

# An embedding-based distance for temporal graphs

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January 24, 2024

## Abstract

We define a distance between temporal graphs based on graph embeddings built using time-respecting random walks. We study both the case of matched graphs, when there exists a known relation between the nodes, and the unmatched case, when such a relation is unavailable and the graphs may be of different sizes. We illustrate the interest of our distance definition, using both real and synthetic temporal network data, by showing its ability to discriminate between graphs with different structural and temporal properties. Leveraging state-of-the-art machine learning techniques, we propose an efficient implementation of distance computation that is viable for large-scale temporal graphs.

**Keywords:** Network science, Temporal networks, Graph distance, Graph embedding

## Introduction

Graphs are ubiquitous mathematical entities formed by a set of *nodes* and one of *edges* connecting them [1–3]. They can model a wide range of interacting systems, such as social [4, 5], technological [6], spatial [7] and biological networks [8] and owe their popularity to their ability to encode the complex relational structure of these systems. Real-world systems, moreover, often have temporal properties that cannot be encoded in static graphs and call for modeling based on time-resolved network representations, known as *temporal graphs* [9]. Examples of these include transportation [10] and ecological networks [11], face-to-face interactions [12–14], collaboration networks [15–17], etc.

Given their ubiquitous use in representing such diverse kinds of systems, it is crucial to be able to compare them. In fact, defining and computing a similarity measure between pairs of graphs [18] underpins many important applications and tasks, including machine learning tasks such as graph classification. However, given graphs' high dimensionality and structural complexity, many different notions of *distance* can be devised, capturing different properties of interest. Because of this, many definitions of distance for static graphs have been introduced, as reviewed in Refs. [19–23]. One of the simplest approaches is the *edit distance* [24] that counts the number of elementary changes (edge or node removal or addition) needed to transform one graph into another. This method only accounts for local information and suffers from the *curse of dimensionality* [25]. Approaches involving the global graph structure are based on matrix inversion [26, 27] but generally have a high computational cost, and approximations are needed to achieve satisfactory computational performance. The above methods are designed for graph pairs with known correspondence between their nodes, a case we will refer to as *matched* graphs. The more general case of *unmatched* graphs involves computing distances for pairs of graphs for which a mapping between nodes is unavailable, and the graphs may have a different size. In this case, one can extract and compare adequately chosen sets of graph features, as done in Refs. [28, 29] or focus on the eigenvalues of appropriate matrix representations [30–33]. Also, in this case, the computational complexity is a bottleneck, and approximate heuristics are often required [19].

In the case of temporal graphs, the temporal dimension adds to the complexity of graph comparison. Many of the aforementioned distance measures for static graphs have been used to study temporal graphs [34], typically to compare the state of the graph at different points in time [35–37]. Here, we study the problem of comparing temporal graphs *as a whole*. In the temporal case, few notions of distance have been proposed: Ref. [38] defines a method to compare temporal graphs based on a set of features that can be tailored to a specific research question; Ref. [39] addresses our same problem of temporal graph comparison but assumes the graphs to be *matched* and is computationally inefficient; Ref. [40] only considers the *unmatched* case and uses the comparison of temporal paths statistics to provide a definition of *dissimilarity* (rather than distance).

Here, we propose a computationally efficient method to compute a distance metric between pairs of temporal graphs, considering both the matched and unmatched cases. We build our comparison on top of graph embeddings, leveraging ideas from both the local and global approaches mentioned above, and encoding differences at the topological as well as at the temporal levels. Commented Python code for implementing our method is available at [github.com/lorenzodallamico/G-DynaDist](https://github.com/lorenzodallamico/G-DynaDist).

## Temporal graphs definitions

Before delving into the details of our main contribution, let us first set some basic definitions.

**Definition 1 (Temporal graph)** *A temporal graph  $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathcal{W})$  is a tuple where  $\mathcal{V}$  is a set of  $n$  nodes,  $\mathcal{E}$  a set of temporal edges between nodes, and  $\mathcal{W}$  a set of edge weights. All edges  $e \in \mathcal{E}$  have the form  $e = (i, j, t)$ , representing an instantaneous interaction between  $i$  and  $j$  at time  $t$ .  $w_e$  indicates the positive weight of edge  $e$ . The graph  $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathcal{W})$  can be represented with a sequence of weighted adjacency matrices,  $\{W_t\}_{t=1, \dots, T}$ , where  $T$  is the number of time points. Each of these matrices has size  $n \times n$  and entries  $(W_t)_{ij} = w_{(i, j, t)}$  if  $(i, j, t) \in \mathcal{E}$  and  $(W_t)_{ij} = 0$  otherwise. In the following, we will refer to these matrices as “snapshots” of the temporal graph at given times, and to  $T$  as the number of snapshots.*

This particular definition is commonly referred to as *snapshot graph* [41]. In a more general description of temporal networks, each interaction may be represented with a tuple  $(i, j, t, \tau)$  where  $\tau \in \mathbb{R}^+$  is an *interaction duration*. We adopt the former notation because it is simpler to handle in the following. The two notations are completely interchangeable whenever the time is discrete and a finite temporal resolution  $t_{\text{res}}$  is set. In fact, all contacts with a duration within  $t_{\text{res}}$  are considered to be instantaneous, and  $(i, j, t, \tau)$  can be represented by a set of interactions of unitary duration:  $\{(i, j, t + \delta)\}_{\delta \in \{0, \dots, \tau-1\}}$ . For this reason, Definition 1 is sufficiently general, as it can also describe interactions lasting more than one temporal unit. For an arbitrary time resolution, the weight  $w_e$  associated with a temporal edge  $e$  may be used to encode the fraction of  $t_{\text{res}}$  the two nodes connected by  $e$  spent in interaction.

Let us now introduce the concept of *matched* and *unmatched* graphs.

**Definition 2 (Matched graphs)** *Let  $\mathcal{G}_1(\mathcal{V}_1, \mathcal{E}_1, \mathcal{W}_1)$  and  $\mathcal{G}_2(\mathcal{V}_2, \mathcal{E}_2, \mathcal{W}_2)$  be two temporal graphs with  $n_1$  and  $n_2$ , respectively. We say that  $\mathcal{G}_1$  and  $\mathcal{G}_2$  are matched if  $n_1 = n_2$  and there exists a known bijective function  $\pi : \mathcal{V}_1 \rightarrow \mathcal{V}_2$  that maps each node of  $\mathcal{G}_1$  to a node of  $\mathcal{G}_2$ . The two graphs are otherwise said to be unmatched.*

When two graphs have the same size, mathematically, there are always many possible mappings  $\pi$  between their nodes, but for the *matched* approach to be valuable, a known mapping associated with an external notion of node identity across the two graphs is necessary (e.g., nodes corresponding to the same persons in two temporal social networks). An implicit consequence of Definition 2 is that all graph pairs with a different number of nodes are considered to be *unmatched*. We now state the requirements for our distance measure and illustrate our main result.

## Main result

In the following, we define two types of distance functions:  $d_m, d_u$  between matched and unmatched graphs, respectively. The inputs to these functions are two temporal graphs,  $\mathcal{G}_1$  and  $\mathcal{G}_2$ , with a potentially different

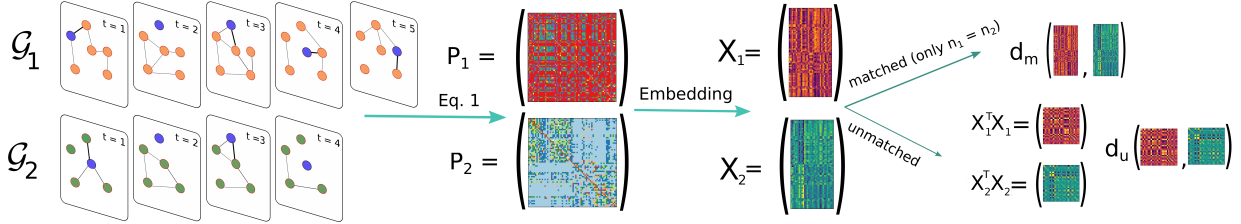


Figure 1: **Distance computation between two temporal graphs.** The inputs to the distance function are two temporal graphs  $\mathcal{G}_1$  (top, orange nodes) and  $\mathcal{G}_2$  (bottom, green nodes), generally with a different number of snapshots ( $T_1 = 5$ ,  $T_2 = 4$ , in the example) and a different number of nodes (here  $n_1 = 6$ ,  $n_2 = 5$ ). Each graph is represented as a matrix  $P \in \mathbb{R}^{n \times n}$ , according to (1), with entry  $(ij)$  encoding the probability that a walker goes from  $i$  to  $j$  following a time-respecting random walk (the walker’s position for each time point is indicated in blue). The matrices  $P_{1,2}$  are then embedded using the EDRep algorithm, mapping them to  $X_1 \in \mathbb{R}^{n_1 \times d}$  and  $X_2 \in \mathbb{R}^{n_2 \times d}$ . Finally, the matched – (3) – and unmatched – (4) – distances are calculated. Notice that a necessary condition to compute  $d_m$  is that  $n_1 = n_2$ .

number of time points (snapshots)  $T_1$  and  $T_2$ . In both cases, the distances should fulfill the following standard requirements [42]: i) non-negativity; ii) separation axiom; iii) symmetry; iv) triangle inequality. In addition, both distances should also be able by design to detect differences induced by the permutation of time indices. The matched distance should also differentiate between temporal networks differing only by a permutation of node indices, while the unmatched one should be invariant with respect to such transformation.

Our proposed distances are computed in two steps: i) we generate a temporal graph embedding, given by a matrix of size  $(n \times d)$  (with  $d$  independent of  $T$ ), that encodes relevant topological and temporal properties by leveraging time-respecting random walks on the temporal network; ii) we define the distance in the embedded space (separately treating the matched and the unmatched cases). The distance computation pipeline is illustrated in Fig. 1, and we now describe the steps outlined above in detail.

## Temporal graph embedding

Graphs are rich data representations, making it challenging to define simple mathematical operations to manipulate them. Graph embeddings provide an interesting avenue for doing so, as they yield a representation in vector space that preserves some of the graphs’ relevant properties [43–46]. In the case of temporal graphs, the additional challenge of dealing with their temporal dimension has been tackled in many different ways: Ref. [47] represents time as an additional dimension of an adjacency tensor; in evolutionary spectral clustering [48–52], a different embedding is obtained for each snapshot, and smoothness conditions are implemented on their temporal evolution; more recent works [53–55] introduced approaches based on time-respecting random walks, which encode relevant temporal properties that are important for dynamical processes occurring on temporal graphs.

We take the latter type of approach as our starting point to generate temporal graph embeddings that are obtained as the solution to an optimization problem. We define a loss function whose argument is a transition matrix  $P$  that is the limiting distribution of time-respecting random walks over the temporal graph  $\mathcal{G}$  to be embedded.  $T$  being the number of snapshots of  $\mathcal{G}$ , we consider an ensemble of random walks of length drawn uniformly at random between 1 and  $T$ , and starting from a randomly chosen node at time  $t = 1$ ; at each time step  $t$ , the walker, situated, e.g., on node  $i$ , can either move to a random neighbor of  $i$  in the snapshot at time  $t$  or stay in place on  $i$ ; if the walker is situated on a node that is not active at time  $t$ , *i.e.* which has no neighbors in this snapshot, the walker stays in place with probability one. The graph snapshots on the left of Fig. 1 show examples of such time-respecting random walks on the input graphs.

Specifically, given a temporal graph  $\mathcal{G}$ , with  $W_t$  the snapshot adjacency matrices of Definition 1 at times  $t = 1, \dots, T$ , we define for each snapshot  $\hat{L}_t = (D_t + I_n)^{-1}(W_t + I_n)$ , where  $D_t$  is the degree matrix  $D_t = \text{diag}(W_t \mathbf{1}_n)$  of the snapshot,  $I_n$  is the identity matrix of size  $n$ , and  $\mathbf{1}_n$  is the  $n$ -sized unity vector. We

then define the matrix  $P$  as

$$P = \frac{1}{T} \sum_{\tau=1}^T \hat{L}_\tau \hat{L}_{\tau-1} \cdots \hat{L}_2 \hat{L}_1, \quad (1)$$

The entries of  $P$  (which is a probability matrix) depend on the graph structure, the distribution of interaction durations, the correlation between nodes' interaction patterns, etc. In particular, they are not invariant under permutations of the time indices. We remark that the random walks used here can be of arbitrary length, hence the matrix  $P$  is sensitive to all the time scales of the temporal graph considered.

Given the above probability matrix  $P$  and a chosen embedding dimensionality  $d$ , we now want to generate, for each node  $i$  of  $\mathcal{G}$ , a unitary node embedding vector  $\mathbf{x}_i \in \mathbb{R}^d$ . To this aim, letting  $X \in \mathbb{R}^{n \times d}$  be the matrix storing in its rows these embedding vectors, we write the loss function as:

$$\begin{aligned} \mathcal{L}_P(X) &= - \sum_{i,j \in \mathcal{V}} \left[ P_{ij} \log Q_{ij}(X) - \frac{\mathbf{x}_i^T \mathbf{x}_j}{n} \right], \\ Q_{ij}(X) &= \frac{e^{\mathbf{x}_i^T \mathbf{x}_j}}{\sum_{k \in \mathcal{V}} e^{\mathbf{x}_i^T \mathbf{x}_k}} := \frac{e^{\mathbf{x}_i^T \mathbf{x}_j}}{Z_i}. \end{aligned} \quad (2)$$

This loss function is the sum of the cross entropies between the distributions in the rows of  $P$  and the variational distributions in the rows of  $Q(X)$ , with the addition of a regularization term. The function  $\mathcal{L}_P$  requires  $\mathcal{O}(n^2)$  operations to be evaluated, since  $Z_i$  is computed in  $\mathcal{O}(n)$  operations for each  $i$ . We adopt the recently proposed EDRep algorithm [56] that proposes an efficient approximation of  $Z_i$ , making it possible to optimize  $\mathcal{L}_P$  in  $\mathcal{O}(n)$  operations. We refer the reader to the *Methods* section for further details.

The matrix  $X$  obtained by optimizing  $\mathcal{L}_P$  defines the embedding of the temporal graph  $\mathcal{G}$ , and we now show how to leverage this embedding procedure to define a distance between temporal graphs.

## Defining a distance between embeddings

We want to define a distance between temporal graph embeddings that quantifies the similarity of the original temporal graphs according to the requirements stated above. Notice that the output embedding vectors  $\mathbf{x}$  are defined up to an orthogonal transformation applied to the rows of  $X$ . In fact, suppose  $R \in \mathbb{R}^{d \times d}$  is an orthogonal matrix, and  $\tilde{\mathbf{x}}_i = R\mathbf{x}_i$ , then  $\mathbf{x}_i^T \mathbf{x}_j = \tilde{\mathbf{x}}_i^T \tilde{\mathbf{x}}_j$  and the loss function of (2) is  $\mathcal{L}_P(\tilde{X}) = \mathcal{L}_P(X)$ . Hence, our distance must be invariant under orthogonal transformations. Moreover, as discussed above, the distance for unmatched graphs must also be invariant with respect to node permutations.

Given these requirements, we now discuss separately our choices to define the matched and unmatched distances. In the *Empirical evaluation* section, we show the efficacy of these choices with numerical tests.

### Distance for matched graphs

Let  $X_1$  and  $X_2 \in \mathbb{R}^{n \times d}$  be the embedding matrices of two matched temporal graphs  $\mathcal{G}_1$  and  $\mathcal{G}_2$ . To satisfy the invariance requirements discussed above, rather than defining our distance directly in terms of the matrices  $X_1$  and  $X_2$ , we use the auxiliary matrices  $M_{X_1} = X_1 X_1^T$  and  $M_{X_2} = X_2 X_2^T$  of size  $n \times n$ . These matrices are by construction invariant with respect to orthogonal transformations of the embedding space and encode the global structure of the corresponding temporal graphs (as the embeddings are generated exploiting the whole networks' structures). We define the distance  $d_m$  between matched temporal graphs as:

$$d_m(\mathcal{G}_1, \mathcal{G}_2) := \|M_{X_1} - M_{X_2}\|_F,$$

where  $\|\cdot\|_F$  is the Frobenius norm. Each matrix  $M$  encodes the similarity in the embedding space between all pairs of nodes of the corresponding temporal graph, and  $d_m$  quantifies thus the difference between these similarity patterns. In the *Methods* section, we show that we actually do not need to compute the large  $(n \times n)$   $M_{X_1}$  and  $M_{X_2}$  matrices, but that the distance can be computed using small  $d \times d$  matrices as follows:

$$d_m(\mathcal{G}_1, \mathcal{G}_2) = \sqrt{\|X_1^T X_1\|_F^2 + \|X_2^T X_2\|_F^2 - 2\|X_1^T X_2\|_F^2}, \quad (3)$$

We can easily verify that  $d_m$  is a distance, as it satisfies all the requirements mentioned above and is generally not invariant under the permutation of node indices.

### Distance for unmatched graphs

In (3), the term  $X_1^T X_2$  implies that  $X_{1,2}$  have the same size and that their rows are ordered according to the same and known indexing of the temporal graphs’ nodes. In the case of *unmatched* graphs, this node correspondence is not available, and the distance, as we discussed, should also be invariant with respect to node permutations. We therefore define the distance between unmatched graphs using auxiliary vectors. Specifically, we denote with  $\lambda(A)$  the vector of ordered eigenvalues of a matrix  $A$  and define our distance between two *unmatched* temporal graphs as

$$d_u(\mathcal{G}_1, \mathcal{G}_2) = \left\| \lambda \left( \frac{X_1^T X_1}{n_1} \right) - \lambda \left( \frac{X_2^T X_2}{n_2} \right) \right\|_2, \quad (4)$$

where  $X_{1,2}$  are, as before, the embeddings matrices of the two graphs, and  $n_{1,2} = |\mathcal{V}_{1,2}|$  are their sizes. The sizes are used to normalize the covariance matrices  $X_1^T X_1$  and  $X_2^T X_2$  so that their eigenvalues are independent from graph size.

The covariance matrices  $X_1^T X_1$  and  $X_2^T X_2$  (of size  $d \times d$ ) are indeed an appropriate argument to define the distance  $d_u$ , since they are independent of the ordering of the nodes and any other orthogonal transformation applied to the columns of  $X$ . However, directly comparing the entries of  $X_1^T X_1$  and  $X_2^T X_2$  requires a one-to-one correspondence between the embedding dimensions (the columns of  $X$ ). This mapping is unavailable because the **EDRep** algorithm makes no guarantees on the correspondence between the dimensions of the embedding spaces of different graphs. As a solution to this issue, we thus compare their spectra, which are invariant with respect to orthogonal transformations of the rows of  $X$ . This choice takes inspiration from the spectral static graph distance definitions – such as Ref. [32] – in which graphs are compared by computing the distance between the ordered sets of the eigenvalues of their matrix representations (e.g., adjacency, Laplacian, non-backtracking, etc.)

### Computational complexity

As discussed in the Methods section, the computational complexity of the embedding step is  $\mathcal{O}(nd^2 + d \cdot \min(n^2, E))$ , where  $E = \sum_t |\mathcal{E}_t|$  is the total number of temporal edges. On top of this, the distance  $d_m$  is then obtained with  $\mathcal{O}(nd^2 + d^2)$  additional operations, while  $d_u$  requires  $\mathcal{O}(nd^2 + d^3)$  additional operations.

## Empirical evaluation

We now proceed to evaluate the distance metrics we introduced, focusing in particular on their ability to capture the differences in topological and temporal properties of empirical temporal graphs. We carry out two evaluation tests using both empirical and synthetic temporal graph data. We use, in particular, empirical temporal graphs published by the **SocioPatterns** collaboration ([sociopatterns.org](http://sociopatterns.org)), that describe time-resolved, close-range proximity interactions of humans and animals in a variety of real-world environments. These data are known to exhibit rich multi-scale network structures, complex temporal activity patterns, correlations between these two, and other complex network features. Hence, they provide a natural benchmark to assess the sensitivity of our distance definitions to specific properties of real-world temporal graphs.

- In the first evaluation test, we consider structurally different synthetic temporal graphs of different sizes, and we cluster them using our temporal graph distance  $d_u$ , checking how well the clusters we find match the graph generating methods we used, irrespective of graph size. We then repeat the same task on empirical labeled data of human proximity in school settings.
- In the second evaluation test, we use the empirical data to elucidate which of the many properties of real temporal graphs are discriminated by the distances we introduced. We proceed as follows: given an empirical temporal graph, we apply a set of randomization operations, where each operation is

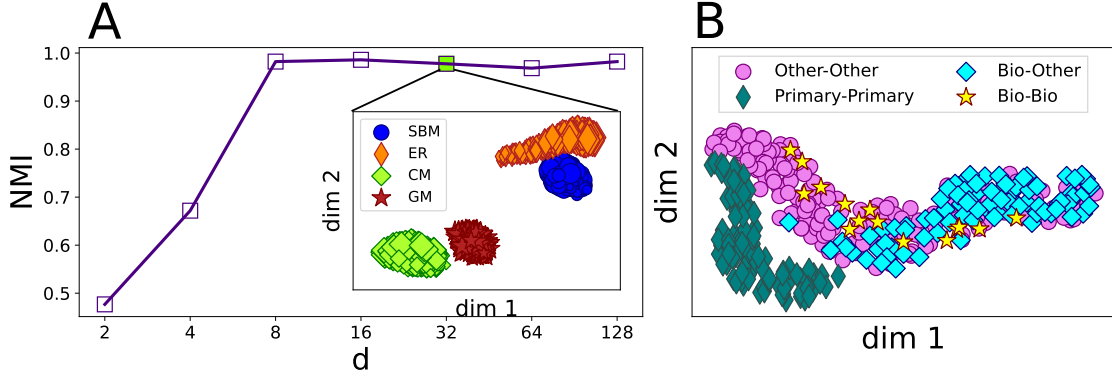


Figure 2: **Validation of  $d_u$  on graphs of varying size.** Panel A: Clustering performance in terms of normalized mutual information (NMI) as a function of the embedding dimensionality  $d$  used in the embedding step shown in Figure 1. The clustering task consists in recognizing four synthetic temporal graph classes with an unsupervised algorithm based on the distance  $d_u$ . The synthetic graphs classes are obtained by generating a graph from either of four models (stochastic block model (SBM), configuration model (CM), Erdős-Renyi (ER), and geometric model (GM)) with constant degree equal to 4.8 and the temporal component is obtained from the activity time series of an empirical graph as detailed in the main text. Inset of panel A: Scatter plot of UMAP dimensionality reduction in two dimensions of the signature vectors  $\lambda$  appearing in the definition of  $d_u$  given in (4), with here  $d = 32$ . Each point refers to a temporal graph; the color and marker code refers to the generative model of its static component, while the marker size is proportional to the number of nodes. Panel B: Each point is the 2-dimensional UMAP embedding of the signature vector  $\lambda$  of the temporal graph obtained selecting two classes and a day of interaction for all possible (`class_1`, `class_2`, `day`) triplets in the `SocioPatterns` data sets describing proximity temporal graphs in schools. The color and marker code are assigned according to the class label: the primary school classes form a group on their own and the other three groups (*Other-Other*, *Bio-Other*, *Bio-Bio*) belong to the high school data sets, where *Bio* are the biology classes, and *Other* the remaining ones. In all cases we use a temporal resolution equal to 10 minutes to create the temporal graphs from the `SocioPatterns` data.

designed to preserve specific properties of the original data (e.g., the activity time series of each node). We then attempt to discriminate the randomized temporal graphs from one another using our distance definitions and quantify the performance of such discrimination task. We test both  $d_m$  and  $d_u$ ; however this evaluation strategy, by design, compares temporal graphs with the same number of nodes.

## Discriminating between temporal graph classes

We define four families of temporal graphs as follows: first, we generate static random graphs of different sizes using four standard generative models; then, we turn these graphs into temporal graphs by assigning to each edge of the static graph the activity time series (*i.e.* the set of timestamps in which that edge was active) of a randomly chosen edge of the *Conference* empirical data set (the largest among the empirical data sets we use). The four generative models we use are: i) the Erdős-Renyi (ER) model [57]; ii) the stochastic block model (SBM), capable of generating graphs with a known community structure [58]; iii) the configuration model (CM), yielding graphs with an arbitrary degree distribution [59]; iv) the geometric model (GM), which generates edges based on proximity in a latent space [60]. Unlike the first three, the latter model yields graphs with a high clustering coefficient. Details on these generative models are provided in the Methods section.

For each model, we generate 250 graphs with size uniformly distributed between  $n = 200$  and  $n = 1800$  and constant average degree. We then deploy our distance definition  $d_u$  to compute a pair-wise distance matrix between all these temporal graphs. We use this matrix as an input for an unsupervised clustering task and check whether this clustering can discriminate the four groups of temporal graphs generated. The unsupervised clustering algorithm only takes the distance matrix and the number of clusters  $k$  (here  $k = 4$ ) as inputs. Here, we first perform a spectral embedding using non-negative matrix factorization (NMF) [61] extracting  $k$  non-negative components and then applying the k-means clustering algorithm with  $k$  classes [62]. We note that successively embedding and clustering is a standard approach, and using NMF is most suited here since the distance matrix is non-negative. Finally, we compare the original temporal graph labels with the partition labels yielded by this unsupervised clustering informed by our temporal graph distances: we

quantify the match between the true partition and the inferred one using the normalized mutual information (NMI), which yields a performance metric ranging between 0 (random guess) and 1 (perfect reconstruction).

Figure 2A shows the normalized mutual information (NMI) between the known temporal graph classes (associated with the four generative models) and the discovered cluster labels as a function of the embedding dimension  $d$ . The discrimination performance is low for small values of  $d$ , but for  $d \gtrsim 8$  the accuracy is high and becomes insensitive to the specific  $d$  value. The inset in Figure 2A shows the output of UMAP algorithm [63] in two dimensions when applied to the vectors  $\lambda \in \mathbb{R}^{32}$  used in the distance  $d_u$ . Each symbol corresponds to one temporal graph, the color and marker shape indicate its generative model, and the marker size is proportional to the number of graph nodes. We observe that graph size does not appear to affect distances systematically, and that the  $\lambda$  vectors used by the distance  $d_u$  allow us to discriminate all four generative models. Indeed, we have verified that the distances  $d_u$  between the graphs and the distances between their respective UMAP embedded vectors are strongly related, with a highly significant Spearman correlation coefficient of  $\sim 0.92$ .

We now carry out a test based on empirical data, using the `SocioPatterns` data sets describing proximity temporal graphs in schools, *i.e.*, *Primary school*, *High school 1*, *High school 2*, *High school 3* (the latter three correspond to data collections carried out in the same school in successive years). In each of these graphs, the nodes are split into classes, and the measurements are taken over multiple days. In the *Primary school* data set there are ten classes, divided into five grades (2 classes per grade). In the *High school* data sets, the classes are split according to the main topics studied, and the data collections involved an increasing number of classes in successive years. Namely, the *High school 1* contains the data of the students of three classes focusing on physics, chemistry and engineering; in *High school 2*, two classes focusing on maths and physics joined the data collection; in *High school 3* an additional maths and physics class and three biology classes also joined. We split each of these data sets into a set of temporal graphs obtained containing the contacts happening on a particular data collection day and involving the nodes of only two classes. We consider all the possible (`class_1`, `class_2`, `day`) triplets, obtaining in this way a family of temporal graphs (with 352 instances) with comparable sizes. While the distance  $d_u$  can compare graphs of arbitrarily different sizes, we want indeed here to set the hardest condition in which these graphs cannot be told apart by simply looking at their size. For each graph, we compute its signature  $\lambda$  of (4) and show the resulting two-component UMAP embedding in Fig. 2B. In this case, the Spearman correlation between the distances  $d_u$  and the distances between the UMAP embedding vectors equals 0.88. The color and marker coding refers in the figure to a labeling denoting the type of the two interacting classes. All primary school classes are treated equally, while in the high school case, we only distinguish between biology classes and all the others. From the plot, one can see that the distance can disentangle the networks formed from primary school data from the ones containing high school data. Moreover, a less neat but still visible distinction exists in the embeddings of (*Bio-Other*), likely because biology students spent more time in the labs and had different interaction patterns. This result confirms the ability of our distance to capture information on the temporal graph at multiple levels.

## Discriminating between temporal graph randomizations

Here, we consider 9 empirical `SocioPatterns` data sets, whose basic properties are summarized in Table 1 of the Methods section. Following Ref. [64], we select 6 types of randomization operations  $R_i$  ( $i = 1, \dots, 6$ ), described in detail in the Methods section. In all cases, we preserve the number of nodes and of snapshots of the original temporal graph.

To quantify the discriminative performance of our temporal graph distance, we proceed as follows, separately for each empirical temporal graph: given the empirical temporal graph and a pair of randomization operations ( $R_i, R_j$ ), we generate a set of 250 realizations using  $R_i$ , labeled as 0, and a set of 250 realizations using  $R_j$ , labeled as 1, for a total of 500 temporal graphs. We then compute the matrix of distances between these 500 graphs and use it to cluster them in 2 clusters, following the same procedure used for Fig. 2a. Figure 3 reports the NMI values between the real labels and the unsupervised algorithm result for each pair of randomizations ( $R_i, R_j$ ) and both the matched distance  $d_m$  (left panel) and the unmatched distance  $d_u$  (right panel). Within each panel, each matrix refers to one empirical temporal graph, and its entries are the NMI values described above. A high NMI entry indicates that our distance discriminates well the temporal graphs generated according to the two randomization procedures in the corresponding row and column of

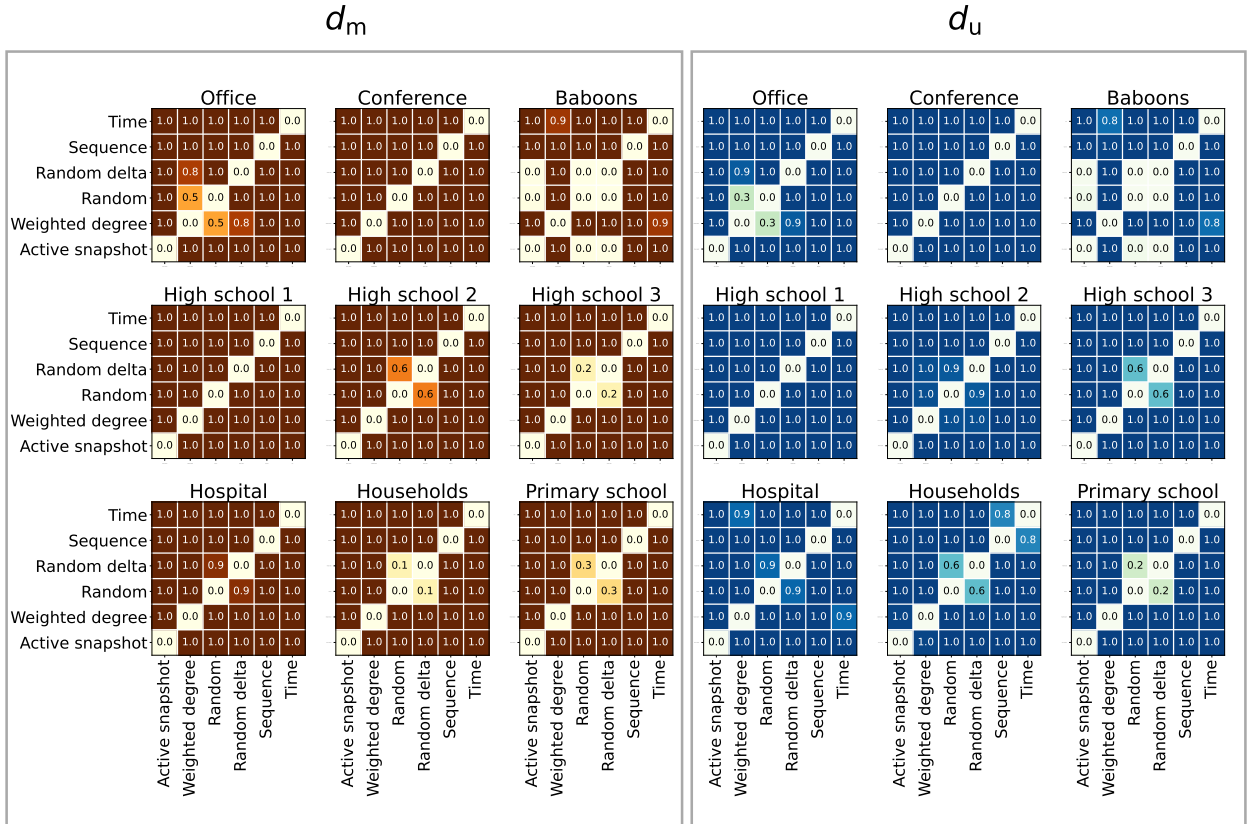


Figure 3: **Distance-based graph clustering for ensembles of graphs generated according to different randomization techniques.** Left panel: results for the matched distance  $d_m$  of (3). Right panel: results for the unmatched distance  $d_u$  of (4). Within each panel, each matrix corresponds to one of the 9 **SocioPatterns** temporal graphs described in Table 1. The rows and columns of each matrix correspond to the same set of 6 randomization techniques we used, described in the Methods sections, and based on the properties they preserve. *Random*: preserves the number of temporal edges; *Random delta*: preserves the number of temporal edges and contact duration distribution; *Active snapshot*: preserves the number of edges at each time-step and activity pattern of each node; *Time*: preserves the aggregated graph structure; *Sequence*: preserves the structure of each snapshot; *Weighted degree*: preserves the nodes’ cumulative interaction time. For each pair of randomizations, we infer the randomization method of each temporal graph via an unsupervised distance-based clustering algorithm, and we compare the inferred randomization method with the known true one. Each matrix entry reports (value and color coding) the accuracy of the inferred labels (randomization methods), quantified as the normalized mutual information (NMI) between the inferred and true labels.

the matrix entry, i.e., that the distance is sensitive to the properties preserved by either  $R_i$  or  $R_j$ . Low NMI values may either correspond to an inability of the distance to capture those properties or simply reflect that the empirical temporal graph is statistically random as far as those properties are concerned, as observed in particular for several pairs of randomizations in the *Baboons* dataset. Thus, it is enough to find one empirical data set for which the distance can distinguish between a pair of randomizations to conclude that the distance is indeed sensitive to the corresponding graph properties.

## Conclusions

We have here introduced a novel definition of distance between pairs of temporal graphs. This definition entails two steps: first, the embedding of the temporal graphs into an Euclidean space, and then the definition of a distance measure in the embedded space. In the first step, we have considered an embedding that exploits time-respecting random walks on the temporal graphs. Indeed, such walks are known to depend on, and encode important structural and temporal properties of these graphs [9, 40, 55, 65]. In the second step, we have proposed two possibilities for the distance definition. On the one hand, if a mapping is known between



the nodes of the graphs to be compared, we consider a distance definition that leverages such mapping. On the other hand, we put forward in the more general case a definition that makes it possible to compare graphs with arbitrarily different sizes (numbers of nodes). Note that in both cases, as the size of the embedding matrix does not depend on the number of temporal graph snapshots, it is possible to embed temporal graphs with different lengths in the same embedding space and thus to compute a distance between them. The evaluation of our pipeline on both synthetic and empirical data sets has shown that the proposed distance can capture structural differences (e.g., degree distribution, clustering coefficient, or presence of communities) as well as temporal differences (e.g., burstiness or node activity patterns) in the temporal graphs being compared.

The methodology we have developed is actually very general and customizable, as several other choices could be made in both steps of the method, namely the choices of the embedding method and of the distance. Our choices are based on two main motivations: i) a theoretical one, given the importance of time-respecting random walks in encoding information on temporal graphs, and thus in generating distributed representations of temporal graphs [9, 55, 65]; ii) a numerical one, which led us to choose the **EDRep** algorithm of Ref. [56] because of its efficiency and scalability and the possibility to obtain definitions of distance that can as well be efficiently computed. Moreover, the results obtained from our evaluation procedures support these choices *a posteriori*.

Our work entails some limitations worth mentioning. First, our evaluation strategy has focused on a limited set of temporal graphs, namely on graphs obtained from data describing proximity events between individuals. These graphs are however known to feature a broad variety of representative complex structural and temporal patterns such as temporally changing community structures, burstiness, broad distributions of event durations, etc [12, 14]. Second, we have considered only the cases either of fully matched graphs (bijection between the sets of nodes) or of no known matching. An interesting intermediate situation would be the one of partially matched graphs, in which only a subset of nodes is matched between the two graphs. Tackling this challenging setting would form an interesting extension of this work.

Defining a distance between temporal graphs opens the door to a wealth of potential applications, of which our evaluation procedures are only possible examples. Such a distance can, on the one hand, support data analysis of temporal graph data by extending the procedure of Fig. 3 to a large set of randomizations [47]. Indeed, as discussed, the inability to distinguish pairs of randomizations of a given temporal graph can be regarded as a statistical property of the graph itself. On the other hand, computing a distance between graphs can provide a crucial model validation tool: many generative models for temporal graphs are proposed based on various mechanisms of interactions, and model validation is often simply based on the comparison of a set of statistical properties [38], while our distance definition makes comparison possible at a global level. In addition, the distance could be used in the process itself of generating synthetic temporal graphs, by informing deep generative models such as *GANS* [66], which have proved extremely powerful in generating realistic data [67, 68]. Generating synthetic contact data with realistic structural and temporal properties could then be used to simulate processes of interest in public health research [69–74]. Finally, empirical (temporal) graphs are hard to anonymize [73, 75, 76] and, to minimize the risk of node re-identification, it might be needed to perform some perturbation operations on the graph before making it publicly available. However, such operations risk destroying some important patterns and information contained in the data. A way to tackle this issue could be to find a trade-off between re-identification risk and information loss, and the distance we have defined could be used to quantify the latter.

## Methods

### The EDRep algorithm

The **EDRep** algorithm [56] was recently proposed to efficiently generate embeddings given a probability matrix encoding the affinity between the embedded items. This is done by optimizing the cost function of (2) under the constraint  $\|\mathbf{x}_i\| = 1$  and obtaining a low-dimensional representation of the information encoded in the matrix  $P$ . A known problem of this type of cost function is the computational complexity because the normalization constants  $Z_i = \sum_{k \in \mathcal{V}} e^{\mathbf{x}_i^T \mathbf{x}_k}$  require  $\mathcal{O}(n^2)$  to be calculated. However, Ref. [56] describes an efficient way to estimate all the  $Z_i$  values in  $\mathcal{O}(n)$ . This is accomplished by first subdividing the nodes into

$q$  groups based on the embedding matrix  $X$ . Here  $q$  is a parameter of the algorithm, and larger  $q$  values generally lead to a higher accuracy, but very good results are obtained already for  $q = 1$ . Second, for each  $a = 1, \dots, q$ , one computes the mean  $\boldsymbol{\mu}_a$  and the covariance matrix  $\Omega_a$  of the set of embedding vectors of the nodes in group  $a$ . Denoting the number of nodes in group  $a$  by  $\pi_a$ , one obtains the estimation of  $Z_i$  as

$$Z_i \approx \sum_{a=1}^q \pi_a \exp \left\{ \mathbf{x}_i^T \boldsymbol{\mu}_a + \frac{1}{2} \mathbf{x}_i^T \Omega_a \mathbf{x}_i \right\} .$$

Coming to the algorithm's computational complexity, given that our choice of  $P$  is the sum of matrix products, the algorithm can be deployed in two forms: one in which  $P$  is never formally computed and the sequence  $\{\hat{L}_t\}_{t=1, \dots, T}$  is fed to the algorithm; and one in which  $P$  is explicitly computed. Letting  $X \in \mathbb{R}^{n \times d}$  be the matrix storing the embedding vectors in its rows, the computational complexity is determined by the matrix product  $PX$  needed to obtain the gradient of  $\mathcal{L}$ . In the former case, this is computed in  $\mathcal{O}(nd^2 + dE)$  operations, where  $E = \sum_{t=1}^T |\mathcal{E}_t|$  is the number of temporal edges. In the second case, instead, the complexity is given by the number of non-zero entries of  $P$ , which cannot exceed  $n^2$ . The former implementation is particularly convenient when  $n$  is large, and the  $\hat{L}_t$  matrices are very sparse. This is because  $P$  may be dense, even if the snapshots are sparse, and for large  $n$ ,  $P$  might not even fit in the computer's memory. Conversely, for small graphs,  $n^2$  may be smaller than the number of temporal edges, making the latter implementation more convenient.

## Matched distance definition

From (3), we have

$$\begin{aligned} d_m^2(X, Y) &= \sum_{i, j \in \mathcal{V}} [(M_X)_{ij} - (M_Y)_{ij}]^2 \\ &= \sum_{i, j \in \mathcal{V}} [(M_X)_{ij}(M_X)_{ij} + (M_Y)_{ij}(M_Y)_{ij} - 2(M_X)_{ij}(M_Y)_{ij}] \\ &\stackrel{(a)}{=} \sum_{i, j \in \mathcal{V}} [(M_X)_{ij}(M_X)_{ji} + (M_Y)_{ij}(M_Y)_{ji} - 2(M_X)_{ij}(M_Y)_{ji}] \\ &= \sum_{i \in \mathcal{V}} [(M_X M_X^T)_{ii} + (M_Y M_Y^T)_{ii} - 2(M_X M_Y^T)_{ii}] \\ &= \text{tr}(M_X M_X^T) + \text{tr}(M_Y M_Y^T) - 2\text{tr}(M_X M_Y^T) \\ &\stackrel{(b)}{=} \text{tr}(X X^T X X^T) + \text{tr}(Y Y^T Y Y^T) - 2\text{tr}(X X^T Y Y^T) \\ &\stackrel{(c)}{=} \text{tr}(X^T X X^T X) + \text{tr}(Y^T Y Y^T Y) - 2\text{tr}(Y^T X X^T Y) \\ &\stackrel{(d)}{=} \|X^T X\|_{\mathbb{F}}^2 + \|Y^T Y\|_{\mathbb{F}}^2 - 2\|X^T Y\|_{\mathbb{F}}^2, \end{aligned}$$

where in (a) we exploited that  $M_X$  and  $M_Y$  are symmetric, in (b) we used the definition of  $M_X, M_Y$ , in (c) we used that property of the trace stating that  $\text{tr}(AB) = \text{tr}(BA)$ , and finally in (d) we applied the definition of the Frobenius norm.

## Temporal graph randomizations

In Table 1 we summarize the properties of the temporal graphs we used to conduct our tests.

We now give a more detailed description of the randomization techniques we adopted, defined in terms of the quantities they preserve. According to the method, it may be more convenient to represent the temporal graph as a sequence of instantaneous interactions  $(i, j, t)$ , as a sequence of interactions with a duration  $(i, j, t, \tau)$ , or as a sequence of weighted adjacency matrices  $W^{(t)}$  [64]. Before randomization, time is discretized at the scale of 10 minutes in each data set, and the cumulative interaction time in each 10-minute window is used as weight.

Table 1: Summary properties of the **SocioPatterns** time-resolved proximity networks used here. *Graph name* is used to identify the graphs; *Description* provides concise information on the context where data were collected;  $n$  is the number of graph nodes; *Duration* is the temporal span of the dataset, and  $T$  is the number of graph snapshots.

Graph name	Description	$n$	Duration	$T$
<i>Primary school</i> [70, 77]	Children of 10 classes of a primary school	242	2 days	194
<i>High school 1</i> [78]	Students of 3 classes of a high school in 2011	126	4 days	453
<i>High school 2</i> [78]	Students of 5 classes of a high school in 2012	180	7 days	1215
<i>High school 3</i> [79]	Students of 9 classes of a high school in 2013	327	5 days	605
<i>Baboons</i> [80]	A group of baboons	13	27 days	3986
<i>Households</i> [81]	People of a village in Malawi	86	26 days	1926
<i>Hospital</i> [82]	Patients and health-care workers of a hospital	75	5 days	579
<i>Conference</i> [12]	People at a medical conference	405	2 days	190
<i>Office</i> [83]	Office workers in an office building	92	19 days	1646

1. *Random*. Temporal edges are represented as  $(i, j, t)$  and all three indices are randomized, avoiding self-edges ( $i$  and  $j$  randomized between 1 and  $n$ , and  $t$  between 1 and  $T$ ).  
**Preserved quantities:** number of temporal edges.
2. *Random delta*. Temporal edges are represented as  $(i, j, t, \tau)$ . Once again,  $i, j, t$  are randomized ( $t$  is sampled between 1 and  $T - \tau$ ), while  $\tau$  is preserved.  
**Preserved quantities:** number of temporal edges and contact duration distribution.
3. *Active snapshot*. At each time step  $t$ , the edges are randomly replaced between active nodes at  $t$ , *i.e.* that had at least one neighbor in the original snapshot.  
**Preserved quantities:** number of edges at each time-step and activity pattern of each node.
4. *Time*. Temporal edges are represented as  $(i, j, t)$  and only the index  $t$  is randomized.  
**Preserved quantities:** aggregated graph structure.
5. *Sequence*. The graph is represented as a sequence of weighted adjacency matrices  $W^{(t)}$  and the randomization acts on the indices  $t$ .  
**Preserved quantities:** the structure of each snapshot.
6. *Weighted degree*. Temporal edges are represented as  $(i, j, t)$  and all three indices are randomized as in *Random* but with the constraint that each node has the same number of contacts as in the original network.  
**Preserved quantities:** nodes weighted degree.

## Synthetic models

We here provide a formal definition of the models used to generate the synthetic graphs under analysis. Even though we considered four models, three of these can be generated from the *degree corrected stochastic block model* [58] by changing its parameters.

**Definition 3 (Degree corrected stochastic block model)** Let  $\mathcal{V}$  be a set of  $n$  nodes and  $\ell \in [k]^n$  be a vector mapping each node to a class. Further let  $C \in \mathbb{R}^{k \times k}$  be a positive symmetric matrix and  $\theta \in \mathbb{R}^n$  be a vector satisfying  $\theta^T \mathbf{1}_n = n$ . The entries of the graph adjacency matrix  $A \in [0, 1]^{n \times n}$  are generated independently (up to symmetry) at random with probability

$$\mathbb{P}(A_{ij} = 1) = \min \left( 1, \theta_i \theta_j \frac{C_{\ell_i, \ell_j}}{n} \right).$$

The vector  $\ell$  contains the labels and gives a community structure in the case in which  $C_{a,a} > C_{a,b}$  for  $b \neq a$ , meaning that there is a higher probability that two nodes in the same community will get connected. The value  $\theta_i$  is proportional to the expected degree of node  $i$ . For this reason, if one chooses  $\theta = \mathbf{1}_n$  and  $\ell = \mathbf{1}_n$ , one gets the Erdős-Renyi model, in which every node has the same expected degree, and there are no communities. The configuration model, instead, is obtained by letting  $\ell = \mathbf{1}_n$ , but changing the value of  $\theta$  to create an arbitrary degree distribution that we choose to be a (properly rescaled) uniform distribution between 3 and 10 raised to the power 4. Finally, the stochastic block model is obtained from a labeling vector different from  $\mathbf{1}_n$  and letting  $\theta = \mathbf{1}_n$ . We consider  $k = 5$  communities of equal size with  $C_{a,b} = 20\delta_{ab} + (1 - \delta_{ab})$ , with  $\delta$  the Kroeneker symbol.

Let us finally introduce the random geometric model.

**Definition 4 (Random geometric model)** Let  $\mathcal{V}$  be a set of  $n$  nodes. For each  $i \in \mathcal{V}$  let  $\mathbf{x}_i \in \mathbb{R}^2$  be a random vector with norm  $\|\mathbf{x}_i\| \leq 1$ . The entries of the graph adjacency matrix  $A \in [0, 1]^{n \times n}$  are generated independently (up to symmetry) at random with probability

$$\mathbb{P}(A_{ij} = 1) = e^{-\beta \|\mathbf{x}_i - \mathbf{x}_j\|},$$

for some positive  $\beta$ .

Note that even though the entries of  $A$  are drawn at random, this model can generate graphs with a high clustering coefficient because the probability depends on the relative distance of a fixed embedding. In our simulations, we set  $\beta = 20$ .

## Acknowledgments

LD and CC acknowledge support from the Lagrange Project of the ISI Foundation funded by CRT Foundation and from Fondation Botnar (EPFL COVID-19 Real Time Epidemiology I-DAIR Pathfinder). AB acknowledges support from the Agence Nationale de la Recherche (ANR) project DATAREDEX (ANR-19-CE46-0008).

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