Temporal Graph Kernels for Classifying Dissemination Processes

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Abstract
Many real-world graphs or networks are temporal, e.g., in a social network persons only interact at specific points in time. This information directs dissemination processes on the network, such as the spread of rumors, fake news, or diseases. However, the current state-of-the-art methods for supervised graph classification are designed mainly for static graphs and may not be able to capture temporal information. Hence, they are not powerful enough to distinguish between graphs modeling different dissemination processes. To address this, we introduce a framework to lift standard graph kernels to the temporal domain. Specifically, we explore three different approaches and investigate the trade-offs between loss of temporal information and efficiency. Moreover, to handle large-scale graphs, we propose stochastic variants of our kernels with provable approximation guarantees. We evaluate our methods on a wide range of real-world social networks. Our methods beat static kernels by a large margin in terms of accuracy while still being scalable to large graphs and data sets. Hence, we confirm that taking temporal information into account is crucial for the successful classification of dissemination processes.

Keywords—Temporal graphs, Classification, Kernels

1 Introduction
Linked data arise in various domains, e.g., in chem- and bioinformatics, social network analysis and computer vision, and can be naturally represented as graphs. Therefore, machine learning with graphs has become an active research area of increasing importance. A prominent method primarily used for supervised graph classification with support vector machines are graph kernels, which compute a similarity score between pairs of graphs. In the last fifteen years, a plethora of graph kernels has been published [17]. With few exceptions, these are designed for static graphs and cannot utilize temporal information. However, real-world graphs often have temporal information attached to the edges, e.g., modeling times of interaction in a social network, which directs any dissemination process, i.e., the spread of information over time, in the temporal graph. Consider, for example, a social network where persons A and B were in contact before persons B and C became in contact. Consequently, information may have been passed from persons A to C but not vice versa. Hence, whenever such implicit direction is essential for the learning task, static graph kernels will inevitably fail.

To further exemplify this, assume that a (sub-)group in a social network suffers from unspecific symptoms, that occurred at some point in time and are probably caused by a disease. Here, nodes represent persons, and the edges represent contacts between them at certain points in time, cf. Figure 1. An obvious question now is whether an infectious disease causes the symptoms. However, dissemination processes are typically complex, since persons may have different risk factors of becoming infected, the transmission rate is unknown and, finally, the network structure itself might suffer from noise. Therefore, this question is difficult to answer by just analyzing a single network. But, assume that similar network data of past epidemics is available. Hence, we can model the detection of dissemination process of a disease as a supervised graph classification problem. In the simplest case, one class contains graphs under a dissemination process of a disease and the other class consists of graphs, where the node labels cannot be explained by the temporal information. Furthermore, notice that infections, or disseminated information in general, often may not be recognized or not reported [37]. Therefore, we additionally consider the scenario where disseminated information is incomplete. Finally, observe that the above learning problem can also model the detection of other dissemination processes in networks, e.g., dissemination of fake news in social media [35] or viruses in computer or mobile phone networks [1].

The key to solving these classification tasks are methods that adequately take the temporal characteristics of such graphs into account. We consider temporal graphs, where edges exist at specific points in time and node labels, e.g., representing infected and non-infected, may change over time.

1.1 Contributions We propose graph kernels for classifying dissemination processes in temporal graphs.
More specifically, our main contributions are:

1. We introduce three different techniques to map temporal graphs to static graphs such that conventional, static kernels can be successfully applied. For all three approaches, we analyze the trade-offs between loss of temporal information and size of the transformed graph.

2. For large-scale problems, we present a stochastic kernel directly based on temporal walks with provable approximation guarantees.

3. We comprehensively evaluate our methods using real-world data sets with simulations of epidemic spread. Our results confirm that taking temporal information into account is crucial for the detection of dissemination processes.

1.2 Related Work

Graph kernels have been studied extensively in the past 15 years, see [17]. Almost all kernels focus on static graphs. Important approaches include random-walk and shortest paths based kernels [7, 32, 4, 18], as well as the Weisfeiler-Lehman subtree kernel [31, 23]. Further recent works focus on assignment-based approaches [16, 27], spectral approaches [15], and graph decomposition approaches [26].

There has been some work considering dynamic graphs. In [20] a family of algorithms to recompute the random walk kernel efficiently when graphs are modified is presented. Wu et al. [38] propose graph kernels for human action recognition in video sequences. To this end, they encode the features of each frame as well as the dynamic changes between successive frames by separate graphs, which are then compared by random walk kernels. Paakken et al. [29] use graph kernels for predicting the next graph in a dynamically changing series of graphs. Using a similar setting, Anil et al. [2] propose spectral graph kernels to predict the evolution of social networks. General spatio-temporal convolution kernels for trajectory data of simultaneously moving objects were introduced in [14]. Wang et al. [36] study the classification of temporal graphs in which both vertex and edge sets can change over time. Here, information propagation is considered as a sequence of individual graphs, where the number of vertices is increasing when an information outburst occurs. They aim to identify such outbursts of information propagation. However, to the best of our knowledge, no graph kernels have been suggested that take temporality of edges and labels, as well as dissemination processes on graphs into account.

An extensive overview of temporal graphs, their static representations, and temporal walks can be found in [12, 21]. In [25] temporal random walks are used to obtain node embeddings for link prediction in evolving networks. In [9], the Katz centrality is extended to temporal graphs using temporal walks. Holme [11] examines how temporal graphs can be used for epidemiological models. The author evaluates different static representations of temporal graphs by comparing predicted and simulated epidemic outbreak sizes.

Identifying vertices that play an important role in dissemination processes has also been studied. For example, Leskovec et al. [19] study the problem of placing sensors in a water distribution network to quickly detect contaminants. Recently, methods for dynamic graphs were proposed where edges may be added to the graph as time progresses. All of these approaches focus on link prediction in single graphs, see, e.g., [25, 33].

Graph neural networks [8] emerged as an alternative for graph classification. Our new approaches can be combined with neural architectures, e.g., see [24].

2 Preliminaries

A labeled, undirected (static) graph $G = (V, E, l)$ consists of a finite set of vertices $V$, a finite set $E \subseteq \{u, v\} \subseteq V \mid u \neq v$ of undirected edges, and a labeling function $l: V \cup E \rightarrow \Sigma$ that assigns a label to each vertex or edge, where $\Sigma$ is a finite alphabet. In a labeled, directed graph $E \subseteq \{(u, v) \in V \times V \mid u \neq v\}$. We use $V(G)$ to denote the set of vertices of $G$. A (static) walk in a graph $G$ is an alternating sequence of vertices and edges connecting consecutive vertices. For notational convenience we sometimes omit edges. The length of a walk $(v_1, v_2, \ldots, v_{k+1})$ is $k$.

A labeled, undirected, temporal graph $G = (V, E, l)$ consists of a finite set of vertices $V$, a finite set $E$ of undirected temporal edges $e = \{(u, v), t\}$ with $u$ and $v$ in $V$, $u \neq v$, availability time (or time stamp) $t \in \mathbb{N}$, and a labeling function. Here the labeling function $l: V \times T \rightarrow \Sigma$ assigns a label to each vertex at each time step $t \in T = \{1, \ldots, t_{\max} + 1\}$ with $t_{\max}$ being the largest time stamp of any $e \in E$. Note that for a temporal graph the number of edges is not polynomially bounded by the number of vertices. For $v \in V$ let $T(v)$
be the set of availability times of edges incident to $v$. For convenience, we regard the set of availability times as a sequence that is ordered by the canonical ordering on the natural numbers. The bijection $\tau_v: T(v) \to \{1, \ldots, |T(v)|\}$ assigns to each time its position in the ordered sequence of $T(v)$ for $v \in V$. The degree $d(v)$ of a vertex $v$ in a temporal graph is the sum of the numbers of edges incident to $v$ over all time steps.

2.1 Kernels for Static Graphs A kernel on a non-empty set $\mathcal{X}$ is a positive semidefinite function $\kappa: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Equivalently, a function $\kappa$ is a kernel if there is a feature map $\phi: \mathcal{X} \to \mathcal{H}$ to a Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$, such that $\kappa(x, y) = \langle \phi(x), \phi(y) \rangle$ for all $x$ and $y$ in $\mathcal{X}$. Let $\mathcal{G}$ be the set of all graphs, then a function $G \times G \to \mathbb{R}$ is a graph kernel. We briefly summarize two well-known kernels for static graphs.

Random walk kernels measure the similarity of two graphs by counting their (weighted) common walks [7, 32]. For a walk $w = (v_1, e_1, \ldots, v_k)$ let $L(w) = (l(v_1), l(e_1), \ldots, l(v_k))$ denote the labels encountered on the walk. Two walks $w_1$ and $w_2$ are considered to be common if $L(w_1) = L(w_2)$. We consider the $k$-step random walk kernel $\kappa_{RW}(G, H) = \langle \phi_{RW}(G), \phi_{RW}(H) \rangle$ counting walks up to length $k$. Here, the feature map $\phi_{RW}$ is defined by $\phi_{RW}(G) = \{|v \in W_l(G) | s = L(w)\}$, where $s \in \Sigma^{2k+1}$ and $W_l(G)$ is the set of walks in $G$ of length $\ell \in \{0, \ldots, k\}$.

Weisfeiler–Lehman subtree kernels are based on the well-known color refinement algorithm for isomorphism testing [31]: Let $G$ and $H$ be graphs, and $l$ be a labeling function $V(G) \cup V(H) \to \Sigma$. In each iteration $i \geq 0$, the algorithm computes a labeling function $l^i: V(G) \cup V(H) \to \Sigma$, where $l^0 = l$. Now in iteration $i > 0$, we set $l^{i+1}(v) = \xi(l^{-1}(v), \{l^{i-1}(w) | w \in N(v)\})$ for $v$ in $V(G) \cup V(H)$. In practice, one maps the above to a unique element from $\Sigma$. The idea of the Weisfeiler–Lehman subtree kernel [31] is to compute the above algorithm for $h \geq 0$ iterations and after each iteration $i$ compute a feature map $\phi_i(G)$ in $\mathbb{R}^{\Sigma^{|\Sigma|}}$ for each graph $G$, where $\Sigma_i \subseteq \Sigma$ denotes the image of $l^i$. Each component $\phi_i(G)_c$ counts the number of occurrences of vertices labeled with $c$ in $\Sigma_i$. The overall feature map $\phi_{WL}(G)$ is defined as the concatenation of the feature maps of all $h$ iterations. Then, the Weisfeiler–Lehman subtree kernel for $h$ iterations is $\kappa_{WL}(G, H) = \langle \phi_{WL}(G), \phi_{WL}(H) \rangle$. This kernel can also be interpreted in terms of walks. A label $l_i(v)$ represents the unique rooted tree of height $i$ obtained by simultaneously taking all possible walks of length $i$ starting at $v$, where repeated vertices visited in the past are treated as distinct.

3 A Framework for Temporal Graph Kernels In the following temporal graphs are mapped to a static graphs such that conventional static kernels can be applied, e.g., the random walk or Weisfeiler-Lehman subtree kernel. To catch temporal information, we use temporal walks, which are time respecting walks. That is, the traversed edges along a temporal walk have strictly increasing availability times. We assume that traversing an edge in a temporal walk does need one unit of time and is not possible instantaneously.

DEFINITION 1. A temporal walk of length $\ell$ is an alternating sequence of vertices and temporal edges $(v_1, e_1 = \{(v_1, v_2), t_1\}, v_2, e_2 = \{(v_2, v_3), t_2\}, \ldots, e_\ell = \{(v_\ell, v_{\ell+1}), t_\ell\}$ such that $t_i < t_{i+1}$ for $1 \leq i < \ell$. For a temporal walk the waiting time at vertex $v_i$ with $1 < i \leq \ell$ is $t_i - t_{i-1}$. The set of temporal walks (of length $\ell$) in a temporal graph $G$ is denoted by $W^\text{tmp}_{\ell}(G)$.

Finally, we define the function $L$ that maps a temporal walk $w$ to the label sequence $L(w) = (l(v_1, t_1), l(v_2, t_2 + 1), l(v_3, t_3 + 2), \ldots, l(v_{\ell-1}, t_\ell + 1), l(v_\ell, t_\ell + 1))$.

Temporal walks enable us to gain insights into the interpretation of the derived temporal graph kernels whenever the static graph kernel can be understood in terms of walks. This is natural in the case of random walk kernels, but also for the widely-used Weisfeiler-Lehman subtree kernel, cf. Section 2.1. We introduce three approaches, that differ in the size of the resulting static graph and in their ability to preserve temporal information as well as to model waiting times, see Table 1 for an overview.

3.1 Reduced Graph Representation First, we propose a straight-forward approach to incorporate temporal information in static graphs. In a temporal graph $G = (V, E, l)$ a pair of vertices may be connected with multiple edges each with a different availability time. In this case, we only preserve the edge with the earliest availability time and delete all other edges. We obtain the subgraph $G' = (V, E', l)$ with $E' \subseteq E$. From this we construct a static, labeled, undirected graph $RG(G) = (V, E, l_s)$ by inserting an edge $e = \{u, v\}$ into $E$ for every temporal edge $e' = \{(u, v), t'\} \in E'$.

We set the new static edge labels $l_s(e)$ to the number of the position $t'$ in the ordered sequence of all (remaining) availability times $t'$ in $E'$. Next, the temporal development of the dissemination is encoded using the vertex labels. Therefore, if the label of a vertex $v \in V$ in $G$ stays constant over time, we set $l_s(v) = 0$. For the remaining vertex labels we take the ordered sequence $T_V$ of all points in time when any vertex label changes for the first time. Then, for each vertex changing its label for the first time at time $t$ we set $l_s(v) = \tau(t)$, where
\( \tau(t_i) \) denotes the position of \( t_i \) in the sequence \( T_V \).

Applying this procedure results in the reduced graph representation \( RG(G) = (V, E, l, \tau) \). Clearly, the transformation may lead to a loss of information. However, notice that \( RG(G) \) is a simple, undirected graph with at most one edge between each pair of vertices. Hence, its number of edges is bounded by \( |V|^2 \), which can be much smaller than \( |E| \).

### 3.2 Directed Line Graph Expansion
In order to avoid a loss of information, we propose to represent temporal graphs by directed static graphs that are capable of fully encoding temporal information.

**Definition 2. (Directed line graph expansion)** Given a temporal graph \( G = (V, E, l) \), the directed line graph expansion \( DL(G) = (V', E', l') \) is the directed graph, where every temporal edge \((u, v, t)\) is represented by two vertices \( n^t_{uv} \) and \( n^t_{vu} \), and there is an edge from \( n^t_{uv} \) to \( n^t_{vu} \) if \( v = x \) and \( t < s \). For each vertex \( n^t_{uv} \), we set the label \( l'(n^t_{uv}) = (l(u, t), l(v, t + 1)) \).

Figure 2b shows an example of the transformation for the graph shown in Figure 2a. The following lemma relates temporal walks in a temporal graph and the static walks in its directed line graph expansion.

**Proposition 3.1.** Let \( G \) be a temporal graph and \( \ell \geq 0 \). The walks in \( W_\ell(DL(G)) \) are in one-to-one correspondence with the temporal walks in \( W^{temp}_{\ell + 1}(G) \).

**Proof.** Let \((v_1, (\{v_1, v_2\}, t_1), v_2, \ldots, (\{v_\ell, v_{\ell + 1}\}, t_\ell), v_{\ell + 1}\) be a temporal walk of length \( \ell \geq 2 \) in \( G \). Then \((n^{t_1}_{v_1v_2}, n^{t_2}_{v_2v_3}, \ldots, n^{t_\ell}_{v_\ell v_{\ell + 1}})\) is a walk of length \( \ell - 1 \) in \( DL(G) \), since the vertices represent temporal edges of \( G \) that are consecutively connected by directed edges in \( DL(G) \) provided that \( t_i < t_{i+1} \) for \( i \in \{1, \ldots, \ell - 1\} \). This holds for every temporal walk.

Vice versa, let \((n^{t_1}_{v_1v_2}, n^{t_2}_{v_2v_3}, \ldots, n^{t_\ell}_{v_\ell v_{\ell + 1}})\) be a walk in \( DL(G) \). Due to the construction of \( DL(G) \) the time stamps satisfy \( t_1 < t_2 < \cdots < t_\ell \) and we can construct a unique temporal walk in \( G \) from the sequence of vertices as above. \( \square \)

Note that for \( \ell = 0 \) the two vertices \( n^1_{uv} \) and \( n^1_{vu} \) representing the same temporal edge \((\{u, v\}, t)\) correspond to two different temporal walks traversing the edge in different directions. In Figure 2b the walk \((n^2_{v_a}, n^2_{v_b}, n^2_{v_c})\) in \( DL(G) \) of length 2 corresponds to the temporal walk \((c, (\{c, a\}, 2), a, (\{a, b\}, 3), b, (\{b, c\}, 7), c)\) of length 3 in the temporal graph \( G \).

The vertex labeling of \( DL(G) \) is sufficient to encode all the label information of the temporal graph \( G \), i.e., two temporal walks exhibit the same label sequence (according to the function \( L \) in Definition 1) if and only if the corresponding walks in the directed line graph expansion have the same label sequence. Therefore, all static kernels that can be interpreted in terms of walks are lifted to temporal graphs and the concept of temporal walks by applying them to the directed line graph expansion. Moreover, the directed line graph expansion supports to take waiting times into account by annotating an edge \((n^2_{uv}, n^1_{vu})\) with the waiting time \( t - s - 1 \) at \( v \). We proceed by studying basic structural properties of the directed line graph expansion.

**Proposition 3.2.** Let \( G = (V, E) \) be a temporal graph and \( DL(G) = (V', E') \) its directed line graph expansion. Then, \( |V'| = 2|E| \) and

\[
|E'| \leq |E| + \frac{1}{2} \sum_{v \in V} d(v) = O(|E|^2),
\]

where \( d(v) \) denotes the degree of \( v \) in \( G \).

**Proof.** The number of vertices directly follows from the construction. The directed line graph expansion \( DL(G) \) of the temporal graph \( G \) is closely related to the classical directed line graph of a modified copy of \( G \) obtained by deleting all time stamps (leading to indistinguishable parallel edges) and replacing all undirected edges by two directed copies. We use the following classical result [10]. For a directed graph \( G = (V, E) \) the number of edges in the directed line graph is \( \sum_{v \in V} d^+(v) \cdot d^+(v) \), where \( d^+(v) \) is the in- and \( d^+(v) \) the outdegree of \( v \). After replacing all undirected edges by two directed copies the in- and outdegrees are equal for each vertex. Furthermore, the directed line graph expansion of \( G \) has at most half the edges, because for the vertices \( n^*_{uv}, n^*_{vu} \) and \( n^t_{uv}, n^t_{vu} \) at most one time constraint \( s < t \) or \( s > t \) can be satisfied. Finally, between \( n^*_{uv} \) and \( n^t_{uv} \) there is no edge, therefore we subtract \( |E| \) and the result follows. \( \square \)

| Transformation                  | Preserves information | Waiting times | Size of static graph |
|---------------------------------|-----------------------|---------------|----------------------|
| Reduced Graph Representation    | \( \times \)          | \( \times \)   | \( O(|V|^2) \)        |
| Directed Line Graph Expansion  | \( \checkmark \)      | \( \checkmark \) | \( O(|E|^2) \)        |
| Static Expansion                | \( \checkmark \)      | \( \star \)    | \( O(|E|) \)          |
Since a cycle in the directed line graph expansion would correspond to a cyclic sequence of edges with strictly increasing time stamps, the directed line graph $DL(G)$ of a temporal graph $G$ is acyclic. Consequently, the maximum length of a walk in the directed line graph expansion is bounded. Therefore, there is no need to down-weight walks with increasing length to ensure convergence, which avoids the problem of halting [32].

### 3.3 Static Expansion Kernel

A disadvantage of the directed line graph expansion is that it may lead to a quadratic blowup w.r.t. the number of temporal edges. Here, we propose an approach that utilizes the static expansion of a temporal graph resulting in a static graph of linear size. The static expansion $SE(G)$ of a temporal graph $G$ is a static, directed and acyclic graph that contains the temporal information of $G$. Similar approaches for static expansions have been used to solve a variety of problems on temporal graphs, see, e.g., [22].

For $G = (V, E, l)$ we construct $SE(G) = (U, E, l')$ with $U$ being a set of time-vertices. Each time-vertex $(v, t) \in U$ represents a vertex $v \in V$ at time $t$. Time-vertices are connected by directed edges that mirror the flow of time, i.e., if an edge from $(v, t) \in U$ to $(v, s) \in U$ exists, then $t < s$. Because edges in $E$ are non-directed, the transformation has to consider both possible directions. It follows, that for each temporal edge $e \in E$, we introduce at most four time-vertices that represent the start and end points of $e$. Next, we add edges that correspond to temporal edges in $E$, and additional edges that represent possible waiting times at a vertex.

**Definition 3. (Static expansion)** For a temporal graph $G = (V, E, l)$, we define the static expansion as a labeled, directed graph $SE(G) = (U, E, l')$, with vertex set $U = \{(u, t), (v, t), (u, t + 1), (v, t + 1) | \{(u, v), t) \in E\}$, and edge set $E = E_N \cup E_W_1 \cup E_W_2$, where

\[
E_N = \{(u, t), (v, t + 1), (v, t), (u, t + 1) | \{u, v\} \in E\},
\]

\[
E_W_1 = \{(w, i + 1), (w, j) | \{w, i + 1\}, (w, j) \in E, i, j \in T(w), \tau_w(i) + 1 = \tau_w(j) \text{ and } i + 1 < j\},
\]

and

\[
E_W_2 = \{(w, i), (w, j) | \{w, i\}, (w, j) \in E, i, j \in T(w), \tau_w(i) + 1 = \tau_w(j) \text{ and } i < j\}.
\]

For each time-vertex $(w, t) \in U$, we set $l'((w, t)) = l(w, t)$. For each edge in $e \in E_N$, we set $l'(e) = \eta$, and for each edge in $e \in E_W_1 \cup E_W_2$, we set $l'(e) = \omega$.

Figure 2c shows an example of the transformation. Notice that the label sequence of a static walk in $SE(G)$ encodes the times of waiting. Since for all edges

\[
((u, t_1), (v, t_2)) \in E \text{ it holds that } t_1 < t_2, \text{ the resulting graph is acyclic. Finally, we have the following result.}
\]

**Proposition 3.3.** The size of the static expansion $SE(G) = (U, E, l')$ of a temporal graph $G$ is in $O(|E|)$.

**Proof.** The size of $U$ is bounded by $4 \cdot |E|$, because at most four vertices for each temporal edge $e \in E$ are inserted. For each $e \in E$, there are at most six edges in $E$. Two edges that represent using $e$ at time $t$ and four possible waiting edges, one for each vertex inserted for edge $e$. Consequently, $|E| \in O(|E|)$.

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### 4 Approximation for the Directed Line Graph Representation

Although the directed line graph expansion preserves the temporal information and is able to model waiting times, see Table 1 and Proposition 3.1, the construction may lead to a blowup in graph size. Hence, we propose a stochastic variant based on sampling temporal walks with provable approximation guarantees.

Let $G = (V, E, l)$ be a temporal graph, the algorithm approximates the normalized feature vector \(\hat{\phi}_RW(G) = \phi_{RW}(G)/||\phi_{RW}(G)||_1\), resulting in the normalized kernel \(\hat{\kappa}_{RW}(G_1, G_2) = \langle \hat{\phi}_{RW}(G_1), \hat{\phi}_{RW}(G_2) \rangle\).

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\(^1\) Section 4 has been updated and improved compared to the conference version [28] of this paper.
for two temporal graphs $G_1$ and $G_2$. The algorithm starts by sampling $S$ temporal walks at random (with replacement) from all possible walks in $G$, where the exact value of $S$ will be determined later. We compute a histogram $\tilde{\phi}_{RW}^k(G)$, where each entry $\tilde{\phi}_{RW}^k(G)_s$ counts the number of temporal walks $w$ with $L(w) = s$ encountered during the above procedure, normalized by $1/|S|$. Algorithm 1 shows the pseudocode.

Algorithm 1

**Input:** A temporal graph $G$, a walk length $k \in \mathbb{N}$, $S \in \mathbb{N}$.

**Output:** A feature vector $\tilde{\phi}_{RW}^k(G)$ of normalized temporal walk counts.

1. Initialize feature vector $\tilde{\phi}_{RW}^k(G)$ to a vector of zeros
2. **parallel for** $1, \ldots, S$ **do**
3. sample $k$-step walk $w$
4. $\tilde{\phi}_{RW}^k(G)_{L(w)} \leftarrow \tilde{\phi}_{RW}^k(G)_{L(w)} + 1/s$
5. **end**
6. **return** $\tilde{\phi}_{RW}^k(G)$

We get the following result, showing that Algorithm 1 can approximate the normalized (temporal) random-walk kernel $\tilde{\kappa}_{RW}^k(G_1, G_2)$ up to an additive error.

**Theorem 4.1.** Let $G$ be a set of temporal graphs with label alphabet $\Sigma$. Moreover, let $k > 0$, and let $\Gamma(\Sigma, k)$ denote an upperbound for the number of temporal walks of length $k$ with labels from $\Sigma$. By setting

$$S = \frac{\log(2 \cdot |G| \cdot \Gamma(\Sigma, k) \cdot 1/\delta)}{2(\sqrt{\Gamma(\Sigma, k)})^2},$$

Algorithm 1 approximates the normalized temporal random walk kernel $\tilde{\kappa}_{RW}$ with probability $(1 - \delta)$, such that

$$\sup_{G_1, G_2 \in G} \left| \tilde{\kappa}_{RW}^k(G_1, G_2) - \langle \tilde{\phi}_{RW}^k(G_1), \tilde{\phi}_{RW}^k(G_2) \rangle \right| \leq 3\lambda.$$

**Proof.** First, by an application of the Hoeffding bound together with the Union bound, it follows that by setting

$$S = \frac{\log(2 |G| \cdot \Gamma(\Sigma, k) \cdot 1/\delta)}{2\varepsilon^2},$$

it holds that with probability $1 - \delta$,

$$\left| \tilde{\phi}_{RW}(G_i)_j - \tilde{\phi}_{RW}(G_i)_j \right| \leq \varepsilon,$$

for all $j$ for $1 \leq j \leq \Gamma(\Sigma, k)$, and all temporal graphs $G_i$ in $G$. Let $G_1$ and $G_2$ in $G$, then

$$\tilde{\kappa}_{RW}^k(G_1, G_2) = \langle \tilde{\phi}_{RW}^k(G_1), \tilde{\phi}_{RW}^k(G_2) \rangle \leq \sum_{i=1}^{\Gamma(\Sigma, k)} (\tilde{\phi}_{RW}(G_1)_i \cdot \tilde{\phi}_{RW}(G_2)_i)$$

$$\leq \sum_{i=1}^{\Gamma(\Sigma, k)} (\tilde{\phi}_{RW}(G_1)_i \cdot \tilde{\phi}_{RW}(G_2)_i) + \varepsilon \cdot \sum_{i=1}^{\Gamma(\Sigma, k)} (\tilde{\phi}_{RW}(G_1)_i + \tilde{\phi}_{RW}(G_2)_i) + \sum_{i=1}^{\Gamma(\Sigma, k)} \varepsilon^2$$

$$\leq \tilde{\kappa}_{RW}^k(G_1, G_2) + 2\Gamma(\Sigma, k) \cdot \varepsilon + \Gamma(\Sigma, k) \cdot \varepsilon.$$

The last inequality follows from the fact that the components of $\tilde{\phi}_{RW}(\cdot)$ are in $[0, 1]$. The result then follows by setting $\varepsilon = \lambda / \Gamma(\Sigma, k)$.

Algorithm 1 can be easily modified for the static (non-temporal) graphs and applied to all three of our kernel approaches.

So far, we assumed that we have access to an oracle to sample the temporal walks uniformly at random from the temporal graph $G$. One possible practical way to obtain the uniformly sampled temporal walks is to use rejection sampling. To this end, we start by uniformly sampling a random edge $e_i = \{(u, v), t_i\} \in E$ and extend it to a $k$-step temporal random walk $w$ starting with probability $1/2$ at node $u$ or node $v$, respectively, and at time $t_i + 1$. At each step, we choose an incident edge uniformly from all edges with availability time not earlier than the arrival time at the current vertex. The probability of choosing a temporal walk $w = (v_1, e_1, \ldots, v_i, e_i = (v_i, v_{i+1}, t_i), \ldots, e_k, v_{k+1})$ from all possible temporal walks of length $k$ is then $P_w = \frac{1}{2} \cdot P_{t_i = 2} \cdot P_{d(v_i, t_i) + 1}$ with $d(v_i, t_i + 1)$ being the number of incident edges to $v_i$ with availability time at least $t_i + 1$, i.e., the arrival time at $v_i$. On the other hand, a lower bound for the probability of any $k$-step temporal walk is $P_{min} = \frac{1}{|V|} \cdot \Delta^{-2}$ with $\Delta$ being the maximal degree in $G$. To obtain uniform probabilities for the sampled walks, we accept a walk only with probability $P_w / P_{min}$. Otherwise, we reject $w$ and restart the walk sampling procedure. Hence, each accepted walk has the uniform probability of $P_w \cdot P_{min} = P_{min}$.

Notice that we can forgo the rejection step in the case that the graphs for which we compute the kernel have similar biases during the walk sampling procedure.

**5 Experiments**

To evaluate our proposed approaches and investigate their benefits compared to static graph kernels, we address the following questions:

**Q1** How well do our temporal kernels compare to each other and static approaches in terms of (a) accuracy and (b) running time?
We used the following real-world temporal graphs and epidemic simulations to reconstruct the Infectious graph represents face-to-face contacts between visitors of the exhibition Infectious: Stay Away [13]. The Highschool graph is a contact network and represents interactions between students in twenty second intervals over seven days.

| Kernel | Data set | Infectious | Tumblr | DBLP | Facebook |
|--------|----------|------------|--------|------|----------|
| Stat-RW | 61.03 ± 2.4 | 63.94 ± 2.3 | 76.40 ± 1.5 | 83.68 ± 1.4 | 83.75 ± 0.8 | 86.43 ± 0.4 |
| Stat-WL | 42.52 ± 2.6 | 45.33 ± 2.7 | 68.95 ± 2.0 | 78.69 ± 1.5 | 78.56 ± 0.8 | 83.41 ± 0.6 |
| RD-RW | 66.20 ± 2.8 | 90.83 ± 1.3 | 90.40 ± 1.0 | 76.15 ± 1.5 | 91.69 ± 0.5 | 83.73 ± 0.8 |
| RD-WL | 83.41 ± 0.5 | 90.06 ± 0.6 | 91.75 ± 1.0 | 70.59 ± 0.9 | 90.55 ± 0.5 | 82.04 ± 0.7 |
| DL-RW | 92.91 ± 0.9 | 97.39 ± 0.7 | 97.95 ± 0.4 | 95.15 ± 0.6 | 98.86 ± 0.1 | 96.46 ± 0.1 |
| DL-WL | 91.68 ± 1.6 | 99.17 ± 0.6 | 98.05 ± 0.4 | 94.19 ± 0.4 | 98.49 ± 0.2 | 96.59 ± 0.2 |
| SE-RW | 88.56 ± 1.0 | 96.89 ± 0.7 | 97.30 ± 1.1 | 95.31 ± 0.5 | 98.46 ± 0.3 | 95.68 ± 0.3 |
| SE-WL | 89.52 ± 1.1 | 97.56 ± 0.7 | 95.40 ± 0.7 | 94.13 ± 1.0 | 97.23 ± 0.2 | 95.26 ± 0.3 |

We chose a subset of the DBLP\footnote{http://www.sociopatterns.org} and Facebook\footnote{snap.stanford.edu/data/memetracker9.html} and epidemic simulations to reconstruct dissemination processes.

**Table 4:** Classification accuracy in percent and standard deviation for the first classification task.

| Kernel | Data set | Infectious | Tumblr | DBLP | Facebook |
|--------|----------|------------|--------|------|----------|
| Stat-RW | 57.71 ± 4.0 | 62.83 ± 2.9 | 66.05 ± 2.4 | 67.35 ± 0.9 | 69.60 ± 1.4 | 67.16 ± 0.6 |
| Stat-WL | 40.77 ± 2.5 | 64.06 ± 2.4 | 64.00 ± 1.3 | 70.11 ± 0.5 | 64.33 ± 0.8 | 69.92 ± 0.3 |
| RD-RW | 60.57 ± 4.7 | 80.06 ± 1.9 | 74.00 ± 1.5 | 69.54 ± 1.0 | 64.24 ± 1.2 | 66.35 ± 0.6 |
| RD-WL | 69.20 ± 1.8 | 83.94 ± 0.7 | 77.40 ± 1.2 | 69.74 ± 0.5 | 67.30 ± 0.5 | 66.66 ± 0.6 |
| DL-RW | 82.64 ± 2.1 | 93.44 ± 1.0 | 88.65 ± 1.2 | 77.21 ± 1.0 | 81.79 ± 0.9 | 79.97 ± 0.5 |
| DL-WL | 36.40 ± 4.0 | 89.33 ± 0.7 | 78.65 ± 1.5 | 78.18 ± 1.3 | 76.45 ± 1.0 | 79.99 ± 0.5 |
| SE-RW | 57.27 ± 3.3 | 93.25 ± 1.3 | 87.20 ± 1.1 | 78.23 ± 0.9 | 83.09 ± 0.6 | 80.15 ± 0.6 |
| SE-WL | 50.79 ± 4.2 | 91.00 ± 1.2 | 79.80 ± 1.5 | 80.64 ± 0.7 | 82.04 ± 0.6 | 75.29 ± 0.5 |
| APPROX (S=50) | 60.41 ± 4.0 | 76.39 ± 3.0 | 74.60 ± 1.8 | 74.73 ± 1.3 | 69.70 ± 0.8 | 72.04 ± 0.7 |
| APPROX (S=100) | 65.41 ± 4.2 | 83.83 ± 1.8 | 75.60 ± 1.9 | 76.49 ± 1.5 | 74.50 ± 0.7 | 73.08 ± 0.6 |
| APPROX (S=250) | 66.93 ± 2.5 | 90.39 ± 1.8 | 78.60 ± 2.1 | 78.44 ± 1.3 | 76.44 ± 0.9 | 77.88 ± 0.6 |

**Q2** How does the approximation for the directed line graph approach compare to the exact algorithm?

**Q3** How is the classification accuracy affected by incomplete knowledge of the dissemination process?

### 5.1 Data Sets

We used the following real-world temporal graph data sets representing different types of social interactions.

*Infectious* and *Highschool*: Two data sets from the SocioPatterns project\footnote{http://www.sociopatterns.org}. The Infectious graph represents face-to-face contacts between visitors of the exhibition Infectious: Stay Away [13]. The Highschool graph is a contact network and represents interactions between students in twenty second intervals over seven days.

*Facebook* and *Tumblr*: The first graph is a subset of the activity of the New Orleans Facebook community over three months [34]. The Tumblr graph contains quotes between Tumblr users and is a subset of the Memetracker data set. Rozenstein et al. [30] used these graphs and epidemic simulations to reconstruct dissemination processes.

*DBLP*: We used a subset of the DBLP database to generate temporal co-author graphs. The subset was chosen by considering publications in proceedings of selected machine learning conferences. The time stamp

**MIT**: A temporal graph of interactions among students of the Massachusetts Institute of Technology [6].
of an edge is the year of the joint publication.

To obtain data sets for supervised graph classification, we generated induced subgraphs by starting a BFS run from each vertex. We terminated the BFS when at most 20 vertices in case of the MIT, 50 vertices in case of the Infections, 60 vertices in case of the Highschool, Tumblr or DBLP, and 100 vertices in case of the Facebook graph had been added. Using the above procedure, we generated between 97 and 995 graphs for each of the data sets. See Table 2 for data set statistics. All data sets will be made publicly available. In the following we describe the model for the dissemination process and the classification tasks.

**Dissemination Process Simulation** We simulated a dissemination process on each of the induced subgraphs according to the susceptible-infected (SI) model—a common approach to simulate epidemic spreading, e.g., see [3]. In the SI model, each vertex is either susceptible or infected. An infected vertex is part of the temporal dissemination process. An initial seed of $s$ vertices is selected randomly and labeled as infected. Infections propagate in discrete time steps along temporal edges with a fixed probability $0 < p \leq 1$. If a vertex is infected it stays infected indefinitely. A newly infected vertex may infect its neighbors at the next time step. The simulation runs until at least $|V| \cdot I$ vertices with $0 < I \leq 1$ are infected, or no more infections are possible.

**Classification Tasks** We consider two classification tasks. The first is the discrimination of temporal graphs with vertex labels corresponding to observations of a dissemination process and temporal graphs in which the labeling is not a result of a dissemination process. Here, for each data set, we run the SI simulation with equal parameters of $s = 1$, $p = 0.5$ and $I = 0.5$ for all graphs. We used half of the data set as our first class. For our second class, we used the remaining graphs. For each graph in the second class, we counted the number $V_{inf}$ of infected vertices, reset the labels of all vertices back to uninfected, and finally infected $V_{inf}$ vertices randomly at a random time.

The second classification task is the discrimination of temporal graphs that differ in the dissemination processes itself. Therefore, we run the SI simulation with different parameters for each of the two subsets. For both subsets we set $s = 1$ and $I = 0.5$. However, for the first subset of graphs we set the infection probability $p = 0.2$ and for the second subset we set $p = 0.8$. The simulation runs repeatedly until at least $|V| \cdot I$ vertices are infected or no more infections are possible. Notice that a classification by only counting the number of infected vertices is impossible for the classification tasks.

In order to evaluate our methods under conditions with incomplete information, we generated additional data sets based on Infections for both classification tasks. For each graph, we randomly set the labels of $\{10\%, \ldots, 80\%\}$ of the infected vertices back to non-infected. We repeated this ten times resulting in 80 data sets for each of the two classification tasks.

**5.2 Graph kernels** As a baseline we use the $k$-step random walk (Stat-RW) and the Weisfeiler-Lehman subtree (Stat-WL) kernel on the static graphs obtained by interpreting the time stamps as discrete edge labels, and assigning to each vertex the concatenated sequence of its labels. To evaluate the three approaches of Section 3, we use the $k$-step random walk and the Weisfeiler-Lehman subtree kernel, resulting in the following kernel instances: (1) RD-RW and RD-WL, which use the reduced graph representation (Section 3.1), (2) DL-RW and DL-WL, which use the directed line graph expansion (Section 3.2), and (3) SE-RW and SE-WL, which use the static expansion (Section 3.3). We evaluate the approximation (APPROX) for the directed line graph expansion, proposed in Section 4, with sample sizes $S = 50$, $S = 100$ and $S = 250$.

**5.3 Experimental Protocol** For each kernel, we computed the normalized Gram matrix. We report the classification accuracies obtained with the C-SVM implementation of LIBSVM [5], using 10-fold cross validation. The C-parameter was selected from $\{10^{-3}, 10^{-2}, \ldots, 10^2, 10^3\}$ by 10-fold cross validation on the training folds. We repeated each 10-fold cross validation ten times with different random folds, and report average accuracies and standard deviations. The number of steps of the random walk kernel ($k \in \{0, \ldots, 5\}$) and the number of iterations of the Weisfeiler-Lehman subtree kernel ($h \in \{0, \ldots, 5\}$) were selected by fold-wise 10-fold cross-validation. All experiments were conducted on a workstation with an Intel Xeon E5-2640v3 with 2.60GHz and 128GB of RAM running Ubuntu 16.04.6 LTS using a single core. We used GNU C++ Compiler 5.5.0 with the flag -O2. To compare running times, we set the walk length of DL-RW to $k = 2$, and for DL-WL we set the number of iterations to $h = 2$.

**5.4 Results and Discussion** In the following we answer questions Q1 to Q3.

Q1 Table 3 and Table 4 show that taking tempo-
Table 5: Running times in ms for the first classification task, random walk length $k = 3$ ($k = 2$ for DL-RW) and number of iterations of WL $h = 3$ ($h = 2$ for DL-WL).

| Kernel | Data set     | Stat-RW | Stat-WL | RD-RW | RD-WL | DL-RW | DL-WL | SE-RW | SE-WL | APPROX (S=50) | APPROX (S=100) | APPROX (S=250) |
|--------|--------------|---------|---------|--------|-------|--------|-------|-------|-------|---------------|---------------|---------------|
|        | MIT          | 50330   | 87      | 22     | 25    | 2647614| 71366 | 7211  | 581   | 188           | 363           | 896           |
|        | Highschool   | 124060  | 106     | 84     | 83    | 33643  | 1972  | 3660  | 382   | 301           | 412           | 1589          |
|        | Infectious   | 130630  |         | 10259  | 96    | 10764  |        | 4973  | 262   | 309           | 399           | 1451          |
|        | Tumblr       |         | 129     | 145    | 96    | 2887   | 847   | 2018  | 302   | 409           | 429           | 1901          |
|        | Dblp         | 29209   | 164     | 145    | 145   | 6715   | 429   | 6454  | 1097  | 1261          | 1242          | 5044          |
|        | Facebook     | 1090141 | 410     | 405    | 405   | 5050   | 429   | 6454  | 1359  | 1926          | 1131          | 7607          |

Table 6: Running times in ms for the second classification task, random walk length $k = 3$ ($k = 2$ for DL-RW) and number of iterations of WL $h = 3$ ($h = 2$ for DL-WL).

| Kernel | Data set     | Stat-RW | Stat-WL | RD-RW | RD-WL | DL-RW | DL-WL | SE-RW | SE-WL | APPROX (S=50) | APPROX (S=100) | APPROX (S=250) |
|--------|--------------|---------|---------|--------|-------|--------|-------|-------|-------|---------------|---------------|---------------|
|        | MIT          | 48497   | 73      | 294    | 25    | 26274726| 71181 | 7462  | 575   | 185           | 361           | 897           |
|        | Highschool   | 107947  | 106     | 4516   | 83    | 32919  | 2121  | 3743  | 369   | 360           | 573           | 1706          |
|        | Infectious   | 139620  |         | 18432  | 98    | 10590  |        | 4820  | 369   | 305           | 595           | 1525          |
|        | Tumblr       | 32353   | 128     | 18436  | 141   | 2890   | 806   | 1792  | 261   | 305           | 395           | 1869          |
|        | Dblp         | 1266452 | 164     | 114842 | 385   | 2800   | 423   | 1792  | 293   | 476           | 807           | 5993          |
|        | Facebook     | 529073  | 401     | 114842 | 385   | 9548   | 1196  | 6173  | 846   | 1170          | 2318          | 7318          |

Lead to improvements in accuracy over all data sets. In most cases the improvement is substantial. For the first classification task, DL-RW and DL-WL reach the best accuracies for all but the Tumblr data set, here SE-RW is best. However, also for the other data sets SE-RW and SE-WL are on par with slightly lower accuracies. For the second classification task, we have a similar situation, our approaches beat the static kernels in all cases. The Stat-RW and Stat-WL kernels have a significantly lower accuracy for all data sets and are not able to successfully detect dissemination processes. This classification task poses a greater challenge for the temporal kernels which reach less good results compared to the first classification task. Especially the Mit data set seems to be hard, only the DL-RW reaches an accuracy of over 80%. However, it also has the overall highest running time for this data set due to its quadratic blowup. See Table 5 for the running times of the first classification task (Table 6 shows similar values for the second task). The running times for the random walk kernels are by orders of magnitude higher than the ones of the Weisfeiler-Lehman kernels. The reduced graph kernels cannot compete with our other approaches in terms of accuracy. In particular for the second classification task the loss of temporal information led to lower accuracies. However, the running times, especially of RD-WL are low. For a lower average number of temporal edges and vertex degree, its advantage gained by reducing the number of edges decreases, and with larger data sets the running times increase. RD-RW and RD-WL deliver slightly worse results for the Facebook data set compared to the static kernels for both tasks.

Q2 For a sample size of $S = 50$ APPROX performs better than the static kernels. And, the accuracies are on par or better than the ones of the reduced graph kernels. With a larger sample sizes of $S = 100$ and $S = 250$ the gap between the accuracies of APPROX and DL-RW is reduced for all data sets in both classification tasks. Table 5 shows that the running time of the approximation algorithm is by orders of magnitude faster than the Mit data set. For $S = 50$ and $S = 100$ there is an improvement in running times for all data sets. For $S = 250$ the running times of the exact algorithm for the Facebook data set is faster.

Q3 We ran the Weisfeiler-Lehman subtree kernels for the Infectious data sets where formerly infected
vertices were randomly set to non-infected. For the first classification task DL-WL and SE-WL keep high average accuracy, see Figure 3a. The Stat-WL kernel falls under 50% accuracy. For the second task the SE-WL kernel achieves better average accuracy than the DL-WL kernel for up to 70% of reset labels, see Figure 3b. Only for 80% the DL-WL kernel achieves better average accuracy.

6 Conclusion
We introduced a framework lifting static kernels to the temporal domain, and obtained variants of the Weisfeiler-Lehman subtree and the k-step random walk kernel. Furthermore, we introduced a stochastic kernel directly based on temporal walks with provable approximation guarantees. We empirically evaluated our methods on real-world social networks showing that incorporating temporal information is crucial for classifying temporal graphs under consideration of dissemination processes. Moreover, we showed that the approximation approach performs well and is able to speed up computation by orders of magnitude. Additionally, we demonstrated that our proposed kernels work in scenarios where information of the dissemination process is incomplete or missing. We believe that our techniques are a stepping stone for developing neural approaches for temporal graph representation learning.

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