

# GoT-WAVE: Temporal network alignment using graphlet-orbit transitions

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## Abstract

Global pairwise network alignment (GPNA) aims to find a one-to-one node mapping between two networks that identifies conserved network regions. GPNA algorithms optimize node conservation (NC) and edge conservation (EC). NC quantifies topological similarity between nodes. Graphlet-based degree vectors (GDVs) are a state-of-the-art topological NC measure. Dynamic GDVs (DGDVs) were used as a dynamic NC measure within the first-ever algorithms for GPNA of *temporal* networks: DynaMAGNA++ and DynaWAVE. The latter is superior for larger networks. We recently developed a different graphlet-based measure of temporal node similarity, graphlet-orbit transitions (GoTs). Here, we use GoTs instead of DGDVs as a new dynamic NC measure within DynaWAVE, resulting in a new approach, GoT-WAVE.

On synthetic networks, GoT-WAVE improves DynaWAVE's accuracy by 25% and speed by 64%. On real networks, when optimizing only dynamic NC, each method is superior  $\approx 50\%$  of the time. While DynaWAVE benefits more from also optimizing dynamic EC, only GoT-WAVE can support *directed* edges. Hence, GoT-WAVE is a promising new temporal GPNA algorithm, which efficiently optimizes dynamic NC. Future work on better incorporating dynamic EC may yield further improvements.

# 1 Introduction

Network alignment (NA) aims to find similar (conserved) regions between compared networks. These regions are not expected to be perfect fits, and thus, NA deviates from the traditional subgraph isomorphism problem [41]. Then, NA can be used for knowledge transfer from a well-known system to a poorly-studied system between their conserved network regions [8]. For example, in computational biology, NA can be used to identify topologically similar (and possibly also sequence-similar) regions of molecular networks of different species and to predict functions of currently unannotated proteins based on functions of their aligned partners in another network [12].

NA produces either: (a) a many-to-many mapping of highly conserved but small network regions or (b) a one-to-one mapping that covers every node of the smaller network and equally many nodes from the other network and is thus large, but is often suboptimally conserved [8, 10]. Both NA types, called local and global, respectively, have (dis)advantages [30, 17]. We focus on global NA.

Global NA can be pairwise [24], resulting in aligned pairs of nodes between two networks, or multiple [13, 46], resulting in aligned node clusters between three or more networks. Multiple NA is more computationally complex than pairwise NA and, furthermore, recent work suggests that multiple NA is also less accurate than pairwise NA [44]. So, here, we focus on pairwise NA, and in particular on global pairwise NA (GPNA).

GPNA consists of two algorithmic components: 1) an objective function, typically node conservation (a measure of node similarity) combined with edge conservation, and 2) an optimization strategy (also called alignment strategy) that aims to maximize the objective function.

Regarding the first component and specifically the node conservation part, graphlet degree vectors (GDVs) [36, 33] have been widely used as topological properties (features) to measure node conservation in GPNA due to the rich topological information that graphlets capture [32, 29, 47]. GDV-based node conservation was shown to be superior in the task of GPNA under the same optimization strategy to other node conservation/similarity measures: IsoRank’s PageRank and GHOST’s spectral signature measures from the biological domain [12, 7], or node2vec and struc2vec network embedding measures from the social domain [16]. Regarding the first component and specifically the edge conservation part, several established measures of edge conservation exist:  $S^3$ , which rewards an alignment when edges are aligned to each other and penalizes it when an edge is aligned to a non-edge [39], and weighted edge conservation (WEC), which is high if many edges are aligned to each other *and* the nodes of the aligned edges are similar with respect to node conservation [40].

Regarding the second component, existing GPNA algorithms have one of two types of optimization strategy. One type is seed-and-extend, where first two highly similar nodes (with respect to node conservation) are aligned, i.e., seeded. Then, the seed’s network neighbors that are similar are aligned, the seed’s neighbor’s neighbors that are similar are aligned, and so on. The exten-

sion around the seed and exploration of the seed’s neighbors aims to improve both node and edge conservation of the resulting alignment. The extension continues until all nodes in the smaller network are aligned, i.e., until a one-to-one (injective) node mapping is produced. WAVE is a representative state-of-the-art seed-and-extend optimization strategy (that we focus on for reasons discussed below), which by default optimizes GDV-based node conservation and WEC [40]. The other type of optimization strategy is a search algorithm. Here, instead of aligning node by node as with the seed-and-extend approach, entire alignments are explored and the one with the best objective function score is returned. MAGNA++ [47] is a representative state-of-the-art search algorithm (that we focus on for reasons discussed below), which uses a genetic algorithm to, by default, optimize GDV-based node conservation and  $S^3$ . Importantly, a typical optimization strategy, including WAVE and MAGNA++, can optimize any objective function, i.e., it is not limited to e.g., GDV-based node conservation and  $S^3$  or WEC. Note that in a recent comprehensive evaluation of different methods [30], WAVE and MAGNA++ rose to the top, although newer GPNA methods have appeared since, such as SANA [27].

Traditional GPNA methods align *static* networks [44]. However, because most of real-world systems evolve over time and thus exhibit a dynamic nature, they are intrinsically not static. As such, they can only be truly understood by accounting for their evolution [19]. The first-ever methods for GPNA of *temporal* networks (see below) were proposed only recently. This could be due to limitations of current biotechnologies for data collection, which have resulted in a lack of temporal network data on molecular systems, such as protein-interaction networks (PINs), that are the systems to which static GPNA methods have been extensively applied [23, 32, 47]. However, as initial temporal PIN data begin to emerge [11, 49], and as other temporal network data become available, e.g., brain, ecological, or social networks [14, 5, 34, 37], temporal GPNA will gain increasing importance.

The only temporal GPNA methods currently available are DynaMAGNA++ [43] and DynaWAVE [45], temporal extensions of MAGNA++ and WAVE. DynaWAVE was shown to be more accurate and faster than DynaMAGNA++ on medium- and large-size networks; DynaMAGNA++ was more accurate (yet slower) on small-size ( $\approx 100$ -node) networks. Since most of real-world networks are not small, we focus on DynaWAVE. This method uses the same seed-and-extend optimization strategy as static WAVE, but it uses it to optimize *dynamic* node and edge conservation. As its dynamic node conservation, DynaWAVE uses a temporal extension of GDVs, dynamic GDVs (DGDVs), which were originally proposed for tasks of node and network classification by [21]. DGDV of a node uses dynamic graphlets to describe the node’s neighborhood in a temporal network. Comparing nodes’ DGDVs yields a measure of similarity between the nodes’ evolving neighborhoods, i.e., dynamic node conservation. As its dynamic edge conservation, DynaWAVE uses dynamic WEC (DWEC), a temporal analog of WAVE’s WEC that generalizes an aligned edge to an aligned event (temporal edge) [45]. Just as WAVE, DynaWAVE can use its optimization strategy in combination with any objective function.

We recently developed graphlet-orbit transitions (GoTs) [3], a different temporal graphlet measure of node similarity. GoTs describe how a node’s neighborhood is evolving by measuring how its participation in different graphlet positions (orbits) changes with time. For example, GoTs can capture when a node in the center of a  $k$ -node star at time  $t$  becomes a part of a  $k$ -node clique at time  $t + 1$ . So far, we used GoTs for network classification. Here, we aim to use GoTs for temporal GPNA as a new dynamic node conservation measure within DynaWAVE. We refer to our GoT-modified version of DynaWAVE as GoT-WAVE.

We evaluate whether GoT-WAVE improves upon DynaWAVE by mimicking the evaluation from the DynaWAVE study. Namely, we evaluate on synthetic data containing 50 temporal networks produced by dynamic versions of five well known graph models. Here, we align all pairs of networks to each other. A good temporal GPNA method should identify as similar those networks that originate from the same model and as dissimilar those networks that originate from different models. Also, we compare the methods on eight real-world networks from biological and social domains. Here, we align each network to its noisy version, in which a percentage of the original network’s edges is rewired. Since the aligned networks have the same nodes, we know which nodes should be mapped to which nodes. The more nodes are correctly mapped, the better the method. In all evaluation tests, we compare the two methods when they optimize: 1) only their respective dynamic node conservation measures (GoTs versus DGDVs), to *fairly* evaluate the two measures against each other, and 2) both node and edge conservation, to give each method the *best-case* advantage (it was already shown that DynaWAVE performs better when it optimizes both rather than only one of node and edge conservation).

We find that on synthetic networks, under both the fair and best-case scenario, GoT-WAVE is more accurate than DynaWAVE by 25% and faster by 64%. On real networks, under the fair scenario, GoT-WAVE is more accurate than DynaWAVE for four of the eight networks, performing better on the denser networks and worse on the sparser ones. We observe the opposite in terms of their running times, i.e., GoT-WAVE is slower than DynaWAVE for denser networks and faster for sparser networks. Thus, the two methods are complementary. Under the best-case scenario, DynaWAVE’s performance is more enhanced than GoT-WAVE’s when dynamic edge conservation is considered as well, as DynaWAVE is now better for all eight networks. However, because GoTs is the only current temporal graphlet-based measure of node similarity that supports edge direction, GoT-WAVE is the only temporal GPNA method that can deal with directed networks (DGDVs and thus DynaWAVE always assume that edges are undirected).

Thus, GoT-WAVE is a promising new temporal GPNA method that efficiently optimizes dynamic node conservation. Finding new measures of dynamic edge conservation better suited for GoT-WAVE could further enhance its performance, which is the subject of future work. Also, GoTs, when used as node conservation within any newer or future GPNA optimization strategies, such as SANA, could yield further improvements.

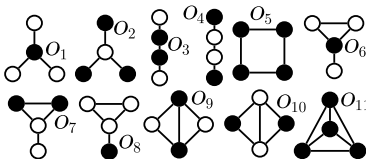


Figure 1: All 11 orbits of all six undirected 4-node graphlets. Nodes that are in the same orbit (i.e., are topologically equivalent) in a given graphlet are colored in black. For example,  $o_1$  and  $o_2$  are two possible orbits of a 4-node star, orbits  $o_3$  and  $o_4$  are two possible orbits of a 4-node chain, etc.

## 2 Methods

### 2.1 Concepts and terminology

A network or *graph*  $G$  is comprised of a set of *vertices* or *nodes*,  $V(G)$ , and a set of *edges*,  $E(G)$ . Nodes represent entities and edges correspond to relationships between the entities. Edges are represented as pairs of vertices of the form  $(a, b)$ , where  $a, b \in V(G)$ . In *directed* graphs, edges  $(i, j)$  are *ordered pairs* (translated to “ $i$  goes to  $j$ ”), whereas in *undirected* graphs there is no order since nodes are always reciprocally connected. Our proposed methodology (see below) is applicable to both undirected and directed graphs [2]. A temporal network comprises  $s$  consecutive network snapshots. We denote the set of all snapshots of a temporal network  $G$  by  $\mathcal{S}(G)$ , and the  $i^{\text{th}}$  snapshot as  $\mathcal{S}_i(G)$ . A temporal network can gain/lose nodes/edges from  $\mathcal{S}_i(G)$  to  $\mathcal{S}_{i+1}(G)$ . We denote the number of nodes in snapshot  $i$  by  $N_i$ .

Graphlets are small non-isomorphic subgraphs. Different node positions (or symmetry groups) in a graphlet are called orbits. For example, it is different to be at the center of a star or at its periphery. All orbits of all undirected graphlets with four nodes are illustrated in Figure 1. Graphlets are a general concept (e.g., not specific to a given size, and edge direction can be incorporated). We denote by  $u\mathcal{O}_k$  the set of all orbits of all  $k$ -node undirected graphlets, and by  $d\mathcal{O}_k$  the equivalent for directed graphlets. We use the simpler  $\mathcal{O}$  notation when the concept is general. The GDV of node  $v$ ,  $\text{GDV}(v)$ , counts how many times node  $v$  appears in (i.e., touches) each orbit  $o \in \mathcal{O}$  (Figure 2). The notion of graphlets and GDVs has been extended from the static to temporal context, into dynamic graphlets and DGDVs. For details, see [21].

### 2.2 Static and temporal GPNA

Static GPNA produces an injection  $f : V(G) \rightarrow V(H)$ , where  $V(G)$  is not bigger than  $V(H)$ , maximizing node or edge conservation between aligned node pairs. Temporal GPNA, extending static GPNA, aims to optimize dynamic node or edge conservation. As dynamic node conservation, we optimize similarity between nodes’ temporal graphlet-based features, namely GoTs, which we define in Section 2.3. We compare nodes’ GoTs as described in Section 2.4. As dy-

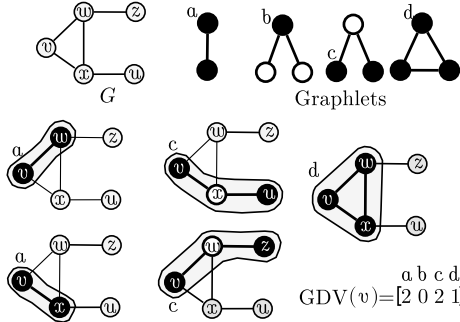


Figure 2: Illustration of  $\text{GDV}(v)$  that counts how many times  $v$  participates in each of the orbits  $a$ ,  $b$ ,  $c$  and  $d$  of all undirected 2-3-node graphlets. In this example,  $v$  touches orbit  $a$  twice (i.e., has degree of two), the periphery of a 3-node chain (orbit  $c$ ) twice, and a triangle (orbit  $d$ ) once.

dynamic edge conservation, when we also optimize this measure, we use DWEC, just as DynaWAVE does. That is, compared to DynaWAVE, the only aspect that we modify is its DGV-based dynamic node conservation measure, replacing it with our GoT-based measure. This ensures a fair comparison between GoTs and DGDVs as two different temporal graphlet-based node features.

### 2.3 Graphlet orbit-transitions (GoTs)

Just like DGDVs, GoTs only account for connected graphlets. Consider the two possible 3-node undirected connected graphlets (chain and triangle) and their orbits from Figure 3. A chain has two possible orbits, i.e., a node can be either at the center of the chain or in one of its leaves. A triangle has

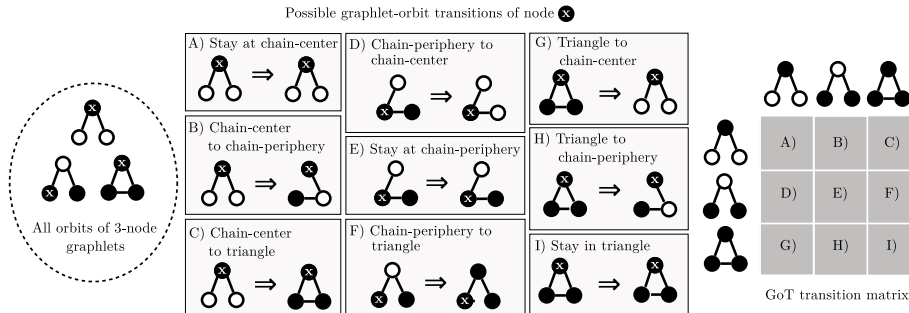


Figure 3: All possible graphlet-orbit transitions (GoTs) of 3-node undirected graphlets and the corresponding GoT matrix. Node  $x$  is the node being considered (whose GoT matrix is shown), and black nodes are in the same orbit as  $x$ . Each cell  $(i, j)$  of the GoT matrix represents the number of times node  $x$  transitions from orbit  $i$  to orbit  $j$ .

a single orbit, as all of its nodes are topologically equivalent. GoTs are the matrix of changes (transitions) between every possible pair of orbits across two consecutive snapshots. There are a total of  $3 \times 3 = 9$  possible orbit transitions in Figure 3. A node can remain in its previous orbit, be it a (A) chain-center, (D) chain-periphery or (I) triangle-node. Or, it can transition from the chain-center to the chain-periphery (B) or to a triangle-node (C), etc. All possibilities for the 3-node graphlets are illustrated in Figure 3; in practice, we use larger graphlets as well (see below). The matrix from Figure 3 illustrates the GoTs of node  $x$  that we use as  $x$ 's feature vector. This matrix offers rich topological information that can be used for various tasks [3]. Here, we use it in the task of temporal GPNA.

Regarding the considered graphlet size, [21] recommended the use of all DGDVs with up to four nodes and six events (temporal edges). This is what we do, to give the best-case advantage to DynaWAVE. For a fair comparison, to account for as similar as possible amount of network topology with both DGDVs and GoTs, we also use all undirected GoTs with up to four nodes, unless explicitly stated otherwise.

## 2.4 GoT-WAVE

For each node, we compute its GoT matrix, flatten the matrix to a vector, and use the vector as the node's features. The feature vectors over all nodes in a network form a  $\#Nodes \times \#Transitions$  matrix. For two networks being aligned, this results in two corresponding matrices with the same number of columns, whose rows are then joined together. Due to high dimensionality and sparsity of the joined matrix, we perform dimensionality reduction on the matrix using principal component analysis, keeping 99% of its variance. Then, we compute the topological similarity between every two nodes from different networks as the cosine similarity between the nodes' PCA-reduced feature vectors. GoT-WAVE uses the resulting node similarities as the dynamic node conservation part of the objective function, which is then optimized using WAVE. In all of the above steps, we do exactly what DynaWAVE does to produce DGDV-based node similarities and perform DGDV-based temporal GPNA.

GoT-WAVE, like DynaWAVE, can optimize dynamic node conservation (i.e., GoTs for GoT-WAVE, DGDVs for DynaWAVE), dynamic edge conservation (DWEC), or both. Its objective function is  $\alpha S_E + (1 - \alpha) S_N$ , where  $S_E$  and  $S_N$  are dynamic edge and node conservation measures, respectively, and  $\alpha \in [0, 1]$  controls how important each measure is. We use: 1)  $\alpha = 0$ , to *fairly* evaluate the two measures against each other, meaning that only dynamic node conservation is considered, or 2)  $\alpha = \frac{1}{2}$ , to give each method the *best-case* advantage, since this  $\alpha$  value seems to work the best for DynaWAVE [45].

## 3 Results and discussion

Results were gathered on a Intel i7-6700 CPU at 3.4GHz with 16GB of RAM. Execution times were obtained using a single core for computation. In the fol-

lowing tests we measure potential improvement of GoT-WAVE over DynaWAVE as follows. Let us denote by  $S_G$  the (accuracy or running time) score of GoT-WAVE, and by  $S_D$  the score of DynaWAVE. Also, let us denote by  $G_A$  the relative gain of GoT-WAVE over DynaWAVE in terms of accuracy, and by  $G_T$  the relative gain GoT-WAVE over DynaWAVE in terms of running time. Since for accuracy, a larger score is better, we define  $G_A = \frac{S_G - S_D}{\min(S_G, S_D)} \times 100\%$ . On the other hand, since for running time, a lower score is better, we define  $G_T = \frac{S_D - S_G}{\min(S_G, S_D)} \times 100\%$ . In both cases, positive gain (i.e., a positive  $G_A$  or  $G_T$  value) would indicate improvement of GoT-WAVE compared to DynaWAVE, and negative gain (i.e., a negative  $G_A$  or  $G_T$  value) would indicate degradation of GoT-WAVE compared to DynaWAVE. For example, in terms of accuracy, if GoT-WAVE has accuracy of 1 and DynaWAVE has accuracy of 0.7, then  $G_A = \frac{1 - 0.7}{0.7} \times 100\% = 43\%$  (i.e., GoT-WAVE is superior to DynaWAVE). On the other hand, if GoT-WAVE has accuracy of 0.7 and DynaWAVE has accuracy of 1, then  $G_A = \frac{0.7 - 1}{0.7} \times 100\% = -43\%$  (i.e., GoT-WAVE is inferior to DynaWAVE). As another example, in terms of running time, if GoT-WAVE takes 2 seconds and DynaWAVE takes 6 seconds, then  $G_T = \frac{6 - 2}{2} \times 100\% = 200\%$  (i.e., GoT-WAVE is superior to DynaWAVE). On the other hand, if GoT-WAVE takes 6 seconds and DynaWAVE takes 2 seconds, then  $G_T = \frac{2 - 6}{2} \times 100\% = -200\%$  (i.e., GoT-WAVE is inferior to DynaWAVE).

### 3.1 Evaluation using synthetic networks

As often done [35, 32, 21], we compare DynaWAVE and GoT-WAVE on a set of synthetic networks from different graph models. We develop temporal versions of well-known models: Erdős-Rényi random graphs [9], Barabási-Albert preferential attachment [4], Watts-Strogatz small-world networks [48], geometric gene duplication model with probability cutoff [35] and scale-free gene duplication [42]. A good GPNA method should identify networks from the same model as being more topologically alike (that is, a having higher alignment quality, i.e., objective function score) than networks from different models.

#### 3.1.1 Synthetic networks

We generate networks with 24 snapshots each ( $T = 24$ ). In each snapshot, new nodes arrive at the network and new edges are added to it until the desired edge density is reached. Node arrival is either linear ( $N_t = \frac{N_T - N_1}{T - 1} \cdot (t - 1) + N_1$ ) or exponential ( $N_t = N_1 \cdot e^{\frac{(t-1)}{10}}$ ), where  $t$  is the index of the snapshot,  $T$  is the total number of snapshots,  $N_1$  is the number of nodes at the start and  $N_t$  is the number of nodes at snapshot  $t$ . We set the arrival function of each model according to what was reported as the observed node arrival function for similar models [25]. How new edges are added (i.e., which nodes they connect) is specific to each model. Edge density is set at  $\approx 1\%$  for all models, mimicking real-world networks (such as PPIs, internet routing and email networks [28]), and remains stable for all snapshots (e.g., this stability was observed in online



social networks by [20]). Each network starts with 100 nodes and grows to 1,000 nodes. We generate ten networks for each of the five graph models, giving us 50 networks with 24 snapshots each, totaling to 1200 snapshots.

### 3.1.2 Performance on synthetic networks

With each of GoT-WAVE and DynaWAVE, we align all pairs of synthetic networks. We compute objective function scores of all alignments. We consider an objective score threshold of  $k$ . Then, a pair of networks is: i) a true positive if their alignment’s objective score is  $k$  or higher and the networks belong to the same model, ii) a false positive if their alignment’s objective score is  $k$  or higher but the networks belong to different models, iii) a false negative if their alignment’s objective score is lower than  $k$  but the networks belong to the same model, and iv) a true negative if their alignment’s objective score is lower than  $k$  and the networks belong to different models. By varying  $k$ , we compute the area under the precision-recall (AUPR) or receiver operating characteristic (AUROC) curve. We compare GoT-WAVE and DynaWAVE with respect to these measures. Note that given the five graph models, the expected AUROC by chance is 0.2.

Under the fair-case scenario, when optimizing solely node conservation ( $\alpha = 0$ ), GoT-WAVE’s AUPR and AUROC are higher by 25% and 32%, respectively, than DynaWAVE’s (Table 1 (a)).

For this particular dataset, also optimizing edge conservation (i.e.,  $\alpha = \frac{1}{2}$ ) decreases performance of both methods, even though it was previously argued that  $\alpha = \frac{1}{2}$  is the best-case scenario [45, 43]. Actually, we also verify that  $\alpha = \frac{1}{2}$  is indeed the best-case scenario on our considered real networks (Section 3.2). It is just that on our considered synthetic networks,  $\alpha = 0$  happens to be both the fair and best-case scenario for both methods, and under this scenario, GoT-WAVE is superior to DynaWAVE.

On synthetic networks, we also find that extracting GoT features is overall 64% faster than extracting DGDV features (Table 1 (b)). Because both methods use their features in the same alignment strategy (WAVE), their alignment times

Table 1: Results on synthetic networks when only node conservation is optimized ( $\alpha = 0$ ) or when node and edge conservation are optimized ( $\alpha = \frac{1}{2}$ ). In parentheses, we show relative improvement (positive gain) or degradation (negative gain) in performance of GoT-WAVE compared to DynaWAVE.

AUPR		
$\alpha$	DynaWAVE	GoT-WAVE
0	0.63	<b>0.79</b> (+25%)
$\frac{1}{2}$	0.59	0.53 (-11%)
AUROC		
$\alpha$	DynaWAVE	GoT-WAVE
0	0.59	<b>0.78</b> (+32%)
$\frac{1}{2}$	0.54	0.70 (+30%)

(a) Accuracy.

Model	DGDVs	GoTs
<b>Random</b>	26s	<b>22s</b> (+18%)
<b>ScaleFree</b>	<b>22s</b>	25s (-14%)
<b>Small-world</b>	23s	<b>4s</b> (+475%)
<b>Geo-GD</b>	34s	<b>11s</b> (+210%)
<b>ScaleFree-GD</b>	16s	<b>12s</b> (+33%)
Total	121s	<b>74s</b> (+64%)

(b) Feature extraction times.

are similar, as expected.

Note that we also performed a subset of all tests for synthetic networks, and specifically those under the fair evaluation scenario ( $\alpha = 0$ ), using the other existing DGDV-based temporal GPNA method, DynaMAGNA++, and a GoT-modified version of it, which we refer to as GoT-MAGNA++. Here, we used the following values of MAGNA++’s parameters: population size of 1000 and 1000 generations. These results are qualitatively similar to those reported above: GoT-MAGNA++’s AUPR and AUROC are 16% and 22% higher, respectively, than DynaMAGNA++’s. However, we maybe did not give DynaMAGNA++ the best-case advantage, because this method was shown to work the best for  $\alpha = \frac{1}{2}$ , and under larger values of its parameters than those that we were able to consider due to MAGNA++’s high running time. So, it is possible that the performance of DynaMAGNA++ (and GoT-MAGNA++) could be improved. However, testing this would take too much computational time, and it would do so unnecessarily, given that DynaWAVE was already shown to outperform DynaMAGNA++ in terms of both accuracy and running time on all networks but the smallest ones (with  $\approx 100$  nodes). So, we believe that our detailed tests against DynaWAVE are sufficient.

### 3.2 Evaluation using real-world networks

Section 3.1 studies GPNA at the network level (whether networks are from the same model), while here we study GPNA at the node level (whether nodes are correctly aligned). A typical process to evaluate GPNA at the node level on a real network is to insert artificial noise into the network, that is, rewire a percentage of its temporal edges (events), and align the original network to the noisy version [45]. Then, since the aligned networks have the same nodes, we can measure the percentage of all nodes that are correctly aligned.

To randomize a dynamic network, we use 3 different randomization schemes. For undirected networks, we use an established randomization scheme [18], which we refer to as *undirected randomization*. This scheme chooses two random events and swaps their time stamps with some probability. For directed networks, we use a variation of the above scheme that has an additional parameter that controls the probability of switching the edge directions of the events, which we refer to as *directed randomization*. For directed networks, we use an additional randomization scheme that only swaps the edge direction of events but not their time stamps, which we refer to as *pure directed randomization*. For a given scheme, we study 10 randomization (i.e., noise) levels, from 0% to 20% in increments of 2%. At each noise level, we produce five random network instances and average the results over the five runs.

First, for a given method, at each noise level, for each alignment, we compute the corresponding objective function score. Ideally, the objective score should decrease as the network is aligned to progressively noisier versions. Furthermore, since we know the perfect alignment between the original network and each of its randomized versions (as their nodes are the same), we compute the ideal objective score – the quality of the perfect alignment, as measured by

DynaWAVE’s and GoT-WAVE’s objective function. We denote the objective scores of the ideal and method-produced alignments for noise  $n$  by  $S_{i,n}$  and  $S_{p,n}$ , respectively. The expectation is that a good method’s produced objective score should be similar to the method’s ideal objective score, i.e.,  $|S_{p,n} - S_{i,n}|$  should be as close as possible to 0. Also, since we want to account for scaling (e.g., the difference of 0.1 between 0.9 and 0.8 is not the same as the difference of 0.1 between 0.3 and 0.2), we divide the difference between the produced and ideal alignment by their maximum, i.e.,  $\max(S_{p,n}, S_{i,n})$ . With these points in mind, we compute the distance  $dis(S_p, S_i)$  over all considered noise levels  $n$  (from 0% to 20%) as:  $dis(S_p, S_i) = \sum_{n=0\%}^{20\%} \frac{|S_{p,n} - S_{i,n}|}{\max(S_{p,n}, S_{i,n})}$

For each network, we compute this distance for each of GoT-WAVE and DynaWAVE. Then, we summarize gain of GoT-WAVE compared to DynaWAVE: let us denote by  $S_G$  the distance score of GoT-WAVE, and by  $S_D$  the score of DynaWAVE. Since a lower distance score is better, we compute the relative gain of GoT-WAVE over DynaWAVE, denoted by  $G_O$ , as:  $G_O = \frac{S_D - S_G}{\min(S_G, S_D)} \times 100\%$ . Positive gains mean that GoT-WAVE is superior to DynaWAVE and negative gains mean that GoT-WAVE is inferior to DynaWAVE.

Second, we compare GoT-WAVE and DynaWAVE in terms of node correctness (see above). Let us denote by  $S_G$  the node correctness of GoT-WAVE, and by  $S_D$  the node correctness of DynaWAVE. Since higher node correctness is better, we compute the relative gain of GoT-WAVE over DynaWAVE, denoted by  $G_{NC}$ , as:  $G_{NC} = \frac{S_G - S_D}{\min(S_G, S_D)} \times 100\%$ . Again, positive gains mean that GoT-WAVE is superior to DynaWAVE and negative gains mean that GoT-WAVE is inferior to DynaWAVE.

### 3.2.1 Real-world temporal networks

We analyze eight real networks (Table 2). Six of them are undirected, three of which are biological networks from the DynaWAVE study, and three are social networks. Due to the lack of directed biological temporal networks, we use two directed temporal networks from other fields.

### 3.2.2 Performance on real undirected networks

In terms of the objective score (Figure 4 both DynaWAVE and GoT-WAVE show adequate behavior, i.e., the objective score decreases as we add more noise. When optimizing solely node conservation ( $\alpha = 0$ ), we observe that:

Table 2: Real temporal networks used in our experiments.

Network	Nodes	Events	Snaps.	Description
<b>zebra</b> [38]	27	500	57	Zebra proximity network
<b>yeast</b> [43]	1,004	10,403	8	Yeast PIN
<b>aging</b> [11]	6,300	76,666	38	Human aging PIN
<b>school</b> [15]	327	7,388	5	School proximity network
<b>gallery</b> [22]	420	22,476	16	Gallery proximity network
<b>arxiv</b> [26]	2,504	138,495	7	Paper co-authorships
<b>emails</b> [31]	167	8,771	9	E-mail communication
<b>tennis</b> [1]	876	103,938	42	Player dominance network

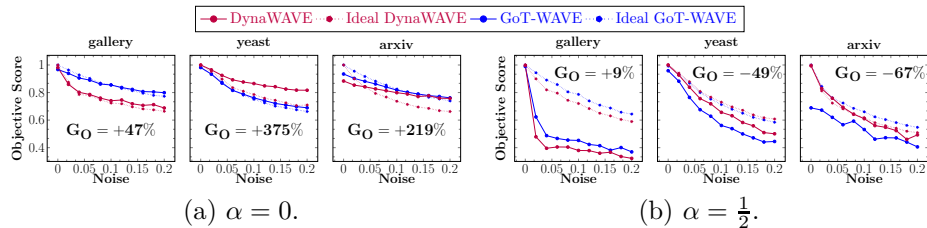


Figure 4: Comparison between GoT-WAVE and DynaWAVE on undirected networks in terms of how well their alignments’ objective scores match the objective scores of ideal alignments, when (a) only node conservation is optimized ( $\alpha = 0$ ) and (b) both node and edge conservation are optimized ( $\alpha = \frac{1}{2}$ ). Recall that  $G_O$  is the relative gain of GoT-WAVE over DynaWAVE (positive: GoT-WAVE is superior; negative: DynaWAVE is superior).

(i) for **gallery** and **zebra** networks, both methods closely match their ideal alignments over all noise levels; (ii) for **yeast** and **aging** networks, both methods closely match their ideal alignments for low noise levels, but for high noises levels, DynaWAVE drifts away from its ideal alignments while GoT-WAVE still closely matches its ideal alignments; and (iii) for **arxiv** and **school** networks, both methods are far from their ideal alignments for low noise levels, but for high noise levels, GoT-WAVE closely matches its ideal alignments while DynaWAVE is still far from its ideal alignments. In other words, in terms of the total gain  $G_O$ , GoT-WAVE improves upon DynaWAVE, more closely matches its ideal alignments than DynaWAVE, for all six networks. When optimizing both node and edge conservation ( $\alpha = \frac{1}{2}$ ), GoT-WAVE more closely matches its ideal alignments for two out of the six networks (**gallery** and **aging**). So, the two methods can be seen as complementary.

In terms of node correctness (Table 3, Figure 5), for  $\alpha = 0$ , the two methods are again complementary - each is the best for three of the six networks. For  $\alpha = \frac{1}{2}$ , DynaWAVE’s node correctness improves more substantially than GoT-WAVE’s, which is why now DynaWAVE is superior for most (though not all) of the networks. In short, GoT-WAVE already captures some of the informa-

Table 3: Node correctness when aligning an undirected real network to itself (noise = 0). In parentheses, we show relative improvement (positive gain) or degradation (negative gain) in performance of GoT-WAVE compared to DynaWAVE. In bold, we show the best result for each network.

	(a) $\alpha = 0$		(b) $\alpha = \frac{1}{2}$	
Network	DynaWAVE	GoT-WAVE	DynaWAVE	GoT-WAVE
<b>zebra</b>	<b>0.926 ± 0.05</b>	0.578 ± 0.09 (-60%)	0.911 ± 0.04	0.615 ± 0.14 (-48%)
<b>yeast</b>	<b>0.966 ± 0.01</b>	0.924 ± 0.01 (-5%)	<b>0.966 ± 0.01</b>	0.919 ± 0.01 (-5%)
<b>aging</b>	0.912 ± 0.01	0.942 ± 0.01 (+3%)	<b>0.959 ± 0.01</b>	0.955 ± 0.01 (-0.4%)
<b>arxiv</b>	0.340 ± 0.02	0.446 ± 0.02 (+31%)	<b>0.658 ± 0.01</b>	0.602 ± 0.04 (-9%)
<b>gallery</b>	0.507 ± 0.03	0.485 ± 0.03 (-5%)	<b>0.557 ± 0.01</b>	0.531 ± 0.01 (-5%)
<b>school</b>	0.735 ± 0.03	0.861 ± 0.03 (+17%)	<b>0.973 ± 0.01</b>	0.971 ± 0.01 (-0.2%)

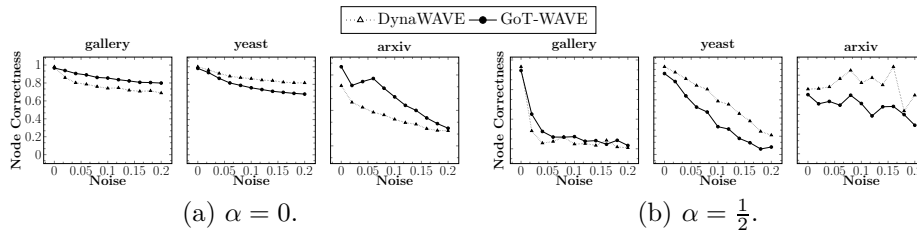


Figure 5: Comparison between GoT-WAVE and DynaWAVE on undirected networks in terms of node correctness, when (a) only node conservation is optimized ( $\alpha = 0$ ) and (b) both node and edge conservation are optimized ( $\alpha = \frac{1}{2}$ ). The higher the node correctness, the better the method.

tion that DWEC captures and thus does not benefit much from using it, while DynaWAVE captures different information from DWEC and thus benefits more from using it. Note that the superiority of one method over the other one is typically consistent over all noise levels, for both  $\alpha = 0$  and  $\alpha = \frac{1}{2}$ .

In terms of running time, extracting GoT features is faster than extracting DGDV features for the sparser networks (**zebra**, **aging** and **school**) and slower for the denser networks (**aging**, **arxiv** and **gallery**). Denser networks induce more GoTs than dynamic graphlets, and thus, GoTs are computationally heavier. Just as for synthetic networks, because both methods use the same alignment strategy (WAVE), their alignment times are similar.

### 3.2.3 Performance on real directed networks

As expected, since this scheme only rewires edge direction, the original network and the noisy networks have identical topology when ignoring edge directions. Because of this, and because DGDVs are undirected, DynaWAVE can not differentiate between the networks, while GoT-WAVE can, since GoTs accounts for edge directions. The rest of this section focuses on the other, directed randomization scheme, where not only edge directions but also time stamps are rewired.

Table 4: Node correctness when aligning a directed network to itself (noise = 0), for  $\alpha = 0$ . In parentheses, we show relative improvement (positive gain) or degradation (negative gain) in performance of GoT-WAVE compared to DynaWAVE. Node correctness results over all noise levels, using the best GoT-WAVE version (3-node directed GoTs), are shown in Figure 6 (a) and (b) for  $\alpha = 0$  and  $\alpha = \frac{1}{2}$ , respectively.

Network	DynaWAVE	GoT-WAVE		
	Undirected-4	Undirected-4	Directed-3	Directed-4
<b>emails</b>	<b>0.85 ± 0.02</b>	0.81 ± 0.03	0.83 ± 0.01 (-2%)	0.81 ± 0.02
<b>tennis</b>	0.74 ± 0.01	0.84 ± 0.03	<b>0.85 ± 0.02 (+15%)</b>	0.81 ± 0.02

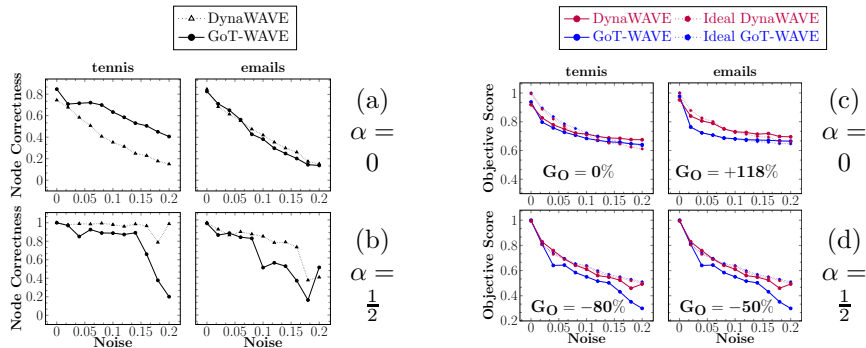


Figure 6: Comparison between GoT-WAVE and DynaWAVE on directed networks in terms of (a,b) node correctness and (c,d) how well their alignments’ objective scores match the objective scores of ideal alignments, when (a,c) only node conservation is optimized ( $\alpha = 0$ ) and (b,d) both node and edge conservation are optimized ( $\alpha = \frac{1}{2}$ ). For panels (a,b), the higher the node correctness value, the better the method. For panels (c,d), recall that  $G_O$  is the relative gain of GoT-WAVE over DynaWAVE (positive: GoT-WAVE is superior; negative: DynaWAVE is superior).

Unlike previous sections, we first address node correctness and only then objective score. We choose this organization because, on directed networks, we do experiments with different sets of GoTs (i.e., 4-node undirected GoTs, 3-node directed GoTs, and 4-node directed GoTs) in an effort to find the best set. For simplicity, we choose the best GoTs as those with the highest node correctness when aligning the original network to a noiseless version for  $\alpha = 0$ . We find that 3-node directed GoTs are the best for both of the directed networks (Table 4). Thus, henceforth, we use 3-node directed GoTs (for DGDVs, we still use four nodes and six events, as recommended by the DGDV authors).

In terms of node correctness, for  $\alpha = 0$ , we observe that GoT-WAVE has higher correctness than DynaWAVE for **tennis** over noise levels, and overall comparable node correctness for **emails**, depending on the noise level (Figure 6 (a)). We hypothesize that GoT-WAVE’s performance depends on subgraph overlap between (consecutive) snapshots of the input network. Subgraph overlap is expected to be higher in the **tennis** network than in the **emails** network, because tennis players tend to have the same opponents every year, while one might not necessarily email the same people in different time periods. Indeed, these are exactly the trends that our two networks show. The same trend was already observed for an alternative email network [6]. Networks with low subgraph overlap such as our **emails** network have fewer transitions (i.e., lower GoTs frequencies), and thus provide less information to GoT-WAVE. For  $\alpha = \frac{1}{2}$ , DynaWAVE’s node correctness is higher for both networks over most noise levels (Figure 6 (b)).

In terms of the objective score, for  $\alpha = 0$ , GoT-WAVE more closely matches its ideal alignments than DynaWAVE does for **emails**, and the two are compa-

rable for **tennis** (Figure 6 (c)). For **tennis**, GoT-WAVE mismatches the ideal alignments at lower noise levels but matches them at higher noise levels, while DynaWAVE mismatches the ideal alignments at both lower and higher noise level. For  $\alpha = \frac{1}{2}$ , DynaWAVE’s performance is again better for both networks (Figure 6 (d)).

In terms of running time, results are qualitatively similar to those for undirected networks.

## 4 Conclusion

We propose GoT-WAVE as a new algorithm for temporal GPNA. Our results suggest that GoTs are an efficient measure of dynamic node conservation. While DynaWAVE benefits more from also optimizing dynamic edge conservation, only GoT-WAVE can support directed edges. Future work on better incorporating dynamic edge conservation into GoT-WAVE may yield further improvements. Also, GoTs could be used under newer alignment strategies instead of WAVE. Further, on real networks, each of GoTs and DGDVs is superior half the time and the two dynamic node conservation measures are thus complementary. So, a deep understanding of each measure’s (dis)advantages could perhaps guide development of a new, improved measure. As more temporal real data continue to become available, which is inevitable, dynamic network analyses, including temporal GPNA, will continue to gain importance.

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## References

- [1] APARÍCIO, D., RIBEIRO, P., AND SILVA, F. A subgraph-based ranking system for professional tennis players. In *Complex Networks VII*. Springer, 2016, pp. 159–171.
- [2] APARÍCIO, D., RIBEIRO, P., AND SILVA, F. Extending the applicability of graphlets to directed networks. *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 14, 6 (2017), 1302–1315.
- [3] APARÍCIO, D., RIBEIRO, P., AND SILVA, F. Temporal network comparison using graphlet-orbit transitions. *arXiv preprint arXiv:1707.04572* (2017).
- [4] BARABÁSI, A.-L., AND ALBERT, R. Emergence of scaling in random networks. *Science* 286, 5439 (1999), 509–512.

- [5] BARRAT, A., AND CATTUTO, C. Sociopatterns. <http://www.sociopatterns.org/datasets/>, 2018. Accessed: 2018-08-11.
- [6] CRAWFORD, J., AND MILENKOVIĆ, T. Cluenet: Clustering a temporal network based on topological similarity rather than denseness. *PloS one* 13, 5 (2018), e0195993.
- [7] CRAWFORD, J., SUN, Y., AND MILENKOVIĆ, T. Fair evaluation of global network aligners. *Algorithms for Molecular Biology* 10, 1 (2015), 19.
- [8] ELMSALLATI, A., CLARK, C., AND KALITA, J. Global alignment of protein-protein interaction networks: A survey. *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 13, 4 (2016), 689–705.
- [9] ERDŐS, P., AND RÉNYI, A. On the evolution of random graphs. *Publ. Math. Inst. Hung. Acad. Sci* 5, 1 (1960), 17–60.
- [10] FAISAL, F. E., MENG, L., CRAWFORD, J., AND MILENKOVIĆ, T. The post-genomic era of biological network alignment. *EURASIP Journal on Bioinformatics and Systems Biology* 2015, 1 (2015), 3.
- [11] FAISAL, F. E., AND MILENKOVIĆ, T. Dynamic networks reveal key players in aging. *Bioinformatics* 30, 12 (2014), 1721–1729.
- [12] FAISAL, F. E., ZHAO, H., AND MILENKOVIĆ, T. Global network alignment in the context of aging. *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 12, 1 (2015), 40–52.
- [13] FLANNICK, J., NOVAK, A., DO, C. B., SRINIVASAN, B. S., AND BATZOGLOU, S. Automatic parameter learning for multiple local network alignment. *Journal of computational biology* 16, 8 (2009), 1001–1022.
- [14] GAO, W., GILMORE, J. H., GIOVANELLO, K. S., SMITH, J. K., SHEN, D., ZHU, H., AND LIN, W. Temporal and spatial evolution of brain network topology during the first two years of life. *PloS one* 6, 9 (2011), e25278.
- [15] GEMMETTO, V., BARRAT, A., AND CATTUTO, C. Mitigation of infectious disease at school: targeted class closure vs school closure. *BMC infectious diseases* 14, 1 (2014), 695.
- [16] GU, S., AND MILENKOVIĆ, T. Graphlets versus node2vec and struc2vec in the task of network alignment. *arXiv preprint arXiv:1805.04222* (2018).
- [17] GUZZI, P. H., AND MILENKOVIĆ, T. Survey of local and global biological network alignment: the need to reconcile the two sides of the same coin. *Briefings in bioinformatics* 19, 3 (2017), 472–481.
- [18] HOLME, P. Modern temporal network theory: a colloquium. *The European Physical Journal B* 88, 9 (2015), 234.



- [19] HOLME, P., AND SARAMÄKI, J. Temporal networks. *Physics reports* 519, 3 (2012), 97–125.
- [20] HU, H., AND WANG, X. Evolution of a large online social network. *Physics Letters A* 373, 12 (2009), 1105–1110.
- [21] HULOVATYY, Y., CHEN, H., AND MILENKOVIĆ, T. Exploring the structure and function of temporal networks with dynamic graphlets. *Bioinformatics* 31, 12 (2015), i171–i180.
- [22] ISELLA, L., STEHLÉ, J., BARRAT, A., CATTUTO, C., PINTON, J.-F., AND VAN DEN BROECK, W. What’s in a crowd? analysis of face-to-face behavioral networks. *Journal of theoretical biology* 271, 1 (2011), 166–180.
- [23] KELLEY, B. P., SHARAN, R., KARP, R. M., SITTLER, T., ROOT, D. E., STOCKWELL, B. R., AND IDEKER, T. Conserved pathways within bacteria and yeast as revealed by global protein network alignment. *Proceedings of the National Academy of Sciences* 100, 20 (2003), 11394–11399.
- [24] KLAU, G. W. A new graph-based method for pairwise global network alignment. *BMC bioinformatics* 10, 1 (2009), S59.
- [25] LESKOVEC, J., BACKSTROM, L., KUMAR, R., AND TOMKINS, A. Microscopic evolution of social networks. In *Proceedings of the 14th ACM SIGKDD international conference on Knowledge discovery and data mining* (2008), ACM, pp. 462–470.
- [26] LESKOVEC, J., KLEINBERG, J., AND FALOUTSOS, C. Graph evolution: Densification and shrinking diameters. *ACM Transactions on Knowledge Discovery from Data (TKDD)* 1, 1 (2007), 2.
- [27] MAMANO, N., AND HAYES, W. B. Sana: simulated annealing far outperforms many other search algorithms for biological network alignment. *Bioinformatics* 33, 14 (2017), 2156–2164.
- [28] MELANCON, G. Just how dense are dense graphs in the real world?: a methodological note. In *Proceedings of the 2006 AVI workshop on BEyond time and errors: novel evaluation methods for information visualization* (2006), ACM, pp. 1–7.
- [29] MEMIŠEVIĆ, V., AND PRŽULJ, N. C-graal: Common-neighbors-based global graph alignment of biological networks. *Integrative Biology* 4, 7 (2012), 734–743.
- [30] MENG, L., STRIEGEL, A., AND MILENKOVIĆ, T. Local versus global biological network alignment. *Bioinformatics* 32, 20 (2016), 3155–3164.
- [31] MICHALSKI, R., PALUS, S., AND KAZIENKO, P. Matching organizational structure and social network extracted from email communication. In *International Conference on Business Information Systems* (2011), Springer, pp. 197–206.

- [32] MILENKOVIĆ, T., NG, W., HAYES, W., AND PRŽULJ, N. Optimal network alignment with graphlet degree vectors. *Cancer informatics* 9 (2010), 121.
- [33] MILENKOVIĆ, T., AND PRŽULJ, N. Uncovering biological network function via graphlet degree signatures. *Cancer informatics* 6 (2008), CIN-S680.
- [34] OLESEN, J. M., BASCOMPTE, J., ELBERLING, H., AND JORDANO, P. Temporal dynamics in a pollination network. *Ecology* 89, 6 (2008), 1573–1582.
- [35] PRŽULJ, N., KUCHAIEV, O., STEVANOVIC, A., AND HAYES, W. Geometric evolutionary dynamics of protein interaction networks. In *Pacific Symposium on Biocomputing* (2010), vol. 2009, pp. 178–189.
- [36] PRŽULJ, N. Biological network comparison using graphlet degree distribution. *Bioinformatics* 23, 2 (2007), e177–e183.
- [37] ROSSI, R., AND AHMED, N. Dynamic networks — network repository. <http://networkrepository.com/dynamic.php>, 2018. Accessed: 2018-08-11.
- [38] RUBENSTEIN, D. I., SUNDARESAN, S. R., FISCHHOFF, I. R., TANTIPATHANANANDH, C., AND BERGER-WOLF, T. Y. Similar but different: dynamic social network analysis highlights fundamental differences between the fission-fusion societies of two equid species, the onager and grevy’s zebra. *PloS one* 10, 10 (2015), e0138645.
- [39] SARAPH, V., AND MILENKOVIĆ, T. Magna: maximizing accuracy in global network alignment. *Bioinformatics* 30, 20 (2014), 2931–2940.
- [40] SUN, Y., CRAWFORD, J., TANG, J., AND MILENKOVIĆ, T. Simultaneous optimization of both node and edge conservation in network alignment via wave. In *International Workshop on Algorithms in Bioinformatics* (2015), Springer, pp. 16–39.
- [41] ULLMANN, J. R. An algorithm for subgraph isomorphism. *Journal of the ACM (JACM)* 23, 1 (1976), 31–42.
- [42] VÁZQUEZ, A., FLAMMINI, A., MARITAN, A., AND VESPIGNANI, A. Modeling of protein interaction networks. *Complexus* 1, 1 (2003), 38–44.
- [43] VIJAYAN, V., CRITCHLOW, D., AND MILENKOVIĆ, T. Alignment of dynamic networks. *Bioinformatics* 33, 14 (2017), i180–i189.
- [44] VIJAYAN, V., KREBS, E., MENG, L., AND MILENKOVIĆ, T. Pairwise versus multiple network alignment. *arXiv preprint arXiv:1709.04564* (2017).
- [45] VIJAYAN, V., AND MILENKOVIĆ, T. Aligning dynamic networks with dynawave. *Bioinformatics* (2017), btx841.

- [46] VIJAYAN, V., AND MILENKOVIĆ, T. Multiple network alignment via multimagna+. *IEEE/ACM transactions on computational biology and bioinformatics* (2017).
- [47] VIJAYAN, V., SARAPH, V., AND MILENKOVIĆ, T. Magna++: Maximizing accuracy in global network alignment via both node and edge conservation. *Bioinformatics* 31, 14 (2015), 2409–2411.
- [48] WATTS, D. J., AND STROGATZ, S. H. Collective dynamics of small-world networks. *Nature* 393, 6684 (1998), 440–442.
- [49] YOO, B., FAISAL, F., CHEN, H., AND MILENKOVIĆ, T. Improving identification of key players in aging via network de-noising and core inference. *IEEE/ACM transactions on computational biology and bioinformatics* (2015).