

TIGGER: Scalable Generative Modelling for Temporal Interaction Graphs

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Abstract

There has been a recent surge in *learning* generative models for graphs. While impressive progress has been made on static graphs, work on generative modeling of *temporal* graphs is at a nascent stage with significant scope for improvement. First, existing generative models do not scale with either the time horizon or the number of nodes. Second, existing techniques are *transductive* in nature and thus do not facilitate knowledge transfer. Finally, due to their reliance on one-to-one node mapping from source to the generated graph, existing models leak node identity information and do not allow *up-scaling/down-scaling* the source graph size. In this paper, we bridge these gaps with a novel generative model called TIGGER. TIGGER derives its power through a combination of *temporal point processes* with *auto-regressive modeling* enabling both transductive and inductive variants. Through extensive experiments on real datasets, we establish TIGGER generates graphs of superior fidelity, while also being up to 3 orders of magnitude faster than the state-of-the-art.

Introduction and Related Work

Modelling and generating graphs find applications in various domains such as drug discovery (Hrinchuk, Popova, and Ginsburg 2020; Li, Zhang, and Liu 2018), anomaly detection (Ranu and Singh 2009), data augmentation (Bojchevski et al. 2018), and data privacy (Casas-Roma, Herrera-Joancomartí, and Torra 2017). Initial works on graph generative modelling relied on making prior assumptions about the graph structure. Examples include *Erdős-Rényi* (Karoński and Ruciński 1997) graphs, *small-world* models (Watts DJ 1998), and *scale-free* graphs (Albert and Barabási 2002). Recently, learning-based algorithms have been developed that circumvent this limitation (You et al. 2018; Goyal, Jain, and Ranu 2020; Hrinchuk, Popova, and Ginsburg 2020; De Cao and Kipf 2018; Liao et al. 2019). Specifically, these algorithms directly learn the underlying hidden distribution of graph structures from training data.

Unfortunately, most of the learning-based generative models are limited to static graphs. In today’s world, there is an abundance of graphs that are *temporal* in nature. Examples include financial transactions (Kumar et al. 2016; Dal Pozzolo et al. 2018), online shopping (He and McAuley

2016), community interaction graphs like Reddit (Liu, Benson, and Charikar 2019), and user behaviour networks (Yang et al. 2013). The interactions (edges) between nodes in a temporal graph are timestamped and the structure of these graphs change with time. The key challenge in generative modelling is therefore to learn the rules that govern their evolution over the time horizon (Michail 2015).

TAGGEN (Zhou et al. 2020) models temporal graphs by converting them into equivalent static graphs by combining node-ids with each of their interaction edge timestamps, and connecting only those nodes in the resulting static graph that satisfy a specified temporal neighbourhood constraint. They perform random walks on this transformed graph, which are then modified using heuristic local operations to generate many synthetic random walks. Finally, the synthetic random walks that are classified by a discriminator as real random walks are collected and combined to construct the generated temporal graph. More recently, DYMOND (Zeno, La Fond, and Neville 2021) presented a non-neural, 3-node motif based approach for the same problem. They assume that each type of motif follows a time-independent exponentially distributed arrival rate and learn the parameters to fit the observed arrival rate.

These approaches suffer from the following limitations:

- **Weak Temporal Modelling:** DYMOND makes two key assumptions: first, the arrival rate of motifs is exponential; and second, the structural configuration of a motif remains the same throughout the time horizon being modeled on. Both these assumptions do not hold in practice – motifs themselves may evolve with time and could arrive with time-dependent rates. This leads to poor fidelity of structural and temporal properties of the generated graph. TAGGEN, on the other hand, does not model the graph evolution rate explicitly. It assumes that the timestamps in the input graph are discrete random variables prohibiting TAGGEN from generating new(unseen in source graph) timestamps. More critically, the generated graph duplicates a large portion of edges from the source graph – our experiments found upto 80% edge overlap between the generated and the source graph. While the design choices of TAGGEN generate graphs that exhibit high fidelity of graph structural and temporal interaction properties, unfortunately it achieves them by generating graphs that are largely indistinguishable from the source graph due to their poor modelling of interaction times.

- **Poor Scalability to Large Graphs:** Both TAGGEN and DYMOND are limited to graphs where the number of nodes are less than ≈ 10000 and the number of unique timestamps are below ≈ 200 . However, real graphs are not only of much larger size, but also grow with significantly high interaction frequency (Paranjape, Benson, and Leskovec 2017). In such scenarios, the key design choice of TAGGEN to convert the temporal graph into a static graph, fails to scale to long time horizons since the number of nodes in the resulting static graph multiplies linearly with the number of timestamps. Further, TAGGEN also requires the computation of the inverse of an $N' \times N'$ matrix, where N' is the number of nodes in the equivalent static graph to impute node-node similarity. This leads to the quadratic increase in memory consumption and even higher cost of matrix inversion, thus making TAGGEN not scalable. On the other hand, DYMOND has an $O(N^3T)$ complexity, where N is the number of nodes and T is the number of timestamps. In contrast, the complexity of the algorithm we propose is in $O(NM)$ for a graph with N nodes and M timestamped edges, and is independent of the time horizon length.

- **Lack of Inductive Modelling:** Inductivity allows transfer of knowledge to unseen graphs (Hamilton, Ying, and Leskovec 2017). In the context of graph generative modelling, inductive modelling is required to (1) upscale or downscale the source graph to a generated graph of a different size, and (2) prevent leakage of node-identity from the source graph. Both TAGGEN and DYMOND rely on one-to-one mapping from source graph node ids to the generated graph and hence are non-inductive.

Contributions: The proposed generative model, TIGGER (Temporal Interaction Graph GEneRator), addresses the above mentioned gaps in existing literature through the following novel contributions:

- **Assumption-free Modelling:** We utilize *intensity-free temporal point processes* (TPP) TPPs (Shchur, Biloš, and Günnemann 2020) to jointly model the underlying distribution of node interactions and their timestamps through *temporal random walks*. Our modelling of time is *assumption-free* as we fit a *continuous* distribution over time. This allows TIGGER to generate timestamps that were not even present in the input graph. Moreover, this empowers TIGGER to sample interaction graphs for future-timestamps. Thus, TIGGER is capable of up-sampling/down-sampling in the temporal dimension.
- **Inductive Modelling:** TIGGER supports inductive modelling through a novel *multi-mode decoder* that learns the distribution over node embeddings instead of learning distribution over node IDs. In addition, through the usage of a WGAN (Arjovsky, Chintala, and Bottou 2017), we support up-sampling/down-sampling of generated graph size. Thus, in contrast to DYMOND and TAGGEN, TIGGER is capable of generating graphs of arbitrary sizes without leaking information from the source graph – potentially useful in many privacy-sensitive applications.
- **Large-scale Empirical Evaluation:** Extensive evaluation over five large, real temporal graphs with up to millions of timestamps comprehensively establishes that TIGGER breaks new ground in terms of its scalability, while also

ensuring superior fidelity of structural and temporal properties of the generated graph.

Problem Formulation

Definition 1 (Temporal Interaction Graph). A *temporal interaction graph* is defined as $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where \mathcal{V} is a set of N nodes and \mathcal{E} is a set of M temporal edges $\{(u, v, t) \mid u, v \in \mathcal{V}, t \in [0, T]\}$. T is the maximum time of interaction.

Problem 1 (Temporal Interaction Graph Generator).

Input: A temporal interaction graph \mathcal{G} .

Output: Let there be a hidden joint distribution of structural and temporal properties from which given \mathcal{G} has been sampled. Our goal is to learn this hidden distribution. Towards that end, we want to learn a generative model $p(\mathcal{G})$ that maximizes the likelihood of generating \mathcal{G} . This generative model, in turn, can be used to generate new graphs that come from the same distribution as \mathcal{G} , but not \mathcal{G} itself.

The above problem formulation is motivated by the *one-shot generative modelling* paradigm i.e., it only requires one temporal graph \mathcal{G} to learn the hidden *joint* distribution of structural and temporal interaction graph properties. Defining the joint distribution of temporal and structural properties is hard. In general, these properties are characterized by inter-interaction time distribution and evolution of static graph properties like degree distribution, power law exponent, no. of connected components, largest connected component, distribution of pair wise shortest distances, closeness centrality etc. Typically, a generative model optimizes over one of these properties under the assumption that the remaining properties are correlated and hence would be implicitly modeled. For example, DYMOND uses small structural motifs and TAGGEN uses random walks over the transformed static graph. In our work, we perform *temporal random walks*, which are then modeled using *point processes*.

TIGGER

Fig. 1 presents the pipeline of TIGGER. Given a source graph, we decompose it through temporal random walks. These random walks are modeled using a recurrent generative neural model. Once the model is trained, it is used to generate synthetic temporal random walks, which are finally merged to form the generated temporal interaction graph. We next formalize each of these sub-steps.

Training Data: Temporal Random Walks

Definition 2 (Temporal Neighborhood). The *temporal neighbourhood* of a node v at time t contains all edges with a higher time stamp. Formally,

$$\mathcal{N}_t(v) = \{e \mid e = (v, u, t') \in \mathcal{E} \wedge t < t'\}$$

Definition 3 (Temporal Random Walk). Given a node v and time t , an ℓ -length temporal random walk starts from v and takes ℓ jumps through an edge in the temporal neighborhood of the current node. More formally, it is a sequence of tuples $S = \{s_1, \dots, s_\ell\}$, where each tuple $s \in S$ is a $(node, time)$ pair such that, $s_1 = (v, t)$ and $\forall i \in [2, \ell]$ the edge $(s_{i-1}.v, s_i.v, s_i.t) \in \mathcal{N}_{s_{i-1}.t}(s_{i-1}.v)$. A walk ends after taking ℓ jumps or if $\mathcal{N}_{s_{i-1}.t}(s_{i-1}.v) = \emptyset$.

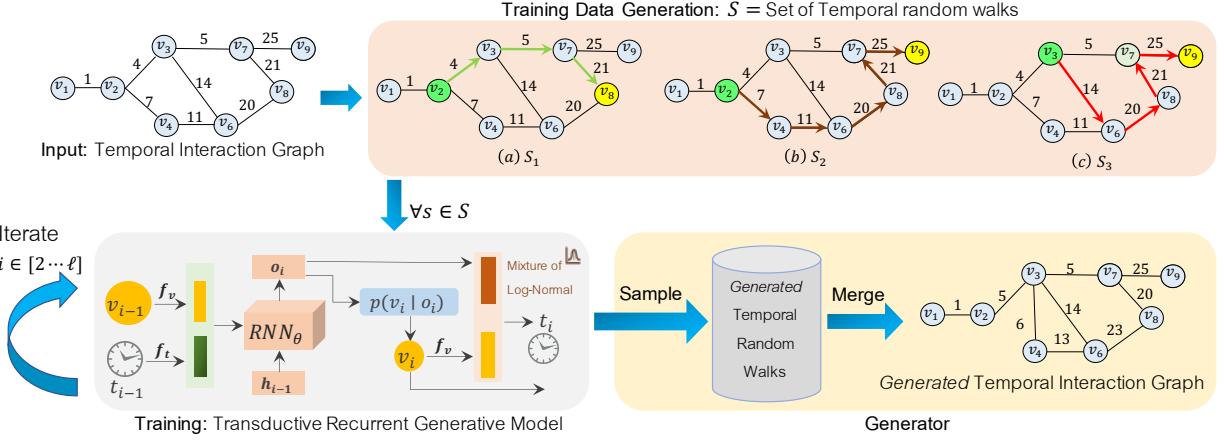


Figure 1: Pipeline of TIGGER in transductive modelling. The highlighted nodes in the Training Data Generation component indicates the start (green) and the ending nodes (yellow) of random walks for different length ℓ .

Since each jump is constrained to edges within the temporal neighborhood, it is guaranteed that $s_i.t > s_{i-1}.t$. To capture the temporal characteristics, the probability of jumping through edge $e \in \mathcal{N}_{s_i,t}(s_i, v)$ decreases exponentially with time gap from (s_i, t) . More formally,

$$p(e = (s_i.v, u, t) | s_i) = \frac{\exp(s_i.t - t)}{\sum_{e' = (s_i.v, u', t') \in \mathcal{N}_{s_i,t}(s_i, v)} \exp(s_i.t - t')}$$

Note that $s_i.t < t$ and hence a smaller gap leads to increased chances of being sampled. While we exponentiate the time gap, other functions, such as linear, may also be used. We use exponentiation due to superior empirical results. A random walk starts from an edge chosen uniformly at random. Examples of temporal random walks are shown in the Data Generation component of Fig. 1.

In Table 3 in appendix, we summarise all the notations used in our work. As per convention, we use boldface symbols to denote learnable vectors and weight matrices.

Modelling Temporal Random Walks

We train a generative model $p(\mathcal{S})$ on a set \mathcal{S} of temporal random walks. Formally,

$$p(\mathcal{S}) = \prod_{S \in \mathcal{S}} p(S)$$

where, $p(S) = p(s_1, \dots, s_\ell)$ (1)

Owing to the *auto-regressive* nature of a sequence, we express $p(S)$ as the product of the conditionals.

$$p(S) = p(s_1) \prod_{i=2}^{\ell} p(s_i | (s_1, \dots, s_{i-1}))$$

We simplify this conditional by decomposing as follows.

$$p(S) = p(s_1) \prod_{i=2}^{\ell} p(s_i.v | (s_1, \dots, s_{i-1})) \quad (2)$$

$$\times p(s_i.t | (s_i.v, (s_1, \dots, s_{i-1}))) \quad (3)$$

To learn the above conditional distribution, we utilize a *recurrent neural network (RNN)* based generator. Formally,

$$\mathbf{h}_i = rnn_{\theta}^{hidden}(\mathbf{h}_1, (s_1, \dots, s_{i-1})) = rnn_{\theta}^{hidden}(\mathbf{h}_{i-1}, s_{i-1})$$

$$\mathbf{o}_i = rnn_{\theta}^{output}(\mathbf{h}_1, (s_1, \dots, s_{i-1})) = rnn_{\theta}^{output}(\mathbf{h}_{i-1}, s_{i-1})$$

Here, $rnn_{\theta}^{output}(\mathbf{h}_{i-1}, x)$ is the output of RNN cell and $rnn_{\theta}^{hidden}(\mathbf{h}_{i-1}, x)$ is the updated hidden state. Both \mathbf{h}_i and \mathbf{o}_i are vectors and we initialize $\mathbf{h}_1 = \mathbf{0}$. Semantically, \mathbf{o}_i captures the *prior* to predict the next node v_i in the temporal random walk. More formally, $p(S)$ in Eq. 3 is re-written as:

$$p(S) = p(s_1) \prod_{i=2}^{\ell} p(s_i.v | \mathbf{o}_i) * p(s_i.t | s_i.v, \mathbf{o}_i) \quad (4)$$

In the following sections, we discuss the internals of the RNN, and formulate how exactly Eq. 4 is learned. We develop two procedures: first is a transductive learning algorithm, and the second is an inductive model.

Transductive Recurrent Generative Model: Given a sequence of node and time pairs s_1, \dots, s_ℓ , we transform $s_i.v$ and $s_i.t$ to vector representations $\mathbf{f}_v(s_i.v) \in \mathcal{R}^{dv}$, $\mathbf{f}_t(s_i.t) \in \mathcal{R}^{dt}$ respectively.

First, we transform the node ids to a vector using $\mathbf{f}_v(v) = \mathbf{W}_v \mathbf{v}$ where $\mathbf{W}_v \in \mathcal{R}^{dv} * \mathcal{R}^N$ is a learnable weight matrix and $\mathbf{v} \in \mathcal{R}^{1 \times N}$ is *one-hot encoding* of the node ID of v . Next, to learn vector representation of time $t \in \mathcal{R}$, we use following TIME2VEC (Kazemi et al. 2019) transformation.

$$\mathbf{f}_t(t)[r] = \begin{cases} \omega_r \cdot t + \zeta_r, & \text{if } r = 0 \\ \sin(\omega_r \cdot t + \zeta_r), & 1 \leq r < d_T \end{cases} \quad (5)$$

where $\omega_1, \omega_2, \dots, \omega_{d_T}, \zeta_1, \zeta_2, \dots, \zeta_{d_T} \in \mathcal{R}$ are trainable weights and shared across each pair of the input sequence. r is the index of $\mathbf{f}_t(t)$. After embedding both $s_{i-1}.v$ and $s_{i-1}.t$, we concatenate them resulting in a vector of \mathcal{R}^{dv+dt} dimension. This vector is fed into the RNN cell along with \mathbf{h}_{i-1} which outputs \mathbf{o}_i and \mathbf{h}_i . We represent $p(s_i.v | \mathbf{o}_i)$ in Eq. 4 as multinomial distribution over $v \in \mathcal{V}$ parameterized by θ_v .

$$\begin{aligned} p(s_i.v = v | \mathbf{o}_i) &= \theta_v(\mathbf{o}_i) \\ &= \theta_v(rnn_{\theta}^{output}(\mathbf{h}_{i-1}, (s_{i-1}.v, s_{i-1}.t))) \\ &= \theta_v(rnn_{\theta}^{output}(\mathbf{h}_{i-1}, (\mathbf{f}_v(s_{i-1}.v) \| \mathbf{f}_t(s_{i-1}.t)))) \\ &= \frac{\exp(\mathbf{W}_v^O \mathbf{o}_i)}{\sum_{\forall u \in \mathcal{V}} \exp(\mathbf{W}_u^O \mathbf{o}_i)} \end{aligned} \quad (6)$$

where $\mathbf{W}_v^O \in \mathcal{R}^{1 \times d_O}$, $\forall v \in \mathcal{V}$ is a node-specific learnable weight vector. d_O is the dimension of o_i .

Temporal point processes (TPP) are de-facto models for modelling distributions of continuous, inter-event time over discrete events in event sequences $\{(e_0, t_0), (e_1, t_1) \dots (e_n, t_n)\}$. TPPs are generally defined using *conditional intensity function* $\lambda(t)$.

$$\lambda(t) = \frac{p(t \mid \mathbf{H}_{t_n})}{1 - F(t \mid \mathbf{H}_{t_n})}$$

Here, $p(t \mid \mathbf{H}_{t_n})$ is the probability distribution of next event time t after observing events till time t_n . $F(t)$ is the cumulative probability distribution corresponding to p . \mathbf{H}_{t_n} is the summary of events till time t_n . $\lambda(t)$ is the expected number of events around infinitesimal interval $[t, t + dt]$ given the history before t . It results in following probability distribution p for next event time (Rizo et al. 2017).

$$p(t \mid \mathbf{H}_{t_n}) = \lambda(t) \exp\left(-\int_{t_n}^{\infty} \lambda(x) dx\right)$$

Resulting log likelihood contains integral due to $p(t)$ which needs to be estimated using *Monte-Carlo sampling* (Mei and Eisner 2017) leading to high variance, unstable updates during training and high computation cost (Omi, Ueda, and Aihara 2019). Motivated by strong performance on event time prediction task by (Shchur, Biloš, and Günnemann 2020), we adopt their TPP formulation, which directly defines $p(t)$ as mixture of *log normal* distribution instead of deriving it from $\lambda(t)$. From Eq. 4,

$$\begin{aligned} p(s_i.t \mid s_i.v, \mathbf{o}_i) &= p(s_i.t - s_{i-1}.t \mid s_i.v, \mathbf{o}_i) \\ &= \theta_t(\Delta t \mid s_i.v, \mathbf{o}_i) \\ &= \sum_{c=1}^C \phi_c^C \frac{1}{\Delta t \sigma_c^C \sqrt{2\pi}} \exp\left(-\frac{(\log \Delta t - \mu_c^C)^2}{2(\sigma_c^C)^2}\right) \end{aligned} \quad (7)$$

where Δt is time difference between s_i and s_{i-1} , $p(t)$ is parameterized by θ_t and $\mu_c^C, \sigma_c^C, \phi_c^C$ are parameters of θ_t .

$$\begin{aligned} \mu_c^C &= \mathbf{W}_c^{\mu C}(f_v(s_i.v) \parallel \mathbf{o}_i), \quad \sigma_c^C = \exp(\mathbf{W}_c^{\sigma C}(f_v(s_i.v) \parallel \mathbf{o}_i)) \\ \phi_c^C &= \frac{\exp(\mathbf{W}_c^{\phi C}(f_v(s_i.v) \parallel \mathbf{o}_i))}{\sum_{j=1}^C \exp(\mathbf{W}_j^{\phi C}(f_v(s_i.v) \parallel \mathbf{o}_i))} \end{aligned}$$

Moreover, C is no. of components in the *log normal* mixture distribution and $\mathbf{W}_c^{\mu C}, \mathbf{W}_c^{\sigma C}, \mathbf{W}_c^{\phi C} \in \mathcal{R}^{(d_V+d_O)}$, $\forall c \in \{1..C\}$. Note that every components' learnable weights are shared across each time-stamp in the sequence.

Training loss: The loss over the set \mathcal{S} of temporal random walks is derived from Eqs. 1, 4, 6 and 7. Specifically,

$$\begin{aligned} \mathcal{L} &= -\log(p(\mathcal{S})) = -\sum_{S \in \mathcal{S}} \log(p(S)) \\ &= -\sum_{S \in \mathcal{S}} \log p(s_1) \sum_{i=2}^{\ell} (\log(p(s_i.v \mid \mathbf{o}_i) \\ &\quad + \log(p(s_i.t \mid s_i.v, \mathbf{o}_i)))) \end{aligned}$$

In the above loss function, $p(s_1) = 1/|\mathcal{E}|$ since the first edge is chosen uniformly at random. $p(s_i.v \mid \mathbf{o}_i)$ and $p(s_i.t \mid s_i.v, \mathbf{o}_i)$ are computed using Eq. 6 and Eq. 7 respectively. A pictorial summary of the training process is available in the training component of Fig. 1.

Inductive Recurrent Generative Model: The primary distinction between transductive and inductive generative models are the construction of node representation and the procedure of learning next node distribution given the past information in the sequence. In the transductive model, a node is represented by its ID $\in \{1, \dots, N\}$ in the form of a one-hot vector. In the inductive model, we use a *Graph Convolution Network (GCN)* to embed nodes.

Node Representations: We first transform the input temporal graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ to a static graph $\mathcal{G}^{static} = (\mathcal{V}, \mathcal{E}^{static})$, where $\mathcal{E}^{static} = \{(u, v) \mid \exists(u, v, t) \in \mathcal{E}\}$. On \mathcal{G}^{static} , we utilize GRAPH SAGE (Hamilton, Ying, and Leskovec 2017) to learn *unsupervised* structural node representations. Details can be found in the appendix.

We denote embedding of node v as $\mathbf{v} \in \mathcal{R}^{d_V}$. Given a temporal walk sequence $S = (s_1, \dots, s_\ell)$, we replace $s_i.v$ with $s_i.v \forall i \in \{1, \dots, \ell\}$. Similar to the transductive variant, in order to learn $p(s_i \mid s_1, \dots, s_{i-1})$, each $s_{i-1}.v$ and $s_{i-1}.t$ is transformed using $\mathbf{f}_v(s_{i-1}.v) = \mathbf{W}s_{i-1}.v$ where $\mathbf{W} \in \mathcal{R}^{d_V} \times \mathcal{R}^{d_V}$ and \mathbf{f}_t using Eq. 5. Both $\mathbf{f}_v(s_{i-1}.v)$ and $\mathbf{f}_t(s_{i-1}.t)$ are concatenated, which is fed into the RNN cell along with the previous hidden state \mathbf{h}_{i-1} . The RNN outputs $\mathbf{o}_i \in \mathcal{R}^{d_O}$ and $\mathbf{h}_i \in \mathcal{R}^{d_H}$. These steps are the same as in the transductive variant.

Multi-mode node embedding decoder: Owing to working with node embeddings, the objective of the RNN is to predict the next node embedding instead of a node ID (in addition to the timestamp). Towards that end, we develop a multi-mode node embedding decoder. Fig. 2 presents the internals. The decoder has three distinct semantic phases. We explain them below.

We first note that node embeddings of a graph may not follow a uni-modal distribution since real-world graphs are known to have communities. The presence of communities would create a multi-modal distribution (Hamilton, Ying, and Leskovec 2017). To model this distribution, we perform K -means clustering on the node embeddings; each cluster would correspond to a community. The appropriate value of K may be learned using any of the established mechanisms (Han, Pei, and Kamber 2011). Next, we design a *multi-mode decoder* that operates in two steps: first, it predicts the cluster that the next node embedding belongs to, and then predicts the node embedding from that cluster.

Formally, we would like to learn probability distribution $p(k_i = k \mid \mathbf{o}_i)$, where k_i denotes the cluster membership of next node $s_i.v$ and $k \in [1, \dots, K]$. From this distribution, k_i is sampled. Given cluster k_i , we next sample a vector \mathbf{z} from $p(\mathbf{z} \mid \mathbf{o}_i, k_i)$. Then, $s_i.v$ is sampled from $p(s_i.v \mid \mathbf{z})$. Since, we need to learn the distribution of $s_i.v$ given \mathbf{o}_i and k_i , we introduce a latent random variable \mathbf{z} in the multi-mode decoder. Mathematically,

$$\begin{aligned} p(s_i.v \mid \mathbf{o}_i) &= p(k_i \mid \mathbf{o}_i) \int_{\mathbf{z}} p(\mathbf{z} \mid \mathbf{o}_i, k_i) p(s_i.v \mid \mathbf{z}) d\mathbf{z} \\ &= p(k_i \mid \mathbf{o}_i) \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z} \mid \mathbf{o}_i, k_i)} [p(s_i.v \mid \mathbf{z})] \end{aligned} \quad (8)$$

where,

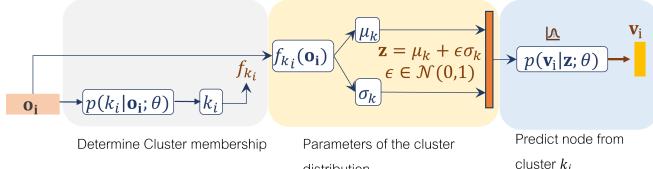


Figure 2: Multi-mode decoder

$$\begin{aligned}
 p(k_i | \mathbf{o}_i) &= \theta_k(\mathbf{o}_i) = \frac{\exp(\mathbf{W}_k^K \mathbf{o}_i)}{\sum_{j=1}^K \exp(\mathbf{W}_j^K \mathbf{o}_i)} \\
 p(\mathbf{z} | \mathbf{o}_i, k_i) &= \mathcal{N}(\mu_{k_i}^K, (\sigma_{k_i}^K)^2) \\
 p(s_i, \mathbf{v} | \mathbf{z}) &= \mathcal{N}(\mu^Z, (\sigma^Z)^2) \\
 \mu_{k_i}^K &= \mathbf{W}_{k_i}^{\mu K} \mathbf{o}_i \quad \sigma_{k_i}^K = \exp(\mathbf{W}_{k_i}^{\sigma K} \mathbf{o}_i) \\
 \mu^Z &= \mathbf{W}^{\mu Z} \mathbf{z} \quad \sigma^Z = \exp(\mathbf{W}^{\sigma Z} \mathbf{z})
 \end{aligned} \tag{9}$$

where $\mathbf{z} \in \mathcal{R}^{dz}$, $\mu_k^K, \sigma_k^K, \mu^Z, \sigma^Z \in \mathcal{R}^{dz}$, $\mathbf{W}^{\mu Z}, \mathbf{W}^{\sigma Z} \in \mathcal{R}^{dz} \times \mathcal{R}^{do}$, $\mathbf{W}_k^{\mu K}, \mathbf{W}_k^{\sigma K} \in \mathcal{R}^{dz} \times \mathcal{R}^{dz}$, $\mathbf{W}_k^K \in \mathcal{R}^{1*do}$ $\forall k \in \{1..K\}$.

We approximate the \mathbb{E} term in Eq. 8 using the reparameterization trick from the auto-encoding *variational bayes* approach (Kingma and Welling 2014) by defining a deterministic function g to represent $\mathbf{z} \sim p(\mathbf{z} | \mathbf{o}_i, k_i)$ as follows:

$$\begin{aligned}
 \mathbf{z} &= g(\mu_{k_i}^K, \sigma_{k_i}^K, \varepsilon) = \mu_{k_i}^K + \varepsilon \sigma_{k_i}^K \quad \varepsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{1}) \\
 \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z} | \mathbf{o}_i, k_i)} [p(s_i, \mathbf{v} | \mathbf{z})] &= \mathbb{E}_{\varepsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{1})} [p(s_i, \mathbf{v} | g(\mu_{k_i}^K, \sigma_{k_i}^K, \varepsilon))] \\
 &\simeq \frac{1}{L} \sum_{j=1}^{j=L} p(s_i, \mathbf{v} | g(\mu_{k_i}^K, \sigma_{k_i}^K, \varepsilon_j)) \quad \varepsilon_j \sim \mathcal{N}(\mathbf{0}, \mathbf{1})
 \end{aligned} \tag{10}$$

Taking the logarithm of Eq. 8, substituting the expectation term using Eq. 10, and assuming $L=1^1$, we get the following:

$$\log p(s_i, \mathbf{v} | \mathbf{o}_i) \simeq \log p(k_i | \mathbf{o}_i) + \log p(s_i, \mathbf{v} | g(\mu_{k_i}^K, \sigma_{k_i}^K, \varepsilon)) \tag{11}$$

$p(s_i, t | s_i, \mathbf{v}, \mathbf{o}_i)$ is modelled the same as Eq. 7 except $\mathbf{f}_v(s_i, \mathbf{v})$, which is replaced by $\mathbf{f}_v(s_i, \mathbf{v})$ where s_i, \mathbf{v} is the vector representation of node s_i, \mathbf{v} .

Training loss is derived from Eqs. 1, 4, 7 and 11 by substituting the log-probabilities below:

$$\begin{aligned}
 \mathcal{L} &\simeq - \sum_{s \in S} \log p(s_1) \sum_{i=2}^{\ell} (\log p(s_i, \mathbf{v} | \mathbf{o}_i) + \log p(s_i, t | s_i, \mathbf{v}, \mathbf{o}_i) \\
 &\quad - \beta \mathcal{D}_{kl}(p(\mathbf{z} | \mathbf{o}_i, k_i) || \mathcal{N}(\mathbf{0}, \mathbf{1}))),
 \end{aligned}$$

where \mathcal{D}_{kl} is KL-Divergence. Empirical observations indicate that adding the regularizer on $p(\mathbf{z})$ helps in reducing over-fitting. Thus, we have added the KL distance regularization on $p(\mathbf{z})$ to restrict its sample space near to the distribution $\mathcal{N}(\mathbf{0}, \mathbf{1})$. Here $\beta \in (0, 1)$ is a hyper parameter, which decides the weightage of the regularizer term. \mathcal{L} is then used to learn the model parameters $\mathbf{W}, \mathbf{W}_k^{\mu K}, \mathbf{W}_k^{\sigma K} \forall k \in \{1 \dots K\}$, $\mathbf{W}^{\mu Z}, \mathbf{W}^{\sigma Z}$ and parameters of $\mathbf{f}_t, \mathbf{f}_v, rnn_{\theta}$.

¹Motivated by (Kingma and Welling 2014), which shows state-of-the-art empirical results on image generation tasks using L=1

Algorithm 1: Sampling synthetic temporal random walks from a trained transductive recurrent generative model

```

Require:  $S_1, \mathbf{f}_v, \mathbf{f}_t, rnn_{\theta}, \theta_v \forall v \in \mathcal{V}, \theta_t, \ell'$ 
Ensure: Synthetic temporal random walks  $\mathcal{S}'$ 
1:  $S' = \{\}$ 
2: for  $s_1 \in S_1$  do
3:    $S' \leftarrow \{\}, (v_1, t_1) \leftarrow s_1, \mathbf{h}_1 \leftarrow \mathbf{0}$ 
4:   for  $i \in \{2, 3 \dots \ell'\}$  do
5:      $\mathbf{o}_i, \mathbf{h}_i \leftarrow rnn_{\theta}(\mathbf{h}_{i-1}, (\mathbf{f}_v(v_{i-1}) \parallel \mathbf{f}_t(t_{i-1})))$ 
6:      $v_i \sim \text{Multinomial}(\theta_{v_1}(o_i), \theta_{v_2}(o_i) \dots \theta_{v_N}(o_i))$  {Sample next node}
7:      $\Delta t \sim \theta_t(t - t_{i-1} | v_i, o_i)$  {Sample next time using eq. 12}
8:      $t_i \leftarrow t_{i-1} + \Delta t$ 
9:      $S' = S' + (v_{i-1}, v_i, t_i)$ 
10:   end for
11:    $\mathcal{S}' = \mathcal{S}' + S'$ 
12: end for
13: Return  $\mathcal{S}'$ 

```

Generating Interaction Graphs

Once the recurrent generative model is trained over the collection \mathcal{S} , we sample synthetic temporal random walks \mathcal{S}' from the trained model. This synthetic collection is then assembled to form the synthetic temporal graph \mathcal{G}' . Similar to (Zhou et al. 2020), from each sequence $S \in \mathcal{S}$, we store the first item s_1 and denote S_1 as the collection of s_1 .

Transductive model: Alg. 1 explains method to sample synthetic temporal random walks using transductive variant of TIGGER. Specifically, in Alg. 1, Δt in line 7 is sampled using below equation (Shchur, Biloš, and Günnemann 2020).

$$\begin{aligned}
 \phi &\sim \text{Categorical}(\{\phi_1^C \dots \phi_C^C\}) \\
 \Delta t &= \exp((\boldsymbol{\sigma}^C)^T \phi \varepsilon + (\boldsymbol{\mu}^C)^T \phi) \quad \varepsilon \sim \mathcal{N}(0, 1)
 \end{aligned} \tag{12}$$

Where $\boldsymbol{\mu}^C = (\mu_1^C \dots \mu_C^C)$ and $\boldsymbol{\sigma}^C = (\sigma_1^C \dots \sigma_C^C)$ and ϕ is one-hot vector of size C .

After collecting synthetic temporal random walks \mathcal{S}' , we assemble them by maintaining the same edge density as in the original graph within time range $t \in [1, T]$. First, we count the frequency of each temporal occurrence in the synthetic random walks. We denote this as $\alpha(v_i, v_j, t)$, i.e. the frequency of occurrence of node pair (v_i, v_j) at time t in \mathcal{S}' . We denote the set of edges present at time t in \mathcal{S}' as \tilde{E}^t . Now, for each uniquely sampled time stamp $t \in [1, T]$, we define the distribution of occurrence on node pairs present at time t in synthetic temporal random walks \mathcal{S}' as follows:

$$p_{v_i, v_j}^t = \frac{\alpha(v_i, v_j, t)}{\sum_{e=(u_i, u_j) \in \tilde{E}^t} \alpha(u_i, u_j, t)} \tag{13}$$

From this distribution, we keep sampling edges till the edge density of the synthetic graph is same as original graph in the temporal dimension.

Inductive model: Sampling from the inductive version follows a similar pipeline as in the transductive variant; the only difference is the presence of an additional step of mapping the generated node embeddings in the synthetic random walks \mathcal{S}' to nodes $v \in \mathcal{G}'$ where $\mathcal{G}' = (\mathcal{V}', \mathcal{E}')$, $|\mathcal{V}'| = N'$, $|\mathcal{E}'| = M'$. \mathcal{G}' is the generated temporal graph. Note that N' and M' are different from the source graph sizes,

and hence allows control over the generated graph size. The pseudocode is provided in Alg. 2 in appendix. First, we train a WGAN (Arjovsky, Chintala, and Bottou 2017) generative model on node embeddings obtained from \mathcal{G}^{static} (Ji et al. 2021). From the trained WGAN model, we sample N' node embeddings to construct \mathcal{V}' . Finally, we match each embedding in S' to its closest node in \mathcal{V}' using cosine similarity.

Theorem 1. *The computation complexities of generating a temporal interaction graph $\mathcal{G}' = (\mathcal{V}', \mathcal{E}')$ through the transductive and inductive versions are $\approx O(M \times \ell' \times (N + C))$ and $\approx O(M \times \ell' \times (K + C + N'))$ respectively.*

PROOF. Provided in Appendix.

Experiments

In this section, we benchmark TIGGER against DYMOND and TAGGEN and establish that it (1) it is up to 2000 times faster, (2) breaks new ground on scalability against number of timestamps, and (3) generates graphs of high fidelity. Our codebase and datasets are available at <https://github.com/data-iitd/tigger>.

Experimental Setup

Datasets: For our empirical evaluation, we use the publicly available datasets listed in Table 1. Columns 2 to 4 of Table 1 summarize the sizes of the temporal interaction graphs. Our datasets span various domains including message exchange platform (**UC Irvine**) (Kunegis 2013a), financial network (**Bitcoin**) (Kumar et al. 2016), communication forum (**Reddit**) (Leskovec and Krevl 2014), shopping (**Ta-feng**) (Bai et al. 2018), and Wikipedia edits (**Wiki**) (Leskovec and Krevl 2014). Further details are provided in Table 5 in appendix. Since DYMOND and TAGGEN do not scale to graphs with large number of timestamps, we sample a smaller subset of Wiki by considering only the first 50 hours. This dataset is denoted as **Wiki-Small**. **Baselines and Training:** We benchmark the performance of TIGGER against DYMOND and TAGGEN. For TIGGER, we denote the inductive version as TIGGER-I. To allow uniform comparison, in TIGGER-I, we generate graph of the same size as the source. For both TAGGEN and DYMOND, we use the code shared by authors. For all algorithms, the entire input graph is used for training and a single synthetic graph is generated. Parameter details along with machine configuration are provided in the appendix.

Evaluation metrics: The performance of a generative model is satisfactory if (1) it runs fast, (2) generates graphs with similar properties as in the source, (3) but without duplicating the source itself. To quantify these three objectives, we utilize the following metrics.

- **Efficiency:** Efficiency is measured through running time of the graph generation component.
- **Fidelity:** To quantify preservation of original graph properties, we compare various graph statistics of the *snapshots* of original graph \mathcal{G}_t and synthetic graph \mathcal{G}'_t for each unique timestamp $t \in \{1 \dots T\}$. We use the following graph statistics (Kunegis 2013b): (i) mean degree, (ii) wedge count, (iii) triangle count, (iv) power law exponent of degree distribution (PLE), (v) relative edge distribution entropy, (vi) largest connected component size (LCC),

(vii) number of components (NC), (viii) global clustering coefficient (CF), (ix) mean betweenness centrality (BC), (x) mean closeness centrality (CC). We explain these metrics in Table 6 in appendix. The *error* with respect to a given graph statistic P is quantified as the *median absolute error*, that is, $Median_{t \in [1 \dots T]} |P(\mathcal{G}_t) - P(\mathcal{G}'_t)|$. We use median instead of mean to reduce the impact of outliers. Nonetheless, the mean absolute errors (MAE) are also reported in the appendix.

- **Duplication:** To capture the level of duplication, we compute the percentage of overlapping edges, i.e., $\frac{|\mathcal{E} \cap \mathcal{E}'|}{|\mathcal{E}|} \times 100$. Measuring duplication is important since an algorithm that duplicates the source graph would obtain perfect scores with respect to property preservation, although the generated graph is of limited use. We note that duplication has not been studied by TAGGEN or DYMOND.

Transductive: Comparison against Baselines

Table 1 presents the performance of all transductive algorithms across all metrics. We summarize the key observations below.

Efficiency and Scalability: TIGGER is by far the most efficient of all models, while DYMOND is the slowest due to its $O(N^3T)$ time complexity. TAGGEN is nearly 2 orders slower than TIGGER. In the inference phase, TAGGEN samples paths from the original graph, uses heuristics to modify these paths and then employs a discriminator to select from the generated paths. This process is prohibitively slow. Additionally, TAGGEN performs an expensive inversion of $N' \times N'$ matrix where N' is number of unique pairs of nodes and their interaction timestamps in \mathcal{G} . Consequently, TAGGEN fails to scale on Wiki and Reddit with millions of timestamps, and on Ta-feng which has much larger node and edge sets (see Table 1). Note that DYMOND fails to complete in all but Wiki-Small, the smallest dataset. TIGGER on the other hand is orders of magnitude faster, and can scale to large datasets, since it simply uses the trained RNN to sample paths, and generates the graph using these paths. In Fig. 3, we plot the growth of running time against the number of timestamps and graph size. As visible, TIGGER is not only faster, but also have a slower growth rate. For this experiment, we sample the desired number of timestamps/temporal edges from the Wiki dataset.

Duplication: TAGGEN consistently duplicates $\approx 80\%$ of the original graph. Hence, the utility of TAGGEN as a graph generator is questionable. Both DYMOND and TIGGER do not suffer from this limitation.

Fidelity: From Table 1, we observe that TIGGER and TAGGEN achieve the best results in majority of graph statis-

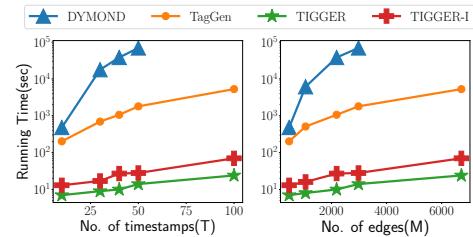


Figure 3: Scalability against # timestamps and # edges in Wiki(hourly). The *y*-axis is in log-scale.

Dataset	N = V	M = E	T	Method	Time(s)	% Edge overlap	Mean degree	Wedge Count	Triangle count	PLE	Edge entropy	LCC	NC	Global CF	Mean BC	Mean CC
Wiki-Small	1.6K	2.9K	50	Median	-	-	1.1064	13.0	0.0	16.4626	0.9912	5.0	44.0	0.0	0.0	0.0122
				DYMOND	69120	0.0	0.2424	8.0	0.0	11.426	0.0075	2.0	32.0	0.0	0.0005	0.0264
				TAGGEN	1800	87.169	0.0674	7.5	0.0	5.6519	0.0042	1.0	0.0	0.0	0.0	0.0004
				TIGGER	14	1.2821	0.0352	5.0	0.0	4.5005	0.0039	1.0	4.0	0.0	0.0	0.0014
UC Irvine	1.8K	33K	194	Median	-	-	1.5714	71.0	0.0	4.634	0.9537	21.0	14.0	0.0	0.0063	0.0701
				TAGGEN	12,480	79.356	0.1806	17.0	0.0	0.7732	0.0062	6.5	1.0	0.0	0.0009	0.0067
				TIGGER	125	25.0	0.076	12.0	0.0	0.4135	0.0102	3.0	3.0	0.0	0.0019	0.013
Bitcoin	3.7K	24K	191	Median	-	-	1.8443	189.5	2.0	3.5607	0.941	50.5	13.0	0.0102	0.0146	0.1003
				TAGGEN	18579	80.0	0.2311	23.0	0.0	0.5207	0.0045	13.0	1.0	0.0016	0.002	0.0133
				TIGGER	128	24.294	0.1217	25.5	1.0	0.294	0.0081	6.0	3.0	0.0078	0.0066	0.0229
Wiki	9.2K	157K	2.6M	Median	-	-	1.1525	33.0	0.0	12.0371	0.9868	7.0	62.5	0.0	0.0	0.0093
				TIGGER	896	25.573	0.072	14.0	0.0	9.4139	0.0057	2.0	10.0	0.0	0.0	0.0017
Reddit	10.9K	662K	2.6M	Median	-	-	1.6693	5955.0	0.0	5.672	0.916	269.0	147.0	0.0	0.0008	0.0217
				TIGGER	4661	0.077	0.1206	704.0	0.0	1.5709	0.0043	128.0	54.0	0.0	0.0006	0.0099
Ta-feng	56K	817K	120	Median	-	-	2.8832	52477.0	0.0	2.6827	0.9289	3798.0	75.0	0.0	0.0011	0.1526
				TIGGER	2722	17.028	0.301	14779.0	0.0	0.0762	0.0147	282.0	295.0	0.0	0.0003	0.045

Table 1: TIGGER’s performance against TAGGEN and DYMOND in terms of graph generation time (Col 6), edge duplication percent (Col 7), and median error across various graph statistics (Cols 8-17). For all performance metrics, lower values are better. For each statistic, we also list the *Median* value over *original graph snapshots* to better contextualize the error values. The best result in each dataset is in boldface. We do not report the results for an algorithm if it does not complete within 24 hours. Errors smaller than five decimal places are approximated to 0.

Metric	Wiki-Small	UC Irvine	Bitcoin
Generation Time(sec)	19	1112	640
%Edge overlap	0	0	0
Mean degree	0.0463/1.1064	0.1949/1.5714	0.4015/1.8443
Wedge Count	7.0/13.0	26.0/71.0	50.0/190
Triangle Count	0.0/0.0	0.0/0.0	1.0/2.0
PLE	5.3916/16.4626	1.1036/4.634	2.0456/3.5607
Edge Entropy	0.0045/.9912	0.0125/.9537	0.0177/.941
LCC	1.0/5	7.0/21.0	16.0/50.5
NC	4.0/44.0	7.0/14.0	18.0/13.0
Global CF	0.0/0.0	0.0/0.0	0.0096/0.0102
Mean BC	0.0/0.0	0.0026/0.0063	0.0113/0.0146
Mean CC	0.0015/0.0122	0.0257/0.0701	0.0594/0.1003

Table 2: Median errors across various graph statistics for inductive version. Each entry, row 3 onwards, denotes (median absolute error/ median value of the corresponding original graph property across snapshots).

tics. However, as we noted above, TAGGEN nearly duplicates the original graph and hence it is not surprising that the graph statistics remain nearly the same. In contrast, TIGGER has an edge overlap of $\approx 20\%$ on average, and yet achieves low errors similar to a near-duplicate graph. While TIGGER-I exhibits higher median error than the transductive TIGGER, it is better than DYMOND (See Wiki-Small in Table 2).

To study how the performance varies with growth of graphs, we study the variation of median error against time in Fig. 4. Consistent with the trends in Table 1, the performance of DYMOND is the weakest. TAGGEN performs marginally better in clustering coefficient (CF), while TIGGER is superior in mean degree and LCC.

Inductive: Performance of TIGGER-I

Before initiating the discussion, we note that TIGGER-I offers an important feature not found in any of the transductive models, *viz.*, the ability to control the size of the generated graph. Table 2 presents the results.

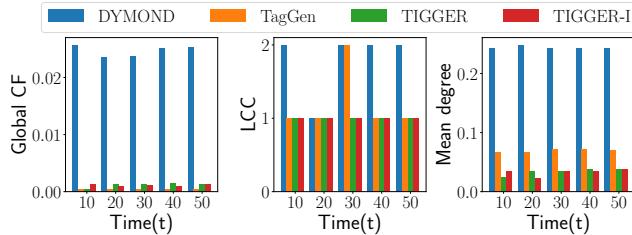


Figure 4: Median error over each consecutive window of 10 graph snapshots in Wiki-Small.

Scalability: TIGGER-I, is orders of magnitude faster than TAGGEN and DYMOND. However, TIGGER-I is 5–8 times slower than transductive TIGGER. This is unsurprising since TIGGER-I needs to perform nearest neighbor search in the inference phase on node embeddings. Additionally, TIGGER-I is challenging to train on large graphs due to its reliance on WGAN, which often fails to converge on large graphs. Hence, we have not reported results on full Wiki, Reddit and Bitcoin. Fig. 3 reveals that the growth rate of running time in TIGGER-I is similar to TIGGER.

Duplication: The edge-overlap of TIGGER-I is 0 across all benchmarked datasets, which is the ideal score.

Fidelity: The modelling task in inductive mode is inherently more difficult due to not having access to node IDs. Despite this challenge, we observe that the errors are low when compared to the median values of graph statistics in the original graph (Table 2). More importantly, despite being inductive, the errors are significantly better than DYMOND and comparable to TAGGEN and TIGGER (compare Tables 2 and 1). This trend is also visible in Fig. 4.

Conclusion

The success of a temporal graph generative model rests on two key properties: (1) Scalability to large temporal graphs since real-world graphs are large, and (2) and the ability to learn the underlying distribution of rules governing graph evolution rather than duplicating the training graph. Existing techniques fail to show the above desired behaviour. As established in our empirical evaluation, the proposed method, TIGGER, achieves the above desiderata. TIGGER derives its power through an innovative use of *intensity-free temporal point processes* to jointly model the node interaction times and the structural properties of the source graph. Additionally, we introduce an inductive version called TIGGER-I, which directly learns the distribution over node embeddings instead of node IDs.

Future Work: The scalability of the inductive model is limited by its graph embeddings and the use of WGAN. Hence, we plan to explore mechanisms that address this limitation and eventually move towards a model that is inductive, scalable and accurate in terms of fidelity.

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