaluate the performance of the explainers are the Area Under the Fidelity-Sparsity Curve (**AUFSC**), and **Best Fid** (best fidelity). The formula for sparsity is given by: $Sp = |\mathcal{R}^k|/|\mathcal{G}^k|$ Sparsity is a ratio between the size of the explanatory subgraph and the input graph $\mathcal{G}^k$.

The formula for Fidelity is given by:

$$Fid(f(\mathcal{G}^k)[e_k], f(\mathcal{R}^k)[e_k]) = \mathbb{1}(Y_k = 1)(f(\mathcal{R}^k)[e_k] - f(\mathcal{G}^k)[e_k]) + \mathbb{1}(Y_k = 0)(f(\mathcal{G}^k)[e_k] - f(\mathcal{R}^k)[e_k]) \tag{4}$$

Fidelity measures the difference between the logit probability output by the temporal network $f(\cdot)$ when the input is the original graph $\mathcal{G}^k$ and when the input is the explanatory subgraph $\mathcal{R}^k$. a logit score of $+1$ implies that the explanatory subgraph is a better prediction than the original graph. The model aims to maximize the fidelity.

The **AUFSC** is a numerical score that measures the area under the graph for the fidelity values at sparsity intervals between 0 and 1 ($|\mathcal{R}^k| = |\mathcal{G}^k|$). A higher value for AUFSC implies the explorer achieves high fidelity, even at a low sparsity threshold.

The goal is to have high fidelity, which means that $f(\mathcal{R}^k)[e_k]$ produces a logit probability that ideally surpasses the original prediction $f(\mathcal{G}^k)[e_k]$, while keeping the explanatory subgraph $\mathcal{R}^k$ as simple as possible. The purpose is not to achieve the same probability output on $f(\mathcal{R}^k)[e_k]$ as $f(\mathcal{G}^k)[e_k]$ (fidelity = 0) but rather to obtain a subset that increases the logit number for this prediction as much as possible (positive fidelity). In a way, we are picking the best events to generate this prediction which we call the "explanatory subgraph".

The metric **Best Fid** simply measures highest fidelity achieved by an explainer, ignoring sparsity altogether. The only limitation is the hyperparameter N_r controlling the maximum amount of nodes allowed.

3.4 Baselines - Other Explainers

The authors compare the performance of the T-GNNExplainer with three baseline explainer methods: PG-Explainer (Luo et al., 2020), ATTN and PBONE (Xia et al., 2023). In contrast to T-GNNExplainer, the baselines are not search-based methods. The original PGExplainer is a parametrized explainer for GNNs that provides a model-level explanation over multiple event predictions. The authors adapt PGExplainer to output explanations for temporal graph structures at an instance-level. The two other explainers were modelled by the authors themselves. Firstly, there is ATTN which is an attention-based explainer that averages the weight values over all attention layers of either TGAT or TGN. PBONE generates an explanation

by removing or "perturbing" one candidate event at a time to compute its importance in a prediction (Xia et al., 2023).

3.5 Target models

The authors test the explainer on two target models, namely TGN and TGAT. TGAT is a temporal graph attention layer that is used in neural networks. This technique uses self-attention and stacks TGAT layers to recognize the node embeddings as functions of time (Xu et al., 2020). Temporal Graph Networks (TGN) is a deep learning framework where dynamic graphs are represented as sequences of timed events (Rossi et al., 2020). TGN consists of a combination of memory modules and graph-based operators. In contrast to TGAT, TGN uses Multi-head Attention in their network.

4 Datasets

The dataset collection consists of bipartite graphs and unipartite graphs, all of which are directed. Bipartite graphs consist of two types of nodes (ex. users and pages). Events in the datasets describe one type of node interacting with the other type (Chang & Tang, 2014). Unipartite graphs consist of one type of node, among which events occur (Chang & Tang, 2014).

In summary, the original paper experiments with two classes of datasets with very distinct characteristics. One is an information-rich, bipartite graph network describing an online collaboration process, and the other is a dataset generated by a statistical process in a small-scale graph with predefined, static relationships.

4.1 Data format

The original paper makes some claims about the data structures that conflict with the implementation in the code. This section highlights implicit assumptions and discrepancies relevant to our discussion in Section 8 about the precise data specifications needed to run the models.

It is first important to note that every dataset used is a directed graph, since the format consist of events that occur from node n_{u_i} to node n_{v_i}. There can be multiple events from node n_{u_i} to node n_{v_i} (ex. a user updates a page multiple times). The original paper states that there could be deletion or internal update events $e_i = \{n_{u_i}, null, t_i, \text{att}_i\}$, however the implementation for the T-GGNExplainer does not allow for null events, therefore there are no self-updates or self-deletions of nodes.

Even though the original paper claims that the T-GNNExplainer takes into account the continuous-time dynamic properties of the data (Xia et al., 2023), only the underlying predictor models do this. Analysis of the methodology and code reveals that T-GNNExplainer only looks at events ordinally, and ignores the amount of time that passes between events.

4.2 Synthetic Datasets

The synthetic datasets are based on a unipartite temporal graph that contains 4 nodes, and 4 possible edge-events. The possible events within this graph adhere to predefined excitory and inhibitory relations. These predefined relations are used in a multivariate Hawkes process to generate a dataset of timestamped events. (Hawkes, 1971) implemented in the Tick Python library (Bacry et al., 2018). A random process is used to generate noise in the form of false events. In summary, the synthetic datasets are relatively small datasets that describe the occurrence of four unique events over time.

4.3 Real-World datasets

The two real-world datasets used in the original paper, Wikipedia and Reddit (Kumar et al., 2019), are bipartite graphs that describe editing processes between users and web pages. In both datasets, this process follows a roughly 1:9 ratio between web pages and users. Each event is accompanied by a 172 numeric features vector that describes the editing process.

It should be noted that although it is claimed these datasets are bipartite, about $\frac{1}{10}$th of the connections are going in both directions. This would disprove the bipartite characteristic. We have not found a reason why this could be the case in the original paper or from the authors who compiled the datasets.(Kumar et al., 2019).

4.4 New dataset

Temporal graph neural networks have the unique ability to infer and predict the developments of evolving network structures (i.e. temporal graphs), in which processes from different scientific disciplines such as ecology and social science (Fortin et al., 2012) (Yu et al., 2018) can be expressed.

Temporal graph data is versatile and expressive, but is, in terms of causality, incredibly complex. A development in the network (i.e. event) arises from an interplay of influences that post-hoc, is difficult to deterministically concretize. Temporal graph explainers such as T-GNNExplainer represent an opportunity to provide transparency to predictions on a data structure with immense expressive power.

In our opinion, a T-GNNExplainer becomes truly useful when it is able to successfully leverage the complex and dynamic inhibitory and excitory influences among events present in real-world processes, to provide end-users with concise and accurate explanations for novel events.

In order to validate the robustness of the claims made by the original authors regarding AUFSC performance, a new dataset is included in the experimentation. **MOOC** is a network representing student interaction from online course content units (Kumar et al., 2019).

MOOC exists in a different and desirable interposition of dataset characteristics with respect to the original datasets. It is equal in size to the originals but has fewer features and can therefore serve to test the generalizability of the proposed methodology on real-world temporal graph processes with limited event information.

A significant amount of time was spent on obtaining another unipartite dynamic dataset and get it to function (Kumar et al., 2018). Unfortunately, we did not succeed due to unclear errors in the code while running.

Table 1: Dataset attributes. Where # represents "Number", so "Number of Events" and "Number of Features".

Name	# of Events	# of Features	Type	Time period	Time granularity
Wikipedia	157,474	172	bipartite	1 month	seconds
Reddit	672,447	172	bipartite	1 month	seconds
MOOC	411,749	4	bipartite	~298 days	seconds
V1	10,000	0	unipartite	~5000 seconds	<seconds
V2	10,000	0	unipartite	~5000 seconds	<seconds

All data sets have a 70% / 15% / 15% train / validation / testing scheme based on timestamps for both TGAT and TGN. The most recent 30% is used for the validation and test sets (Kumar et al., 2018)(Kumar et al., 2019).

5 Hyperparameters

The experimental setup is copied from Section 5.2 and the Appendix of the original paper (see Appendix C below for further details).

For the novel dataset, minor changes have been made. Firstly, in the training of the graph prediction models (TGAT and TGN), the dimensionality for time, memory and node embeddings is adjusted to match the dimensionality of the feature information in the novel datasets. Secondly, the number of training epochs

for training the explainers on MOOC is set to 50. Due to limited compute resources, epoch values were chosen to reflect the ratio of training epochs for the original real-world datasets compared to the dataset size and number of features. In Appendix C.1 we explain our setup of hyperparameter tuning; however, due to limitations in compute resources, we were unable to run this experiment.

6 Experimental setup & Code

The following experiments were performed: 1) Reproduction on the original performance claims, 2) Extension of performance evaluation to one new datasets. 3) Subgraph density analysis, this is the analysis of the relationship between number of nodes in the initial sub graph per test sample and explanation performance.

The repository can be found here https://github.com/chaosido/FACT-course.

6.1 Reproduction

To reproduce the original results, we train the models (TGAT, TGN) on the original datasets (Wikipedia, Reddit, Synthetic V1, Synthetic V2). We then train the explainers (T-GNNExplainer, PGExplainer, ATTN, PBONE) on the trained temporal graph networks from the previous step. Finally, the performance is evaluated using the evaluation methods in the authors' original code to measure AUFSC and Best Fid scores (evaluation detailed in section 3.3).

6.2 Extension with novel datasets

New datasets need to adhere to a number of constraints to train explainer models, data format and content constraints. Before the new dataset can be used in training, it needs to be processed to match the navigator feature vector as described in Section 3.2.2. The full experimental setup of the new datasets is described in Appendix C.

6.3 Subgraph density analysis

An additional part of our experimentation involves the analysis of the relationship between the number of nodes in the initial explanatory subgraph $\mathcal{G}^k$ and the explanatory performance. For each test sample, the number of nodes in the initial explanatory subgraph is compared to the AUSFC for this test sample.

In our temporal graph datasets, multiple events can exist between any two given nodes. (i.e. one user edited the same web page multiple times). Consequently, the number of nodes in the initial subgraph is variable. More information about the construction of the initial explanatory subgraph of an event to be explained can be found in the appendix B1. Because of this variability, for some events, the initial subgraph encapsulates the intensive interaction between two nodes. For other events, it encapsulates non-interconnected duplets of nodes. Discovering the relationship between the number of nodes in the initial subgraph and explanation performance can illuminate certain temporal graph charecteristics that correlate with explainer performance.

Since the number of events in the initial subgraph is set by a hyperparameter. We use 'density' to denote the number of nodes in the intial subgraph.

This experimentation is only performed with real-world datasets. The simulated datasets exists of only 4 possible events between 4 nodes. The upper bound in the number of nodes in the initial subgraph is too small to reveal a relationship between subgraph density and explanation performance.

Since the number of events in the initial subgraph is determined by a hyperparameter, and only the number of nodes is variable, we refer to the number of nodes in the initial subgraph as 'density'.

6.4 Computational Requirements

All experiments were trained on a compute cluster with a 40GB A100 PCie GPU and a cluster of CPUs each equipped with a 24-core AMD EPYC 7F72 24-core Processor @ 3.2 GHz.

Training times were also tracked. The average training time for the models (TGAT,TGN) is 4 hours, for the explainers this averaged at 26 hours. The computational hours required for the results presented in this research can be split up into 88 hours for the training of the models and 345 hours for the training of the explainers.

7 Results

7.1 Results on original paper

In this section we report our reproduced results in Table 2 and Table 3 for the real-world datasets for specific target models. For the remaining results please see the appendix D.

Table 2: Best fidelity and AUFSC achieved by each explainer on Wikipedia for target model TGAT.

	Wikipedia TGAT			
	Best Fid		**AUFSC**	
	old	**new**	**old**	**new**
ATTN	0.891	0.918	0.564	0.626
PBONE	0.027	1.405	-2.227	1.076
PG	1.354	0.642	0.692	-0.653
T-GNN	**1.836**	**1.604**	**1.477**	**1.300**

As shown in the Table 2 and Table 3, T-GNNExplainer still mostly outperforms the 'best baseline', except for Reddit, however nearly all Best Fidelity and AUFSC scores for T-GNNExplainer are lower in our experiment compared to the original paper. Nearly all baselines score higher on both metrics compared to the original findings (see complete tables in the Appendix D).

PBONE has better performance than the original results on almost all AUFSC experiments except TGN/Reddit (Table 10). Most explainers perform worse on the Reddit dataset than the original results, except PBONE/TGAT. TGN has a wider range of AUFSC scores than TGAT, indicating more varied results. The difference between the orginal and reproduced metric values are also largest on average for PBONE across all four original datasets. Tables in the appendix show similar results D.

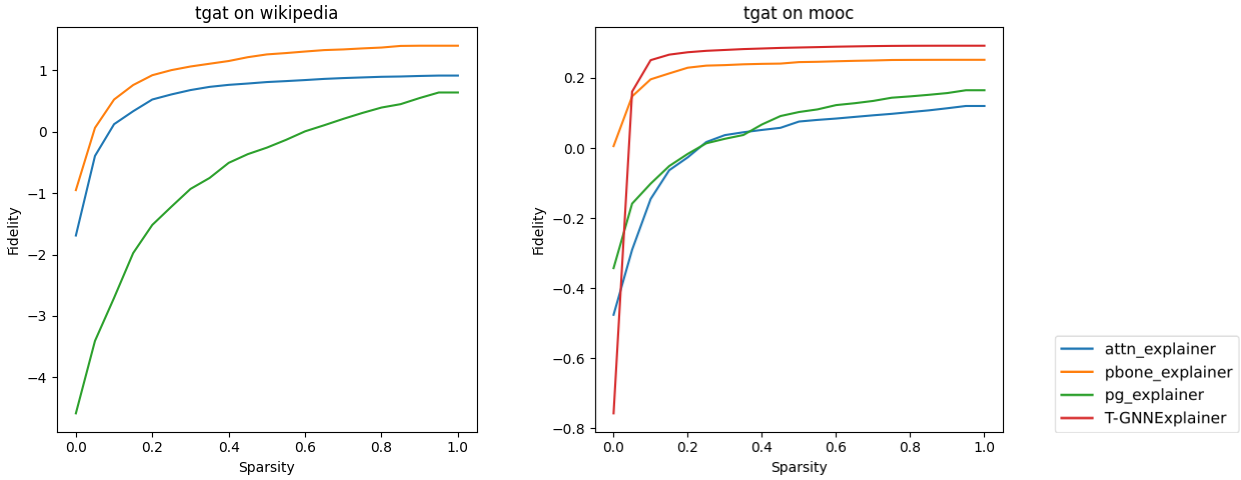
Table 3: Best fidelity and AUFSC achieved by each explainer on Reddit for target model TGN.

	Reddit TGN			
	Best Fid		**AUFSC**	
	old	**new**	**old**	**new**
ATTN	0.575	0.144	0.289	-1.546
PBONE	0.340	0.244	-0.256	**-0.629**
PG	0.679	0.117	0.020	-2.193
T-GNN	**1.362**	**0.251**	**1.113**	-1.060

Performance on the Reddit dataset is an outlier compared to other datasets. The PBONE method outperforms the T-GNNExplainer on this dataset. Both models (TGN and TGAT) have low results on both Best Fid and AUFSC.

7.2 Results beyond original paper

In this section we report our results in Table 4 for the new real-world dataset MOOC. In Figure **??**, we illustrate the fidelity-sparsity curve on the original real-world datasets, as well as the new real-world dataset.



(a) AUFSC curve for TGN on the Synthetic V2 dataset.

(b) AUFSC curve for TGAT on MOOC dataset.

Figure 1: Two graphs for AUFSC curves and corresponding legend for all four explainers. The legend indicaties the lines for each explainer: blue, orange, green and red for ATTN, PBONE and T-GNNExplainer respectively. The scales between (a) and (b) differ.

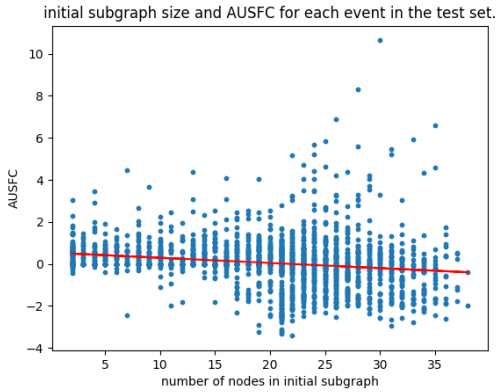
Table 4: Best fidelity and AUFSC achieved by each explainer on MOOC. An emboldened result is the highest result in that column.

MOOC	**TGAT**		**TGN**	
	Best Fid	**AUFSC**	**Best Fid**	**AUFSC**
ATTN	0.120	0.024	0.251	0.186
PBONE	**0.252**	**0.230**	0.418	0.348
PG	0.165	0.059	0.310	0.259
T-GNN	0.224	0.182	**0.478**	**0.437**

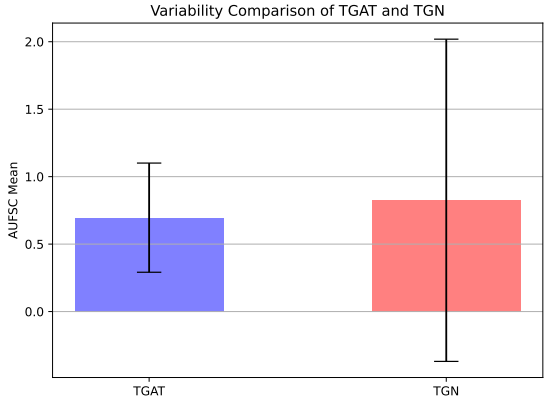
For the MOOC dataset, the T-GNNExplainer outperforms the baselines only for TGN, whereas PBONE outperforms for TGAT (See Table 4). However, all explainers are very close in value on both metrics, and score low.

Figure 3 encompasses results of the reproduction of the original experimentation with of T- T-GNNExplainer. it includes $4 * 500$ =2000 AUSFC scores. A red trend line is constructed by a least squares fit. The decision to use AUSFC as a reflection of explination performance stems from the reasoning that AUSFC encapsulates the fidelity over all sparsity intervals and is therefore a robust metric.

The variability plot shows a higher variability between the underlying models for the T-GNNExplainer. Using TGAT as an underlying model yields less variance in the outcomes over all models in comparison to TGN.



(a) Performance as a function of subgraph density for the T-GNNExplainer on TGAT Reddit, TGN Reddit, TGAT Wikipedia, TGN Wikipedia.



(b) Variability comparison of TGAT and TGN. The mean is taken over all the datasets for the AUFSC metric for each target model, with its standard deviation.

Figure 2: density plot and variation plot

Table 5: This shows the percentage differences between T-GNNExplainer and the best baseline explainer. For example, the first number in the first column indicates that in the original results, T-GNNExplainer outperformed the second best baseline on the Best Fid metric by 35.6%. For the new results, the negative values indicate where T-GNNExplainer performed second best to PBONE.

Percentage % difference between best and best baseline explainer on real-world datasets						
		Wikipedia		**Reddit**		**MOOC**
Model	**Metric**	**Old**	**New**	**Old**	**New**	**New**
TGAT	Best Fid	**35.60**	14.16	**88.81**	9.56	-11.11
	AUFSC	**113.44**	20.82	391.60	-4.11	-20.87
TGN	Best Fid	**80.79**	49.43	**100.59**	2.87	14.35
	AUFSC	**708.22**	177.83	285.12	NA	25.57

8 Discussion

8.1 Main claim

Almost all of the values for the AUFSC and Best Fid metrics differ in our reproduction of the original experiment. Despite lower performance in nearly all the output values on both key metrics compared to the original results (See Tables 4, 9, 10, 11, 12), the reproduced experiments still largely support the claim that the T-GNNExplainer outperforms the PGExplainer and ATTN explainers. However, it does not always outperform PBONE. In both instances where T-GNNExplainer does not outperform the baselines, PBONE performs best (Reddit/AUFSC for both TGAT and TGN). T-GNNExplainer performs second best in these cases.

In our analysis of the main claim that T-GNNExplainer outperforms the leading baseline by up to $\sim 50\%$ on the AUFSC metric, it is unclear how the original authors calculated this value. We calculated the percentage difference using $\left(\frac{(T-\text{GNN})-\text{best baseline}}{|\text{best baseline}|} * 100\right)$, and applied it to the original results (See Tables 9, 10, 11, 12). These new calculations differ from the reported percentage difference in the original paper. For example, the original paper states that the T-GNNExplainer outperforms the leading baseline (PGExplainer) for TGN trained on Wikipedia on AUFSC by 86% whereas we found it outperforms by $\sim 700\%$ (See Table 5). Table 5 and Table 13 show that the percentage difference is consistently lower on all valid comparisons for the new

results compared to the old results. This confirms that the the T-GNNExplainer does not perform as well in the reproduced experiments as in the original results, on both the Best Fid and AUFSC metrics. Please note that since some Best Fid and AUFSC metrics are negative, some percentage difference values could not be calculated.

8.2 MOOC Dataset

Experiments on the MOOC dataset reveal very similar trends to all explainer models (See Table 4), but the variance of the results is much smaller and closer to 0. The underlying T-GNN models did not score a high accuracy on MOOC compared to the other datasets (96% compared to 66% respectively).

Since the prediction of these T-GNN models are used as the "ground truth" for the explainers, the explainer is dependent on the performance of the underlying predictor model. Since the explainer doesn't look "under the hood" at the steps that the T-GNN model takes to make a prediction, and rather uses the T-GNN model to find post-hoc explanations, it follows that when the estimates are noisy, the performance of the explainer suffers.

Considering the low accuracy of both TGN and TGAT on MOOC, this could explain why the variance of the results on MOOC is far smaller than on other datasets.

8.3 Subgraph Density analysis

Figure **??** indicates that the graph explainers included in this research (which are post-hoc instance level) perform better on events that have a two-hop neighbour event history that includes a limited number nodes. For all explainers there exists a negative trend between the number of nodes in the initial subgraph and the explanatory performance as can be seen in Figure **??** and Appendix Section D 9. This discrepancy means that on average, AUSFC is higher when the initial subgraph is more dense (i.e. has fewer nodes). In our understanding, there are two salient reasons to explain this phenomenon:

1. When the number of nodes in the initial subgraph is low, the explainers are more successful at selecting the events that, together, maximize fidelity for this event. The same explainers are less successful at this task when the events are sparsely connected. With this logic, the discrepancy in performance is a result of the explainer methodology.
2. The second reason pertains to event relations structures present in the initial subgraphs. The idea of an event relation structure is analogous to idea of pre-defined event relations visualized in Figure 2 of the original paper. These structures might be more simple, and homogeneous among dense initial subgraphs in comparison to sparse initial subgraphs. They are on average more simple since, the complexity of the event relation structures is limited by the number of nodes in the initial subgraph. They are more homogeneous since the maximum complexity of event relations is lower, resulting in more event relations structure repetition within datasets. This homogeneity and simplicity are conducive to the learning process of explainers. With this logic, the discrepancy can be attributed to temporal graph data characteristics.

It is possible that the observed performance discrepancy is caused by a mixture of the two aforementioned reasons and/or reasons not mentioned.

Given on average, explainers perform best on high density initial subgraph events, it would be interesting to discover whether e_k is separated from the small group of nodes of which e_k's history exists or if it is an interaction among this small, highly interacting group of nodes. We intuit the prior situation is almost always the case, but have no empirical evidence to support this.

Suitable dataset characteristics Given the results found in our experimentation, the most desirable dataset is one where for each event that we're predicting, the 20 most recent events in a two-hop neighbourhood ($\mathcal{G}^k$), involve only a few nodes. This is a datasets where small node groups have intensive interaction, ideally not to close together. Over time, the composition of node groups changes. If change is too quick, the initial explanatory subgraph density decreases, which is undesirable.

The original plan was to run another dataset next to MOOC, which would have added to the gap by being a real-world unipartite dataset. After several days of data cleaning and bug fixing, it was found that it could not be done. It appears that T-GNNExplainer requires a very specific type of data format. For example, in the processing file for the datasets, there are a couple of assertions that are not discussed in the paper, but which limit the data input space. Even when these assertions are fulfilled, the unclear errors can still break the model later on during a run. All of this can be seen as quite limiting. Apart from the real-world applications, there are currently also very few datasets publicly available that adhere to these standards for experimental generalization purposes. It would fruitful to clean more real world datasets or think of more intricate methods to generate synthetic data with the dynamic temporal characteristic for further generalization purposes.

8.4 Model Agnostic Claim

Although the authors claim that T-GNNExplainer is model agnostic, it doesn't seem to stay true for these two SOTA models. Our results show that the explanatory power of T-GNNExplainer differs between the TGAT and TGN models. Figure 2 **??** shows that the T-GNNExplainer performs worse overall on the TGAT model than TGN, however performance on the TGN model has way higher variance, so it also offers less certainty.

8.5 Reddit dataset

All explainers underperform on the Reddit dataset. One possible explanation points to the size of the dataset and the method for splitting the data. Reddit is by far the biggest dataset (~ 260000 bigger than MOOC). When training the T-GNN models, the data is split temporally where the first 85% events are used for training and validation and the last 15% events are used as test data. The problem with this method is that graph data is not independent, so events earlier in time could influence events later in time. Separating the data in this way can lead long-distance predictions that are inherently more uncertain. In line with this is MOOC, which is the second biggest dataset, also resulting in low scores comparatively. A more advanced temporal splitting methods could be used to obtain more valid outcomes (de Bruin et al., 2021).

Another reason could be that the Reddit dataset seems to have mistakes in it. It is said to be a bipartite dataset of users editing pages. However there are nodes that appear in both sets, which is impossible in a bipartite dataset. This could result in worse modeling as the data is not clean.

8.6 Computational efficiency

The authors discuss the computational efficiency of the T-GNNExplainer in comparison to the baseline models in their Appendix. They found that the T-GNNExplainer is significantly slower than the baseline models, none of which are search-based methods. For example, T-GNNExplainer takes 28.2s to explain one instance in the Reddit datset trained on TGAT compoared to 0.39s for PBONE (Appendix by (Xia et al., 2023)). They state that the complexity of the MCTS algorithm is O(NDC) (Appendix by (Xia et al., 2023)), where N is the number of rollouts, D is how far each rollout expands a node, and a constant for inference time. Given that in the code, the hard coded leaf nodes meant that each rollout expanded nodes all the way down to a subgraph containing 1 event, the complexity was very high. Efficiency would likely be improve if this rollout search wasn't continued on to the final node.

8.7 Discrepancy between results

It is unclear why none of the values in the reproduced experiments match the original results. One interesting discrepancy is that in our results PBONE either performs second best, or in some cases outperforms T-GNNExplainer. In the original results, the leading baselines are either ATTN or PGExplainer. PBONE performs best on AUFSC for both models trained on the Reddit dataset. In instances where PBONE performs second best, its evaluation metrics are often close in value to those of T-GNNExplainer.

Since T-GNNExplainer is computationally intensive given the task (i.e. it only provides instance level explanations), it is not clear whether it is model-agnostic, and it requires very precise dataset configurations, it would be valuable to explore other methods to provide explanations for T-GNNs. In comparison to T-GNNExplainer, PBONE is a very simple model that is computationally much faster than T-GNNExplainer. Considering its simplicity, computational efficiency, and its ability to "compete" with T-GNNExplainer, refining this method could be valid avenue for exploration. Justification could be found in similar methods explored by Lucic et al. (2022) where the authors use a perturbation method on GNNs to achieve strong results.

9 What was easy and what was difficult?

What was easy: The authors made their code accessible online, without which the paper would not have been reproducible. Reading the responses on OpenReviews was helpful in providing insight into the difficulties others also had with the paper. The Appendix provided by the authors in response to the OpenReview comments helped clarify questions we had about hyperparameters and implementation.

What was difficult: Discrepancies between the code and the paper, and inconsistencies in the code (missing directories, dependencies, hard-coded hyperparameters, inconsistent nomenclature, etc.) meant the code required a lot of trial-and-error to produce valid results. For example, the λ variable named "c_puct" was reported to be 5 in the paper, but was set to 100 in the config files. This discrepancy was not identified until after the T-GNNExplainer had already been trained. This trial-and-error, combined with the massive compute requirements demanded by the code, meant we ran out of compute resources allocated to our team, and we still had to forego many crucial experiments (hyperparameter tuning) due to lack of computational resources. Using the Machine Learning Emissions Calculator (Lacoste et al., 2019), we estimate that the GPU resources on this project alone emitted at least 51 kg CO2 eq., or equivalent to driving more than 200km by an average ICE car (See Table 6 in Appendix A).

While validating reproducibility is essential in machine learning, there is a serious conversation to be had about the trade-off between these efforts and the societal and environmental costs incurred when the groundwork to enable reproduction is not "baked" into the research process from the start.

Communication with original authors: The authors were contacted, but we did not receive a response.

References

Chirag Agarwal, Owen Queen, Himabindu Lakkaraju, and Marinka Zitnik. Evaluating explainability for graph neural networks, 2023.

Kenza Amara, Rex Ying, Zitao Zhang, Zhihao Han, Yinan Shan, Ulrik Brandes, Sebastian Schemm, and Ce Zhang. Graphframex: Towards systematic evaluation of explainability methods for graph neural networks, 2022.

Emmanuel Bacry, Martin Bompaire, Stéphane Gaïffas, and Soren Poulsen. Tick: a python library for statistical learning, with a particular emphasis on time-dependent modelling, 2018.

Jenna Burrell. How the machine 'thinks': Understanding opacity in machine learning algorithms. *Big Data amp; Society*, 3(1), 2016. doi: 10.1177/2053951715622512.

Chang Chang and Chao Tang. Community detection for networks with unipartite and bipartite structure. *New Journal of Physics*, 16(9), 2014. doi: 10.1088/1367-2630/16/9/093001.

Gerrit Jan de Bruin, Cor J. Veenman, H. Jaap van den Herik, and Frank W. Takes. Experimental evaluation of train and test split strategies in link prediction. In Rosa M. Benito, Chantal Cherifi, Hocine Cherifi, Esteban Moro, Luis Mateus Rocha, and Marta Sales-Pardo (eds.), *Complex Networks & Their Applications IX*, pp. 79–91, Cham, 2021. Springer International Publishing.

Finale Doshi-Velez and Been Kim. Towards a rigorous science of interpretable machine learning, 2017.

Farzan Farnia and David Tse. A minimax approach to supervised learning, 2017.

Marie-Josee Fortin, Patrick James, Alistair MacKenzie, Stephanie Melles, and Bronwyn Rayfield. Spatial statistics, spatial regression, and graph theory in ecology. *Spatial Statistics*, 1:100–109, 05 2012. doi: 10.1016/j.spasta.2012.02.004.

Valeria Gelardi, Didier Le Bail, Alain Barrat, and Nicolas Claidiere. From temporal network data to the dynamics of social relationships. *Proceedings of the Royal Society B: Biological Sciences*, 288(1959), September 2021. ISSN 1471-2954. doi: 10.1098/rspb.2021.1164.

Alan Hawkes. Point spectra of some mutually exciting point processes. *Journal of the Royal Statistical Society. Series B*, 33, 07 1971. doi: 10.1111/j.2517-6161.1971.tb01530.x.

Wenchong He, Minh N. Vu, Zhe Jiang, and My T. Thai. An explainer for temporal graph neural networks, 2022.

Srijan Kumar, William L Hamilton, Jure Leskovec, and Dan Jurafsky. Community interaction and conflict on the web. In *Proceedings of the 2018 World Wide Web Conference on World Wide Web*, pp. 933–943. International World Wide Web Conferences Steering Committee, 2018.

Srijan Kumar, Xikun Zhang, and Jure Leskovec. Predicting dynamic embedding trajectory in temporal interaction networks. In *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery amp; Data Mining*, KDD '19. ACM, July 2019. doi: 10.1145/3292500.3330895.

Alexandre Lacoste, Alexandra Luccioni, Thomas Dandre, and Victor Schmidt. Quantifying the carbon emissions of machine learning, 2019. URL `https://mlco2.github.io/impact/`.

Meng Liu, Youzhi Luo, Limei Wang, Yaochen Xie, Hao Yuan, Shurui Gui, Haiyang Yu, Zhao Xu, Jingtun Zhang, Yi Liu, Keqiang Yan, Haoran Liu, Cong Fu, Bora Oztekin, Xuan Zhang, and Shuiwang Ji. Dig: A turnkey library for diving into graph deep learning research, 2021.

Ana Lucic, Maartje ter Hoeve, Gabriele Tolomei, Maarten de Rijke, and Fabrizio Silvestri. Cf-gnnexplainer: Counterfactual explanations for graph neural networks, 2022.

Dongsheng Luo, Wei Cheng, Dongkuan Xu, Wenchao Yu, Bo Zong, Haifeng Chen, and Xiang Zhang. Parameterized explainer for graph neural network, 2020.

Fabiola Pereira, João Gama, Sandra Amo, and Gina Oliveira. On analyzing user preference dynamics with temporal social networks. *Machine Learning*, 107, 11 2018. doi: 10.1007/s10994-018-5740-2.

Emanuele Rossi, Ben Chamberlain, Fabrizio Frasca, Davide Eynard, Federico Monti, and Michael Bronstein. Temporal graph networks for deep learning on dynamic graphs, 2020.

Claude Elwood Shannon. A mathematical theory of communication. *The Bell System Technical Journal*, 27 (3):379–423, 1948. doi: 10.1002/j.1538-7305.1948.tb01338.x.

Wenwen Xia, Mincai Lai, Caihua Shan, Yao Zhang, Xinnan Dai, Xiang Li, and Dongsheng Li. Explaining temporal graph models through an explorer-navigator framework. In *The Eleventh International Conference on Learning Representations*, 2023. URL `https://openreview.net/forum?id=BR_ZhvcYbGJ`.

Da Xu, Chuanwei Ruan, Evren Korpeoglu, Sushant Kumar, and Kannan Achan. Inductive representation learning on temporal graphs, 2020.

Rex Ying, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. Gnnexplainer: Generating explanations for graph neural networks, 2019.

Bing Yu, Haoteng Yin, and Zhanxing Zhu. Spatio-temporal graph convolutional networks: A deep learning framework for traffic forecasting. July 2018. doi: 10.24963/ijcai.2018/505.

Hao Yuan, Jiliang Tang, Xia Hu, and Shuiwang Ji. Xgnn: Towards model-level explanations of graph neural networks. In *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery amp; Data Mining*, KDD '20. ACM, August 2020. doi: 10.1145/3394486.3403085.

A Machine Learning Emissions Calculator

In Table 6, we provide the specifications for the calculator used to calculate the CO_2 impact.

Table 6: Specifications for the calculator (Lacoste et al., 2019)

Hardware	Hours used	Provider	Carbon Efficiency	Offset Bought
AMD EPYC 7763	400	Private Infrastructure	0.459	0

B Model description

B.1 T-GNNExplainer

We explain the Explorer-Navigator framework below in further detail to provide clarity through a more intuitive understanding of this model.

A temporal graph network predicts whether a target event e_k will occur or not (Rossi et al., 2020)(Xu et al., 2020). The purpose of the T-GNNExplainer is to find a set of preceding events that explain why the model made this prediction.

This subset of events $\mathcal{R}^k$ henceforth referred to as the "explanatory subgraph" is found from a set of candidate events. These candidate events are selected through three hyperparameters. The first hyperparameter (`n_hops` in the code) limits them spatially to be within a k-hop neighborhood of the target event (i.e., 2 hops). The second (`num_neighbors` in the code) restricts them temporally to the target event (i.e., within the 10 most recent events). $\mathcal{R}^k$ finally, is further limited by the hyperparameter N_r, which constrains the maximum number of nodes that the explanatory subgraph can have. In the code, this number is hard coded to 20. The reasoning is that if the subgraph is too large e.g. if $|\mathcal{R}^k| = |\mathcal{G}^k|$, then the explanatory power of $\mathcal{R}^k$ becomes tautological, losing usefulness in its lack of specificity.

The explainer module is made up of two parts, the navigator and the explorer, that work together to "prune" a graph of unimportant events related to the target event e_k, resulting in a graph of only the most relevant events that lead to the prediction of the target event.

B.2 Navigator

The navigator is inspired by the "explanation network for node classification" from the parameterized explainer proposed by Luo et al. (2020). The navigator $h_\theta(e_j, e_k)$ proposed in this paper is a two-layer multi-layer perceptron (MLP) that learns a correlation between two events e_j (the candidate) and e_k (the target).

To infer the relationship between two specific events, the features of both events are concatenated into a vector and input into the network:

$$Z_{e_j,e_k} = [X_{n_{u_k}} \| X_{n_{v_k}} \| \text{Time}(t_k) \| \text{att}_k \| X_{n_{u_j}} \| X_{n_{v_j}} \| \text{Time}(t_k) \| \text{att}_k]^T$$

X represents the node feature matrix, $Time(\cdot)$ is a harmonic function that encodes the real-valued timestamp into a learnable vector adapted from (Xu et al., 2020), and $||$ represents concatenation.

Given that the navigator is an MLP that takes as input the concatenated features of two events to learn a relationship between them, this indicates that the network learns similarities between events. So when the explorer (explained in section B.3 below) uses the navigator to remove "unimportant" events from the search space, the navigator selects dissimilar events to the target event.

B.3 Explorer

The explorer uses a modification of Monte Carlo Tree Search (MCTS). The explorer searches a tree of nodes, where each child node is a subgraph of its parent node, which has one fewer event than the parent before it.

The root node is initialized as a subset of $\mathcal{G}^k$ that satisfies the constraints imposed by temporal and spatial hyperparameters.

Starting from the root node, the explorer selects and expands child nodes. It is important to note that these child nodes are not stored in memory. Rather, the explorer keeps track of a list of previously expanded events at each node $\mathcal{C}(\mathcal{N}^i)$. This entire process is conducted through multiple rounds (i.e. rollouts), a hyperparameter that is set to 500 in this paper.

Each rollout starts with the root node and we prune events until we reach a leaf node, which is a child that satisfies the hyperparameter criteria that it has fewer than 5 events. In the code itself, a leaf node is defined as a subgraph with 1 event in the code, and less than 5 events in the paper.

Child nodes are selected and expanded until a leaf is reached. The search tree of all nodes is not not stored in memory across rollouts, rather each rollout starts with the root and a list of events that were expected and expanded in previous rollouts.

B.4 Node Selection

The search path is selected using the following formula:

$$e^* = \underset{e_j \in \mathcal{C}(\mathcal{N}^i)}{\arg\max} \left(\frac{c(\mathcal{N}^i, e_j)}{n(\mathcal{N}^i, e_j)} + \lambda \frac{\sqrt{\sum_{e_l \in \mathcal{C}(\mathcal{N}^i)} n(\mathcal{N}^i, e_l)}}{1 + n(\mathcal{N}^i, e_j)} \right) \tag{5}$$

Since the nodes themselves are not stored in memory, a child node is "selected" by removing an optimal event e* from the current node N^i. This equation says that from events that have already been expanded, select an event that has a high average reward value from previous rounds (exploitation term) but has not been explored as much (exploration term). The λ is a hyperparameter set by the paper authors that controls how much exploration is encouraged.

B.5 Node Expansion

Instead of generating and searching a tree of all possible subgraphs, the explorer uses the navigator to create subgraphs that are relevant to its search. The navigator finds the least important event in relation to the target/predicted event e_k:

$$e^* = \underset{e_j \in \mathcal{N}^i / \mathcal{C}(\mathcal{N}^i)}{\arg\min} \; h_\theta(e_j, e_k) \tag{6}$$

The explorer then creates a new child node by removing e^* from the current node N_i. It is important to note that the navigator only searches events that were not already removed in previous rollouts, so that we do not end up removing the same event in every rollout.

B.6 Reward & Backpropagation

Child nodes are selected and expanded until we reach a leaf node. Once we have reached this leaf node, a reward is calculated through the negative cross-entropy loss based on the work of Farnia & Tse (2017):

$$\min_{\mathcal{R}^k} - \sum_{c=0,1} \mathbb{1}(Y_k = c) \log P(Y_{new} = c | \mathcal{R}^k) \tag{7}$$

The loss looks at how much the probability of a prediction (Y_k) of the original graph (G_k) changes when the input is limited to a specific subgraph ($\mathcal{R}^k$). If the probability changes a lot, then that subgraph is not a good explanation for the prediction made on event e_k by the original graph. The outcome of the loss

function is seen as the reward for the back-propagation. The back-propagation step itself, consists of adding the cumulative reward value for each subgraph/node $c(\mathcal{N}^i, e_j)$, and how many times it's received a reward $c(\mathcal{N}^i, e_j)$.

B.7 Selecting the explanatory subgraph

The explorer-navigator process is repeated through several rollouts to explore different possible subgraphs. The best explanation for the prediction e_k is the subgraph that has the highest cumulative reward and has the simplest explanation according to the sparsity threshold ($|\mathcal{R}^k| \leq N_r$ in equation 8).

B.8 Optimal explainer

The optimal explainer g^* is the minimum cross-entropy averaged over all predictions for k target events

$$g^* = \arg\min_g -\frac{1}{K}\sum_{k=1}^{K}[\mathbb{1}(Y_k = 1)\log\sigma(f(\mathcal{R}^k)[e_k]) + \mathbb{1}(Y_k = 0)\log(1 - \sigma(f(\mathcal{R}^k)[e_k]))] \tag{8}$$

$$\text{Subject to } \mathcal{R}^k = g(e_k, \mathcal{G}^k, f(\cdot)) \text{ and } \mathcal{R}^k \subseteq \mathcal{G}^k \text{ and } |\mathcal{R}^k| \leq N_r$$

where $\leq N_r$ is the hyperparameter that controls the size of $\mathcal{R}^k$.

C Experimental setup: Novel datasets

Table 7: Hyperparameters used for all models on all datasets.

Hyperparameter	**TGAT**			**TGN**		
	Real-world	**Synthetic**	**MooC**	**Real-world**	**Synthetic**	**MooC**
Hidden Dimension	172	4	4	172	4	4
Attention heads	2	2	2	2	2	2
N degree	10	10	10	10	10	10
Memory dimension	-	-	-	172	4	4
Time dimension	172	4	4	172	4	4
Node feature dimension	172	4	4	172	4	4
Edge feature dimension	172	4	4	172	4	4
Training epoch	10	100	100	10	100	100
Learning rate	$1e^{-4}$	$1e^{-4}$	$1e^{-4}$	$1e^{-4}$	$1e^{-4}$	$1e^{-4}$
Batch size	512	256	512	256	512	256
Dropout probability	0.1	0.1	0.1	0.1	0.1	0.1

The format of the MooC dataset matches the required format of real world datasets. Similar to Reddit and Wikipedia, feature normalization is applied to the dataset. For the Reddit hyperlinks dataset, the concrete preprocessing steps that are taken can be found in the Reddit_hyperlinks_preprocess.ipynb file. In summary, min-max normalization is applied to each feature column individually and the datatypes and column names are changed to match the requirements set by the author's code. Once these two steps are completed the instructions in the Read.me file provided can be used to train to T-GNNExplainer on a novel dataset.

The process.py file ensures the non-feature columns exclusively contain two node indexes, a timestamp and a label. After processing the file is saved in a subdirectory called 'processed'. Secondly, indexes ought to be generated for a real-world dataset. This is done by calling 'python tg_dataset.py -d dataset_name -c index'. The read.me file gives the wrong instruction here. This step randomly samples 500 events from the test split on which the performance of the T-GNNExplainer will be evaluated. Before T-GNNExplainer

can be trained, the GNN's (TGAT and TGN) need to be trained on the new dataset. Make sure that the hyperparameters are correctly specified in the run.sh files. For the inductive event prediction performed by the two GNN's, average precision after each epoch is outputted in the terminal. In our experimentation, the best achieved average precision is recorded (Table 8).

Once TGAT and TGN are trained on all datasets. T-GNNExplainer is ready to be trained. The final step of the Read.me provides adequate instructions. The Fidelity results are outputted in files called model_name_lownumber_to_highnumber.csv.

Table 8: Models' average precision (AP) for the inductive event prediction on all datasets. "NR" is for "Not reported".

		Wikipedia	**Reddit**	**Synthetic v1**	**Synthetic v2**	**MooC**
TGAT	New	0.971	0.982	0.945	0.953	0.626
	Old	0.979	0.975	0.963	0.964	NR
TGN	New	0.947	0.980	0.945	0.960	0.659
	Old	0.985	0.966	0.954	0.969	NR

C.1 Hyperparameter tuning

To validate the robustness of our findings, our intention was to tune the hyperparameters of the experiment as follows: 1) adjusting the learning rate of the navigator, and 2) adjusting the hyperparameter λ controlling the exploration term in the MCTS of the explorer (see equation 1). The rationale for tuning these values is that the the Explorer-Navigator framework is the key to the T-GNNExplainer, so optimizing performance in the explorer and the navigator can give further insight into their functioning.

Due to limitation in compute resources, we were unable to run this experiment.

D Complete AUFSC and Best Fid results for the original datasets

In Table 11 and Table 12 the results for the synthetic datasets, Synthetic v1 and Syntehtic v2, are presented, and in Table 9 and Table 10 the original real-world datasets results are presented.

Table 9: Best fidelity and AUFSC achieved by each explainer on Wikipedia.

	Wikipedia											
	TGAT						**TGN**					
	Best Fid			**AUFSC**			**Best Fid**			**AUFSC**		
	old	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**
ATTN	0.891	0.918	0.027	0.564	0.626	0.062	0.479	0.420	-0.059	0.073	0.205	0.132
PBONE	0.027	1.405	1.378	-2.227	1.076	3.303	0.296	0.528	**0.232**	-0.629	0.212	**0.841**
PG	1.354	0.642	-0.712	0.692	-0.653	-1.345	0.464	0.381	-0.083	-0.231	-1.419	-1.188
T-GNN	**1.836**	**1.604**	-0.232	**1.477**	**1.300**	-0.177	**0.866**	**0.789**	-0.077	**0.590**	**0.589**	-0.001

Table 10: Best fidelity and AUFSC achieved by each explainer on Reddit.

	Reddit											
	TGAT						**TGN**					
	Best Fid			**AUFSC**			**Best Fid**			**AUFSC**		
	old	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**
ATTN	0.658	0.386	-0.272	-0.654	-1.157	-0.503	0.575	0.144	-0.431	0.289	-1.546	-1.835
PBONE	0.167	1.077	**0.910**	-2.492	**0.657**	**3.149**	0.340	0.244	**-0.096**	-0.256	**-0.629**	-0.373
PG	0.804	0.506	-0.298	-0.369	-0.939	-0.570	0.679	0.117	-0.562	0.020	-2.193	-2.213
T-GNN	**1.518**	**1.180**	-0.338	**1.077**	0.630	-0.447	**1.362**	**0.251**	-1.111	**1.113**	-1.060	-2.173

Table 11: Best fidelity and AUFSC achieved by each explainer on Synthetic dataset v1.

	Synthetic v1											
	TGAT						**TGN**					
	Best Fid			**AUFSC**			**Best Fid**			**AUFSC**		
	old	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**
ATTN	0.555	0.636	0.081	0.390	0.522	0.132	2.178	1.506	-0.672	1.624	0.872	-0.752
PBONE	0.044	0.830	**0.786**	-2.882	0.708	**3.590**	0.000	1.826	**1.826**	-3.311	0.755	**4.066**
PG	0.476	0.648	0.172	-0.081	0.380	0.461	2.006	1.426	-0.580	0.626	-0.032	-0.658
T-GNN	**0.780**	**1.120**	0.340	**0.666**	**0.988**	0.322	**2.708**	**2.093**	-0.615	**2.281**	**1.743**	-0.538

Table 12: Best fidelity and AUFSC achieved by each explainer on Syntethic dataset v2.

	Synthetic v2											
	TGAT						**TGN**					
	Best Fid			**AUFSC**			**Best Fid**			**AUFSC**		
	old	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**	**old**	**new**	**delta**
ATTN	0.605	0.193	-0.412	0.291	0.061	-0.230	0.988	1.674	0.686	-0.634	-0.436	0.198
PBONE	0.096	0.328	**0.232**	-4.771	0.296	**5.067**	0.320	2.896	**2.576**	-5.413	0.189	**5.602**
PG	1.329	0.215	-1.114	-0.926	0.152	1.078	1.012	1.251	0.239	-1.338	-1.419	-0.081
T-GNN	**1.630**	**0.401**	-1.229	**1.331**	**0.380**	-0.951	**4.356**	**3.427**	-0.929	**3.224**	**2.415**	-0.809

E Findings on percentage differences for AUFSC and Best Fid on Synthetic Datasets

In Table 13 the percentage differences between best and second best explainer is shown for the two synthetic datasets.

Table 13: This shows the percentage differences between T-GNNExplainer and the best baseline xplainer for the synthetic datasets.

Percentage % difference between best and second best explainer on synthetic datasets					
		Synthetic V1		**Synthetic V2**	
Model	**Metric**	**Old**	**New**	**Old**	**New**
TGAT	Best Fid	**40.54**	34.94	**22.65**	22.26
	AUFSC	**70.77**	39.55	357.39	28.38
TGN	Best Fid	**24.33**	14.62	**330.43**	19.45
	AUFSC	**40.46**	99.89	NA	1177.78

F Suggestions for further research

In the course of our reproducibility research, we have discussed various interesting and valuable paths for extending the study on T-GNNExplainers. Here we elaborate on those different paths that could be explored in further research. We have classed our ideas into distinct subjects for clarity.

Level of explanation: T-GNNExplainer is an instance level explainer. We suggest adapting the T-GNNExplainer to be a graph level explainer (there is evidence in the code that the original authors started and abandoned this implementation).

Models: The authors claim that the T-GNNExplainer is model agnostic. This claim should be validated by testing on more temporal graph network architectures.

Baselines: The authors of the original paper have created two explainers themselves and adapted an existing one to compare to the T-GNNExplainer. In future research, it would be beneficial to compare the results to more baseline methods.

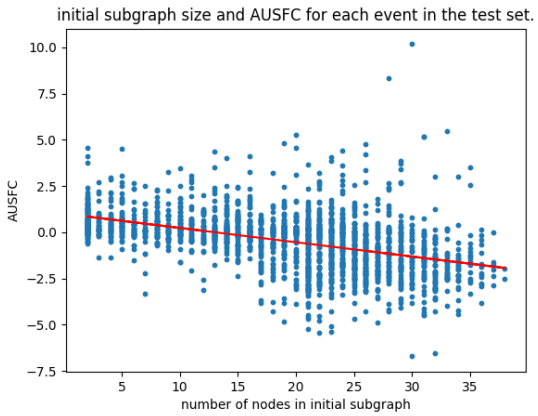
Navigator: Firstly, exploring the impact of different loss functions could solidify current choices or provide a better method. Secondly, in the current study Mutual Information is used as a comparison tool. However, experimenting with other comparison methods, like Shannon Entropy (Shannon, 1948), could contribute fairly to this subfield. Lastly, based on the input to the navigator, it appears to capture "similarity" as a proxy for importance between events. However, the paper mentions temporal importance, which should also be explored.

Explorer: This explorer uses Monte Carlo Tree Search as a base search method. As MCTS is a heuristic search method, further research could include comparing the impact of using different heuristic search-based algorithms. Other types of search-based methods, like uninformed search algorithms and local search methods, could also be explored.

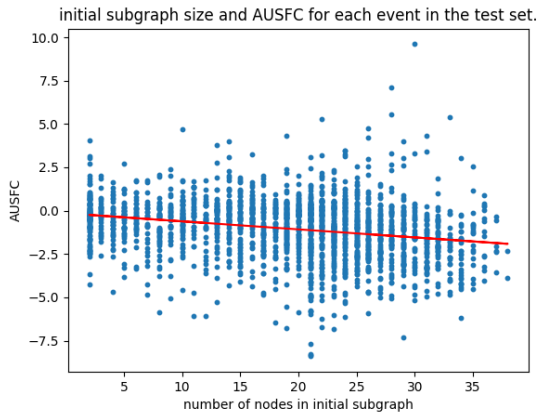
Data: In our paper we extended the study by producing and analysing results on another dataset. This dataset was similar in domain as the original two real-world datasets. For further research, we suggest exploring this more. We recommend experimenting with different feature sizes and domains, but also with the same or similar ones. Furthermore, we have not extended the paper by exploring on the synthetic datasets. We recommend using different methods to simulate datasets.

Evaluation: In the original paper the authors created the AUFSC metric. For future research, the validity of this metric should be validated. We recommend comparing with other metrics.

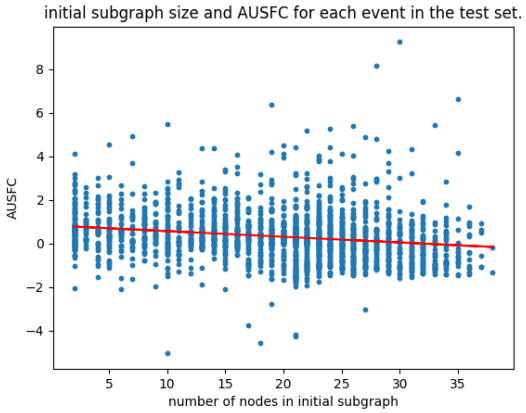
G Subgraph density analysis



(a) Explainer performance as a function of subgraph density for ATTN on reddit, wikipedia

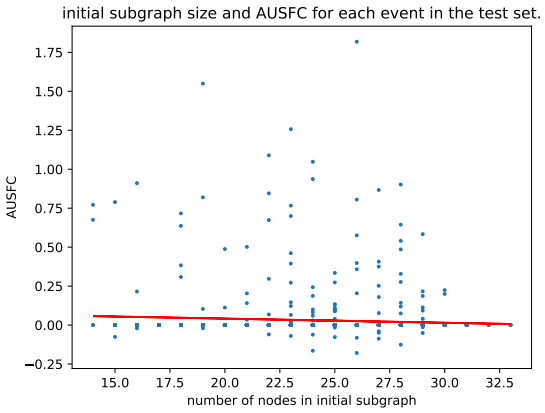


(b) Expainer performance as a function of subgraph density for PG on reddit, wikipedia

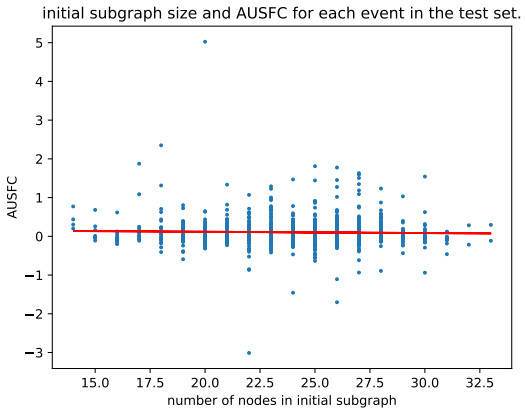


(c) Explainer performance as a function of subgraph density for PBONE on reddit, wikipedia

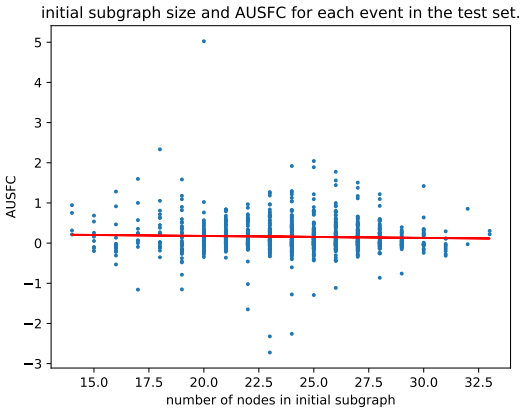
Figure 3: Supplementary results of subgraph density analysis.



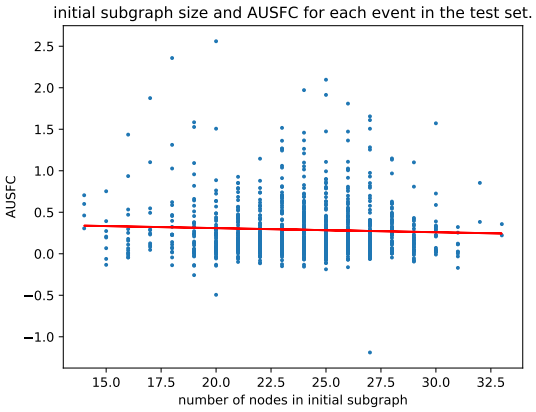
(a) Explainer performance as a function of subgraph density for TGNNExplainer on MOOC



(b) Explainer performance as a function of subgraph density for ATTN on MOOC



(c) Explainer performance as a function of subgraph density for PG on MOOC



(d) Explainer performance as a function of subgraph density for PBONE on MOOC

Figure 4: Supplementary results of subgraph density analysis.