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Dynamic Katz and related network measures

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We study walk-based centrality measures for time-ordered network sequences. For the case of standard dynamic walk-counting, we show how to derive and compute centrality measures induced by analytic functions. We also prove that dynamic Katz centrality, based on the resolvent function, has the unique advantage of allowing computations to be performed entirely at the node level. We then consider two distinct types of backtracking and develop a framework for capturing dynamic walk combinatorics when either or both is disallowed.

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Temporal network
Katz centrality

1. Introduction

Centrality measures play an important role in network analysis by quantifying the importance of each node [8,10]. How to make the notion of importance mathematically precise is highly context dependent, and hence there exists a range of centrality measures. Walk-based centralities constitute a large and widely-used class, motivated by counting the number of walks beginning from each node, with some form of downweighting based on the walk length [6,12]. Different types of weights lead to different families of centralities, such as Katz versus exponential; one or more parameters allow for even further freedom within each family. Moreover, in recent years it has been proposed that one might wish to ignore walks that immediately backtrack, to obtain centrality measures that are better suited for certain applications. Such centrality measures are said to be *non-backtracking* and are known to offer tangible benefits [2–4,16]. In this paper, we present a framework for analyzing and computing walk-based centrality measures, including non-backtracking versions, in the case of time-evolving networks.

Key contributions in this work are as follows.

- A proof that Katz (or resolvent-based) centrality is unique among matrix function-based versions, in that a combinatorially correct expression exists in the form of products of functions of node-level adjacency matrices (Theorem 1); thereby showing that dynamic Katz has a major computational advantage.
- Edge-level expressions for other matrix function-based versions ((12) and (13)) using a block matrix construction, with an accompanying convergence theory (Proposition 3).
- Corresponding computable expressions for non-backtracking versions of matrix function-based temporal centrality measures ((22) and (23)) along with an accompanying convergence theory (Propositions 6 and 7).

The material is organized as follows. Section 2 sets up some notation and explains what we mean by a temporal network. In section 3 we state and prove a unique property of dynamic Katz. Sections 4 and 5 develop a framework in which general matrix function-based centralities can be handled. In section 6 we introduce and study new non-backtracking versions of these measures, focusing on three main variations where backtracking is disallowed within time frames, across time frames, or both. Section 7 concludes with a brief discussion.

2. Background

In this section we review some definitions and notation associated with graphs and some of their matrix representations.

A *network*, or *graph*, is an ordered pair of sets $G = (V, E)$, where V is the set of *nodes* and $E \subset V \times V$ is the set of *edges* among the nodes [10,25]. We consider graphs with unweighted edges and no self-loops. Given an edge $(i, j) \in E$ we will call i its *source* and j its *target*. If the edge (j, i) also exists, we will refer to this as the *reciprocal* of the edge (i, j) and we will say that edge (i, j) is *reciprocated*. Further, we will often denote the directed edge (i, j) by $i \to j$.

Throughout this work I denotes the identity matrix, $\mathbf{1}$ denotes the vector of all ones; the size of both, unless otherwise stated, is chosen such that the resulting expressions in which they appear are coherent. The symbol $\star$ will be used as a placeholder to denote an arbitrary vertex, where appropriate.

Two definitions that are central to our work those of a *walk* and a *(non-)backtracking walk* around a graph. We review them in the following.

Definition 1. A walk of length r is a sequence of r edges $(e_1, e_2, \dots, e_r)$ such that the target of e_ℓ coincides with the source of $e_{\ell+1}$ for all $\ell = 1, 2, \dots, r - 1$.

Remark 1. An equivalent definition can be given in terms of the nodes: namely, a walk of length r can also be seen as a sequence of $r + 1$ nodes $(i_1, i_2, \dots, i_{r+1})$ such that $(i_\ell, i_{\ell+1}) \in E$ for all $\ell = 1, 2, \dots, r$.

Definition 2. Let G be a graph. A walk in G is said to be backtracking if any two consecutive edges in it are reciprocated. The walk is said to be non-backtracking (NBT) otherwise.

2.1. Graphs and matrices

A widely used linear algebraic representation of a graph is its adjacency matrix.

Definition 3. Let $G = (V, E)$ be an unweighted graph with n nodes. Its adjacency matrix $A \in \mathbb{R}^{n \times n}$ is entrywise defined as:

$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$

for all $i, j = 1, 2, \dots, n$.

Other matrices of interest for the purpose of our work are the *source* and *target* (or *terminal*) matrices associated with G and the adjacency matrix of the line graph of G; see, e.g., [10,29,30].

Definition 4. Let G be an unweighted graph with n nodes and m edges. Its source and target (or terminal) matrices $L, R \in \mathbb{R}^{m\times n}$ are entrywise defined as:

$$L_{ei} = \begin{cases} 1 & \text{if edge } e \text{ has the form } i \to \star \\ 0 & \text{otherwise} \end{cases}$$

and

$$R_{ej} = \begin{cases} 1 & \text{if edge } e \text{ has the form } \star \to j \\ 0 & \text{otherwise} \end{cases}$$

respectively, for all $e = 1, 2, \dots, m$ and for all $i, j = 1, 2, \dots, n$.

The *line graph* (or *interchange graph* or *dual graph*) of G is constructed from G as follows: edges in the original graph are regarded as nodes and two nodes $i \to j$ and $k \to \ell$ in this new line graph are connected if $j = k$, that is, if, together, they represent a walk of length two in the original graph G; see, e.g., [26]. The adjacency matrix $W \in \mathbb{R}^{m\times m}$ of the line graph can then be entrywise defined in terms of elements of G as

$$W_{i\to j, k\to \ell} = \delta_{jk},$$

where δ_{jk} is the Kronecker delta. Moreover, we can recover the adjacency matrices of both the unweighted graph G and its associated line graph via the identities $A = L^T R$ and $W = RL^T$ (see e.g. [4]).

2.1.1. Walk-based centrality measures

Katz centrality [21] is a widely used centrality measure that assigns to each node i the ith element of the vector

$$\mathbf{y}(\alpha) = \sum_{r=0}^{\infty} \alpha^r A^r \mathbf{1}. \tag{1}$$

Combinatorially, Katz centrality can be understood as assigning to node i the sum over all possible walk lengths of the number of walks originating from i of length r scaled by α^r, where $\alpha > 0$ is a downweighting parameter. Indeed, it is easy to show that $(A^r)_{ij}$ is the number of walks of length r originating from node i and ending at node j and hence the above interpretation of the entries of $A^r\mathbf{1}$ readily follows. Furthermore, whenever $0 < \alpha < 1/\rho(A)$, where $\rho(A)$ denotes the spectral radius of A, the series appearing in (1) converges and the vector of Katz centralities can be equivalently defined as

$$\mathbf{y}(\alpha) = (I - \alpha A)^{-1}\mathbf{1}.$$

The idea underlying Katz centrality can be generalized to obtain other centrality measures for nodes defined in terms of matrix functions and their entries, or sums thereof; see, e.g., [12] and references therein. Suppose that the analytic function

$$f(z) = \sum_{r=0}^{\infty} c_r z^r \tag{2}$$

has nonnegative Maclaurin coefficients $c_r \geq 0$ and is convergent for $|z| < R$. Then, for any $0 < \alpha < R/\rho(A)$ the matrix power series

$$f(\alpha A) = \sum_{r=0}^{\infty} c_r \alpha^r A^r$$

also converges [19]. Entries and sums of entries of $f(\alpha A)$ can thus be interpreted in terms of the number of walks taking place in the network, with shorter walks being given more weight since $c_r\alpha^r \to 0$ as $r \to \infty$. Because of this combinatorial interpretation, the function f may be used to define centrality measures of nodes:

- *f-total communicability:* $f(\alpha A)\mathbf{1}$; and
- *f-subgraph centrality*, defined as the diagonal of $f(\alpha A)$.

A notable special case is that of $c_r = 1/r!$ or, equivalently, $f(z) = e^z$, which yields the popular *subgraph centrality* and *total communicability* measures for nodes, defined in terms of the diagonal elements and row sums of e^A, respectively [7,13].

2.2. Temporal networks

The definition of a network may be extended in various ways to a time-evolving setting [20]. We consider here the case where, for a fixed collection of nodes, a network is recorded at a discrete set of time frames. This is relevant in many message passing and digital interaction contexts; see, e.g., [5,22,23].

Definition 5. A *temporal network* $\mathcal{G}$ with n nodes is a finite ordered sequence of networks $\mathcal{G} = (G^{[1]}, \ldots, G^{[N]})$ associated with a finite increasing collection of time frames $\mathcal{T}_N = (t_1, \ldots, t_N)$, where each network $G^{[\tau]} = (V^{[\tau]}, E^{[\tau]})$ exists at time $t = t_\tau$ for $\tau = 1, 2, \ldots, N$.

In the following we will assume that $V^{[\tau]} = \mathcal{V} = \{1, \ldots, n\}$ for all $\tau = 1, 2, \ldots, N$; that is, the node set is fixed over time. In principle, nodes which join or leave the temporal network can be accommodated in this framework—they will be isolated nodes when inactive. We further assume that, for all $\tau = 1, 2, \ldots, N$, $G^{[\tau]}$ is unweighted and contains no self-loops. We denote by $m_\tau = |E^{[\tau]}|$ the number of edges appearing in $G^{[\tau]}$.

Further, we denote by $m = \sum_{\tau=1}^{N} m_\tau$ the total number of edges in $\mathcal{G}$. Each of the graphs $G^{[1]}, G^{[2]}, \ldots, G^{[N]}$ appearing in the definition of $\mathcal{G}$ can be described via their adjacency matrices, which we denote by $A^{[\tau]}$ for all $\tau = 1, 2, \ldots, N$. These are implicitly used in [20] to define the *adjacency index* (or *presence function* [9]) of a temporal network $\mathcal{G}$, which is a third-order tensor $\mathcal{A} \in \mathbb{R}^{n\times n\times N}$ entrywise defined as

$$\mathcal{A}_{ij\tau} = (A^{[\tau]})_{ij}$$

for all $i, j \in \mathcal{V}$ and $\tau = 1, 2, \ldots, N$. We will instead work with the separate adjacency matrices $A^{[\tau]}$; furthermore, we will denote by $L^{[\tau]}$ and $R^{[\tau]}$ the corresponding source and target matrices, respectively, and by $W^{[\tau]}$ the adjacency matrix of the line graph of $G^{[\tau]}$.

The definition of a walk across a network can be extended to the setting of temporal graphs as follows.

Definition 6. A walk of length r across a temporal network is defined as an ordered sequence of r edges $(e_1, e_2, \ldots, e_r)$ such that the target of e_ℓ coincides with the source of $e_{\ell+1}$ for all $\ell = 1, \ldots, r-1$ and, moreover, that $e_\ell \in E^{[\tau_1]}, e_{\ell+1} \in E^{[\tau_2]}$ for some $1 \leq \tau_1 \leq \tau_2 \leq N$.

Remark 2. Equivalently, we could see a walk of length r as an ordered sequence of $r+1$ nodes $(i_1, i_2, \ldots, i_{r+1})$ such that for all $\ell = 2, \ldots, r$ it holds that $(i_{\ell-1}, i_\ell) \in E^{[\tau_1]}$ and $(i_\ell, i_{\ell+1}) \in E^{[\tau_2]}$ for some $1 \leq \tau_1 \leq \tau_2 \leq N$.

We stress that nontrivial walks can occur within a time frame and, moreover, a walk is allowed to remain inactive for some of the time frames. We will sometimes use the notation $i \xrightarrow{t_\tau} j$ to denote the edge $i \to j \in E^{[\tau]}$.

In the next section, after reviewing how Katz centrality was extended in [17] to the temporal setting by simply considering multiplications of matrix functions of the form $(I - \alpha A^{[\tau]})^{-1}$, we prove that Katz centrality is indeed the only centrality measure for which this approach can be employed. Generalizations to the temporal setting of other centrality measures, such as, e.g., total communicability, may be computed using the matrix construction that we present in section 4 in order to respect the combinatorics of walks.

3. Walk-based centrality measures in temporal networks

A generalization of Katz centrality to temporal networks is proposed in [17] using the dynamic communicability matrix

$$\mathcal{Q} := \prod_{\tau=1}^{N} (I - \alpha A^{[\tau]})^{-1} \tag{3}$$

We note here that when given a product of elements from a ring that are indexed by some subset of the natural numbers, as is the case in (3), we take it to mean that each subsequent term multiplies all the previous terms from the right. This assigns to node i the ith element of the vector

$$\boldsymbol{y}(\alpha) = \mathcal{Q}\mathbf{1} = (I - \alpha A^{[1]})^{-1} \cdots (I - \alpha A^{[N]})^{-1}\mathbf{1}. \tag{4}$$

It can be checked that for $0 < \alpha < (\max_\tau\{\rho(A^{[\tau]})\})^{-1}$, the component $\boldsymbol{y}(\alpha)_i$ corresponds to the weighted sum of all walks that emerge from node i, where walks of length r are weighted as α^r; see [17] for more details.

We note that this combinatorial interpretation, where walks of length r are weighted by the appropriate coefficient c_r in (2), may fail if we were to consider matrix functions other than the resolvent in the expression (4). For example, the exponential case $c_r = \beta^r/r!$ in (2), for some $\beta > 0$, was extended to the time-dependent setting using a quantum physics motivation to give [11]

$$\prod_{\tau=1}^{N} e^{\beta A^{[\tau]}} = e^{\beta A^{[1]}} e^{\beta A^{[2]}} \cdots e^{\beta A^{[N]}}.$$

However, *from a combinatorial viewpoint* this generalization has the drawback of not weighting walks consistently with their length. Consider for example a walk of length five from i to j that is realized by traveling two edges at time $t = t_1$, one edge at time $t = t_2$, and two edges at time $t = t_3$. Because of its length, we would expect this walk to be weighted as $\frac{\beta^5}{5!}$ in keeping with the theory that we have seen for static networks. However, it is straightforward to check that the (i, j) entry of $e^{\beta A^{[1]}} e^{\beta A^{[2]}} e^{\beta A^{[3]}}$ is weighted as $\frac{\beta^2}{2!}\frac{\beta^1}{1!}\frac{\beta^2}{2!} = \frac{\beta^5}{4}$. Furthermore, this walk of length five is weighted differently from another walk of length five that travels, say, one edge at times $t = t_1, t_2$ and three edges at time $t = t_3$. Indeed, the weight of this second walk is $\frac{\beta}{1!}\frac{\beta}{1!}\frac{\beta^3}{3!} = \frac{\beta^5}{6}$. Thus, the generalization to the temporal setting presented in [11] not only fails to respect the combinatorics of walks, with walks of length r not weighted as $\frac{\beta^r}{r!}$, but is also inconsistent in weighting different walks of the same length.

In the following subsection we show that resolvent-based centrality measures are unique in this regard: they are the only functions that respect the combinatorics of walks when translated to the temporal setting with the simple expression

$$f(\alpha A^{[1]}) f(\alpha A^{[2]}) \cdots f(\alpha A^{[N]}).$$

3.1. A remarkable property of Katz centrality

Is it possible for choices of f other than the resolvent (including the popular $f(z) = e^z$) to compute f-centralities on a time-evolving network directly using products of functions of adjacency matrices? While the example above clarified that the exponential subgraph and total communicability on a time-evolving network cannot be computed by simply multiplying the matrix exponential of each adjacency matrix, it is still *a priori* possible that they could be computed by multiplying some *other* function of each adjacency matrix, say, via $\prod_{\tau=1}^{N} g(\alpha A^{[\tau]})$ for some $g(z)$. More generally, posing this question for f-centrality measures is equivalent to the following combinatorial problem: Given the function $f(z) = \sum\limits_{r=0}^{\infty} c_r z^r$, $c_r \geq 0$, find a function $g(z)$ such that

$$\sum_{r=0}^{\infty} c_r \alpha^r h_r(x_1, \ldots, x_N) = \prod_{i=1}^{N} g(\alpha x_i), \tag{5}$$

where

$$h_r(x_1, \ldots, x_N) = \sum_{i_1+\cdots+i_N=r} x_1^{i_1} \ldots x_N^{i_N}$$

is the rth complete homogeneous symmetric polynomial in $N \geq 2$ variables. Indeed, finding a solution to this scalar problem would imply that the weights assigned to a walk in the matrix $\prod_{\tau=1}^{N} g(\alpha A^{[\tau]})$

- depend only on the total walk length and not, for example, on how it is split between time frames; and
- hold for any possible time evolving graph.

It turns out that this is essentially (up to a multiplicative constant and a linear change of variable) only possible if $f(z)$ is the resolvent. For example, there is no way to correctly compute the combinatorics of exponential centrality on time-evolving graphs by directly multiplying some functions of the adjacency matrix.[4] The theorem below gives a formal proof of this claim.

Theorem 1. *Given the sequence of nonnegative real numbers* $(c_r)_r$, *let* $f(z) = \sum_{r=0}^{\infty} c_r z^r$ *and let* $N \geq 2$. *The functional equation* (5) *has a solution* $g(z)$ *if and only if there exist nonnegative constants* $\gamma, \delta \geq 0$ *such that* $c_r = \gamma \delta^r$ *for all* r, *i.e., if and only if* $f(z) = \gamma(1 - \delta z)^{-1}$. *Moreover, in that case the solution is*

$$g(z) = \sqrt[N]{\gamma}\, (1 - \delta z)^{-1}.$$

[4] Of course, this does not mean that computing exponential centralities on time evolving graphs is not possible: indeed, the multilayer approach proposed in this paper is an example of a combinatorially exact, albeit potentially computationally demanding, way to compute it.

Proof. Suppose first that $c_r = \gamma\delta^r$ for some $\gamma, \delta \geq 0$, then (see also [17] and [27, Ch. 7])

$$\sum_{r=0}^{\infty} c_r \alpha^r h_r(x_1, \dots, x_N) = \gamma \sum_{r=0}^{\infty} \alpha^r h_r(\delta x_1, \dots, \delta x_N) = \gamma \prod_{i=1}^{N} \sum_{r=0}^{\infty} (\delta x_i \alpha)^r = \gamma \prod_{i=1}^{N} \frac{1}{1 - \alpha\delta x_i},$$

so taking $g(\alpha x_i) = \sqrt[N]{\gamma}(1 - x_i\delta\alpha)^{-1}$ yields a solution to (5).

Conversely suppose that (5) has a solution $g(z)$, and assume that $f(0) = 1$. In doing so we do not lose generality, for it is clear that $g(z)$ solves (5) for $f(z)$ if and only if, for all $\gamma \geq 0$, $\sqrt[N]{\gamma}\, g(z)$ solves it for $\gamma f(z)$. Recall now the following (classic) property of complete homogeneous symmetric polynomials [27, Sec. 7.5]:

$$h_r(\underbrace{1, \dots, 1}_{\ell \text{ variables}}, \underbrace{0, \dots, 0}_{(N-\ell) \text{ variables}}) = \#\{\text{monomials of degree } r \text{ in } \ell \text{ variables }\} = \binom{\ell + r - 1}{r}.$$

Then, evaluating (5) at $(x_1, \dots, x_N) = (0, \dots, 0)$ yields $g(0) = 1$. Next, we evaluate (5) at $(x_1, x_2, \dots, x_N) = (1, 0, \dots, 0)$ and conclude that $f(z) = g(z)$. Finally, by evaluating (5) at $(x_1, x_2, x_3, \dots, x_N) = (1, 1, 0, \dots, 0)$, we obtain

$$\sum_{r=0}^{\infty} (r+1) c_r \alpha^r = \sum_{r=0}^{\infty} \alpha^r \sum_{k=0}^{r} c_k c_{r-k}. \tag{6}$$

Now define $\delta := c_1$ and proceed by induction. We begin with $c_1 = \delta^1$. Let us then assume that $c_k = \delta^k$ for all $1 \leq k \leq r - 1$; equating the coefficients of α^r in (6) we get

$$(r+1)c_r = \sum_{k=0}^{r} c_k c_{r-k} = 2c_r + \sum_{k=1}^{r-1} \delta^r \quad \Longrightarrow \quad c_r = \delta^r. \quad \square$$

Motivated by this result, in sections 4 and 5 we introduce a block upper-triangular matrix $M \in \mathbb{R}^{m \times m}$ which will allow us to generalize f-subgraph centrality and f-total communicability to treat temporal networks while respecting the combinatorics of walks. These results will then be generalized to the non-backtracking setting in section 6.

4. The global temporal transition matrix

We start by re-interpreting the results in [17] via the line graph construction. To build intuition, suppose for simplicity that $N = 2$ and let $A^{[1]}$ and $A^{[2]}$ be the adjacency matrices of the graphs appearing at time frames $t_1 < t_2$ in the temporal network $\mathcal{G}$. For any adjacency matrix A and adjacency matrix W of the associated line graph, it holds that $A = L^T R$ and $W = RL^T$. These immediately yield

$$(A^r)_{ij} = (L^T W^{r-1} R)_{ij} \tag{7}$$

for all $i, j \in V$ and for all $r \geq 1$; see [4,29,30].

Remark 3. Equation (7) above summarizes the fact that taking $r \geq 1$ steps in the node space, i.e., on the original graph G, corresponds to taking $r-1$ steps in the edge space, i.e., on the line graph associated with G.

Equation (7) together with (3) and the assumption that $0 < \alpha < (\max_{\tau=1,2}\{\rho(A^{[\tau]})\})^{-1}$, yields

$$\begin{aligned}
\mathcal{Q} &= (I - \alpha A^{[1]})^{-1}(I - \alpha A^{[2]})^{-1} \\
&= \left(I + \sum_{r=1}^{\infty} \alpha^r {A^{[1]}}^r\right)\left(I + \sum_{r=1}^{\infty} \alpha^r {A^{[2]}}^r\right) \\
&= (I + \sum_{r=1}^{\infty} \alpha^r {L^{[1]}}^T {W^{[1]}}^{r-1} R^{[1]})(I + \sum_{r=1}^{\infty} \alpha^r {L^{[2]}}^T {W^{[2]}}^{r-1} R^{[2]}) \\
&= (I_n - \alpha {L^{[1]}}^T (I_m - \alpha W^{[1]})^{-1} R^{[1]})(I_n - \alpha {L^{[2]}}^T (I_m - \alpha W^{[2]})^{-1} R^{[2]}),
\end{aligned}$$

and hence

$$\begin{aligned}
\mathcal{Q} = I_n &+ \alpha\left(\sum_{\tau=1}^{2} {L^{[\tau]}}^T (I_m - \alpha W^{[\tau]})^{-1} R^{[\tau]}\right) \\
&+ \alpha^2 {L^{[1]}}^T (I_m - \alpha W^{[1]})^{-1} W^{[1,2]} (I_m - \alpha W^{[2]})^{-1} R^{[2]},
\end{aligned} \tag{8}$$

where $W^{[1,2]} := R^{[1]}(L^{[2]})^T$. The combinatorial role of each term appearing in (8) is as follows:

- I_n counts walks that do not involve any edge within either graph, i.e., walks of length zero.
- $\alpha\left(\sum_{\tau=1}^{2} {L^{[\tau]}}^T (I - \alpha W^{[\tau]})^{-1} R^{[\tau]}\right)$ counts walks that use at least one edge within one of the two graphs, and no edges within the other: note that necessarily these walks have length at least one.
- $\alpha^2 {L^{[1]}}^T (I_m - \alpha W^{[1]})^{-1} W^{[1,2]} (I_m - \alpha W^{[2]})^{-1} R^{[2]}$ counts walks that use at least one edge within each graph; note that necessarily these walks have length at least two, and, moreover, that at some point necessarily the walk has passed over an edge that exists at time t_1 to a subsequent edge that exists at time t_2, with the target of the time t_1 edge matching the source of the time t_2 edge (this is encoded in $W^{[1,2]}$).

Consider now the following block-triangular matrix:

$$M^{[1,2]} = \begin{bmatrix} W^{[1]} & W^{[1,2]} \\ 0 & W^{[2]} \end{bmatrix}. \tag{9}$$

The following result holds.

Proposition 1. *Suppose $M^{[1,2]}$ is defined as in* (9)*. Then, when* $0 < \alpha < (\max_{\tau=1,2}\{\rho(A^{[\tau]})\})^{-1}$,

$$(I - \alpha M^{[1,2]})^{-1} = \begin{bmatrix} (I-\alpha W^{[1]})^{-1} & \alpha(I-\alpha W^{[1]})^{-1}W^{[1,2]}(I-\alpha W^{[2]})^{-1} \\ 0 & (I-\alpha W^{[2]})^{-1} \end{bmatrix}.$$

Proof. Note that the rth power of $M^{[1,2]}$ is given by

$${M^{[1,2]}}^r = \begin{bmatrix} W^{[1]} & W^{[1,2]} \\ 0 & W^{[2]} \end{bmatrix}^r = \begin{bmatrix} {W^{[1]}}^r & \sum_{s=0}^{r-1} {W^{[1]}}^s W^{[1,2]} {W^{[2]}}^{r-1-s} \\ 0 & {W^{[2]}}^r \end{bmatrix}.$$

Thus

$$\sum_{r=0}^{\infty} \alpha^r {M^{[1,2]}}^r = I_{2m} + \sum_{r=1}^{\infty} \begin{bmatrix} \alpha^r {W^{[1]}}^r & \alpha^r \sum_{s=0}^{r-1} {W^{[1]}}^s W^{[1,2]} {W^{[2]}}^{r-1-s} \\ 0 & \alpha^r {W^{[2]}}^r \end{bmatrix}.$$

Since the spectral radius of $W^{[\tau]}$ coincides with that of $A^{[\tau]}$ by Flanders' theorem, it follows that, when $0 < \alpha < (\max_{\tau=1,2}\{\rho(A^{[\tau]})\})^{-1}$, the diagonal blocks of the matrix on the right-hand side equal $(I - \alpha W^{[\tau]})^{-1}$, for $\tau = 1, 2$, respectively.

Finally, the non-zero off-diagonal block is such that

$$\begin{aligned} \sum_{r=1}^{\infty} \alpha^r \sum_{s=0}^{r-1} {W^{[1]}}^s W^{[1,2]} {W^{[2]}}^{r-1-s} &= \alpha \sum_{r=0}^{\infty} \alpha^r \sum_{s=0}^{r} {W^{[1]}}^s W^{[1,2]} {W^{[2]}}^{r-s} \\ &= \alpha \left(\sum_{s=0}^{\infty} \alpha^s {W^{[1]}}^s \right) W^{[1,2]} \left(\sum_{s=0}^{\infty} \alpha^s {W^{[2]}}^s \right) \\ &= (I_m - \alpha W^{[1]})^{-1} \alpha W^{[1,2]} (I_m - \alpha W^{[2]})^{-1}. \end{aligned}$$

The above, together with the fact that

$$(I_{2m} - \alpha M^{[1,2]})^{-1} = I_{2m} + \sum_{r=1}^{\infty} \alpha^r {M^{[1,2]}}^r,$$

concludes the proof. □

If we now let

$$\mathcal{L} = \begin{bmatrix} L^{[1]} \\ L^{[2]} \end{bmatrix} \quad \text{and} \quad \mathcal{R} = \begin{bmatrix} R^{[1]} \\ R^{[2]} \end{bmatrix}$$

it follows from (7) and Proposition 1 that

$$\mathcal{Q} = I + \alpha \mathcal{L}^T (I - \alpha M^{[1,2]})^{-1} \mathcal{R}.$$

This alternative description of $\mathcal{Q}$ is not useful in this context, since $\mathcal{Q}$ can be easily computed by working in the node space, i.e., directly from the adjacency matrices $A^{[\tau]}$; however, this construction, appropriately generalized, will allow us to define and compute f-centrality measures for temporal networks for all functions f and NBT versions for temporal networks.

These two points will be addressed in sections 5 and 6 below. In the reminder of this section, we will extend the definition of the matrices $M = M^{[1,2]}$, $\mathcal{L}$, and $\mathcal{R}$ to treat the case of $N \geq 2$ time frames. To gain further intuition, we will also describe how the generalization of the matrix M can be interpreted as the adjacency matrix of a static multilayer network.

We begin by extending the definitions and results above to the case of $N \geq 2$.

Definition 7. Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with N time frames $t_1 < t_2 < \cdots < t_N$, with $G^{[\tau]} = (\mathcal{V}, E^{[\tau]})$. The backtrack-allowing transition matrix $W^{[\tau_1,\tau_2]}$ where $1 \leq \tau_1 < \tau_2 \leq N$, is defined entrywise as follows:

$$(W^{[\tau_1,\tau_2]})_{i\to j,k\to\ell} = \delta_{jk}$$

for all $i \to j \in E^{[\tau_1]}$ and $k \to \ell \in E^{[\tau_2]}$.

These matrices are generally non-square and encode in their entries the presence of temporal walks of length two that take place across two distinct, but not necessarily consecutive, time frames.

Proposition 2. *Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with N time frames $t_1 < t_2 < \cdots < t_N$. Let moreover $L^{[\tau]}$ and $R^{[\tau]}$ be the source and target matrices associated with graph $G^{[\tau]}$. Then for all $\tau_1 < \tau_2$ we have*

$$W^{[\tau_1,\tau_2]} = R^{[\tau_1]} {L^{[\tau_2]}}^T.$$

Proof. The result may be established straightforwardly by working entrywise. □

We now extend the definition of $M^{[1,2]}$ to the case of $N \geq 2$ as follows.

Definition 8. Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with N time frames $t_1 < t_2 < \cdots < t_N$. The global temporal transition matrix associated with $\mathcal{G}$ is the $m \times m$ block matrix:

$$M := M^{[1,2,\ldots,N]} = \begin{bmatrix} W^{[1]} & W^{[1,2]} & W^{[1,3]} & \ldots & W^{[1,N]} \\ 0 & W^{[2]} & W^{[2,3]} & \ldots & W^{[2,N]} \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \ldots & \ldots & 0 & W^{[N]} \end{bmatrix}.$$

We mention in passing that this is the adjacency matrix of a multilayer graph associated with the line graph of $\mathcal{G}$; see subsection 4.1 for more details. Similar constructions, although at node level, have been used over the years as a means to incorporate the temporal aspect in block-matrix representations of $\mathcal{G}$; examples include [1,15,24,28]. We note however that the adjacency matrix presented in Definition 8 does not correspond to the adjacency matrix of the line graph of any of the networks underlying the matrices presented in these references. Indeed, the number of nonzeros in the matrices presented in these references is strictly larger than the number of edges in the temporal graph, due to the presence of “artificial edges” described in the off-diagonal blocks. Therefore the adjacency matrix of the associated line graph would be of larger dimension than the matrix in Definition 8

Definition 9. Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with N time frames $t_1 < t_2 < \cdots < t_N$ and let $L^{[\tau]}$ and $R^{[\tau]}$ be the source and target matrices of $G^{[\tau]}$ for $\tau = 1, 2, \ldots, N$. The global source and global target matrices to N time frames associated to $\mathcal{G}$ are

$$\mathcal{L} = \mathcal{L}^{[1,\ldots,N]} = \begin{bmatrix} L^{[1]} \\ L^{[2]} \\ \vdots \\ L^{[N]} \end{bmatrix} \quad \text{and} \quad \mathcal{R} = \mathcal{R}^{[1,\ldots,N]} = \begin{bmatrix} R^{[1]} \\ R^{[2]} \\ \vdots \\ R^{[N]} \end{bmatrix},$$

respectively.

It can be verified that, for all $\alpha \in (0, (\max_\tau\{\rho(A^{[\tau]})\})^{-1})$, Katz centrality (4) on a time-evolving network with global temporal transition matrix $M = M^{[1,\ldots,N]}$ can be rewritten as

$$\boldsymbol{y}(\alpha) = \mathcal{Q}\mathbf{1} = [I + \alpha\mathcal{L}^T(I - \alpha M)^{-1}\mathcal{R}]\mathbf{1} = \mathbf{1} + \alpha\mathcal{L}^T(I - \alpha M)^{-1}\mathbf{1}, \tag{10}$$

where we have used the fact that $\mathcal{R}\mathbf{1} = \mathbf{1}$.

As we mentioned earlier in the section, this construction is not actually needed to compute $\boldsymbol{y}(\alpha) = \mathcal{Q}\mathbf{1}$. However, it will be instrumental to the generalizations to f-centrality measures and their NBT equivalent. One observation that emerges from the above is that walks around the temporal graph $\mathcal{G}$ can be enumerated by counting walks around the graph underlying M and then projecting to the node space appropriately. We explore this connection in the next subsection.

4.1. Multilayer interpretation of M

The motivation for the definition of the block matrices above is that we can view walks across multiple time frames in the following way. Recall that given any graph G, one can construct the line graph associated with G whose adjacency matrix is the matrix

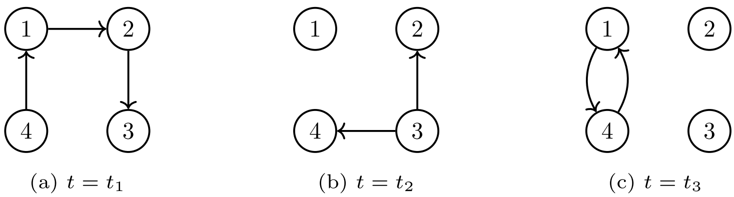

Fig. 1. Small temporal network $\mathcal{G} = (G^{[1]}, G^{[2]}, G^{[3]})$.

W. The nodes of the line graph are the edges of G and any two nodes are connected if the concatenation of the corresponding edges in G forms a walk of length two across the original graph. Katz centrality of a node can then be computed by counting walks on the line graph, summing them using appropriate weights, and then using the source and target matrices to "translate" the obtained result from the edge space (represented by the line graph) to the node space (represented by G). The key result that allows this approach is (7) or, equivalently, the fact that a walk of length r in the line graph corresponds to a walk of length $r+1$ in G.

To mirror this construction in the case of temporal networks, one begins by constructing the line graphs of each $G^{[\tau]}$ appearing in $\mathcal{G}$. The new graph representation of $\mathcal{G}$ in the edge space will now contain $m = \sum_\tau m_\tau$ nodes, labeled as $i \xrightarrow{t_\tau} j$ and hence identified by the source and target of each edge and by the time frame at which the connection occurs. Two nodes in this new graph are connected by a directed edge if their concatenation forms a walk of length two in the graph corresponding to the time frame $t = t_\tau$, i.e., if they form a walk of length two in $G^{[\tau]}$. Consider for example the graph in Fig. 1. The construction built so far is presented in the left-hand panel of Fig. 2. Clearly, this construction is incomplete, as the walks that we are able to represent, and hence count, at this stage are only those that take place entirely in one of the $G^{[\tau]}$, for some $\tau = 1, 2, \ldots, N$. Walks of length two in temporal networks may also take place *across* time frames, and these are not accounted for by the construction of the line graphs $W^{[\tau]}$. For example, the temporal walk $4 \xrightarrow{t_1} 1 \xrightarrow{t_3} 4$ in Fig. 1 is not accounted for in the edge space representation of Fig. 2a.

The graph built so far, whose adjacency matrix is block-diagonal with $W^{[\tau]}$, $\tau = 1, 2, \ldots, N$ as diagonal blocks, thus needs to be adapted to allow for walks that happen across time frames: directed edges are added to connect nodes of the form $i \xrightarrow{t_{\tau_1}} j$ to edges of the form $j \xrightarrow{t_{\tau_2}} k$ if $\tau_1 < \tau_2$. The resulting graph is now a multilayer network which encodes all possible temporal walks of length two taking place in $\mathcal{G}$. For example, in the (partial) temporal line-graph construction presented in Fig. 2a associated with the graph in Fig. 1 one needs to add the dashed and dotted edges pictured in Fig. 2b.

Here, dashed lines represent connections that happen across two consecutive time frames which are stored in $W^{[1,2]}$ and $W^{[2,3]}$, while dotted lines represent walks of length two that start at time t_1 and finish at time t_3 and these connections are stored in $W^{[1,3]}$.

If we now turn our attention to the adjacency matrix of this multilayer, it is easy to see that this is indeed the matrix M that we presented in Definition 8.

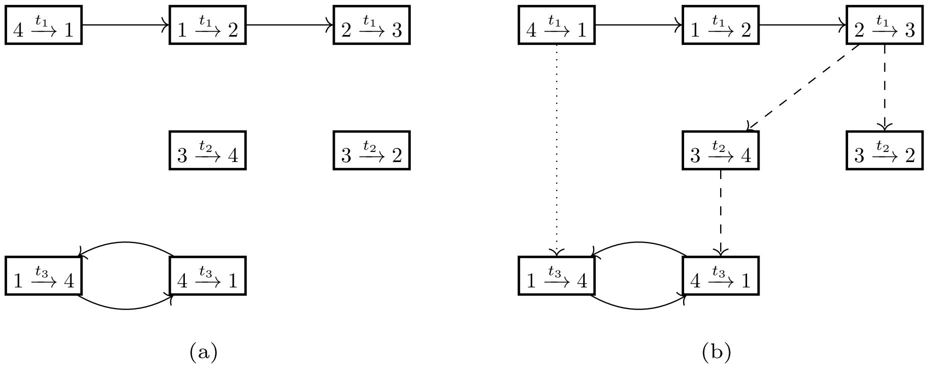

Fig. 2. (a) Partial line graph construction associated to $\mathcal{G}$ in Fig. 1, as described in subsection 4.1. (b) Multilayer graph underlying the matrix M in Definition 8 associated with the graph in Fig. 1.

Remark 4. As in the case of static networks, a temporal walk of length r in the graph associated to M corresponds to a temporal walk of length $r+1$ in $\mathcal{G}$.

Because of this interpretation of M as the adjacency matrix of a network associated with $\mathcal{G}$, one can expect to be able to compute dynamic walk-based centrality measures using M by counting walks in its associated multilayer graph, summing these walks with appropriate weights, and then projecting the result to the node space using the global source and target matrices. This was achieved in (10) for Katz centrality, and will be generalized to other matrix functions in the next section.

5. *f*-total communicability and *f*-subgraph centrality on time-evolving networks

In this section, we consider generalization of the proposed block-matrix approach to walk-based centralities with weights induced by some suitable analytic functions f via their Maclaurin series.

Suppose that $\mathcal{G}$ is a temporal network and let $M = M^{[1,\dots,N]}$ be its global temporal transition matrix. Suppose moreover that, for all $|z| < R$, the series $f(z) = \sum_{r=0}^{\infty} c_r z^r$ converges. Extending our treatment of the $N = 2$ case in section 4, we define the temporal f-subgraph centrality of node i as

$$\boldsymbol{x}(\alpha)_i = \left(c_0 I_n + \alpha \mathcal{L}^T \sum_{r=1}^{\infty} c_r (\alpha M)^{r-1} \mathcal{R} \right)_{ii}$$

and the temporal f-total communicability of node i as

$$\boldsymbol{y}(\alpha)_i = \left(c_0 I_n + \alpha \mathcal{L}^T \sum_{r=1}^{\infty} c_r (\alpha M)^{r-1} \mathcal{R}\mathbf{1} \right)_i .$$

The following result now follows immediately from the definition of M.

Proposition 3. *If the power series $f(z) = \sum_{r=0}^{\infty} c_r z^r$ converges with radius of convergence R, then the series $\sum_{r=1}^{\infty} c_r(\alpha M)^{r-1}$ also converges for all $\alpha \in [0, R/\rho)$, where $\rho = \max_\tau\{\rho(A^{[\tau]})\}$. Moreover,*

$$\sum_{r=1}^{\infty} c_r(\alpha M)^{r-1} = \partial f(\alpha M),$$

where ∂ is the functional operator

$$\partial f(z) := \sum_{r=0}^{\infty} c_{r+1} z^r = \begin{cases} \frac{f(z)-f(0)}{z} & \text{if } z \neq 0 \\ f'(0) & \text{if } z = 0. \end{cases} \tag{11}$$

Using this result we can now formally define temporal f-subgraph centrality and temporal f-total communicability for any analytic function f as follows.

Definition 10. Let $\mathcal{G}$ be a temporal network and let $M = M^{[1,\dots,N]}$ be its global temporal transition matrix. Let f be a function which is analytic in a neighborhood of zero with Maclaurin series $f(z) = \sum_{r=0}^{\infty} c_r z^r$, such that $c_r \geq 0$ for all r, and such that f is defined on the spectrum of M. Moreover, let ∂ be the functional operator defined in (11). Temporal f-subgraph centrality of node i is defined as

$$\mathbf{x}(\alpha)_i = \left(c_0 I + \alpha \mathcal{L}^T \partial f(\alpha M)\mathcal{R}\right)_{ii}. \tag{12}$$

Additionally, temporal f-total communicability of node i is defined as the ith entry of the following vector:

$$\mathbf{y}(\alpha) = c_0 \mathbf{1}_n + \alpha \mathcal{L}^T \partial f(\alpha M)\mathbf{1}_m. \tag{13}$$

These formulae count the number of walks across the temporal network in the required manner: the factor $c_r\alpha^r$ is applied to all walks of length r. This follows from the one-to-one correspondence between walks of length r, weighted as $c_r\alpha^r$, in the original time-evolving graph and walks of length $r-1$, weighted as $c_r\alpha^{r-1}$, in the graph associated with M; see Remark 4. Indeed, the role of the operator ∂ is to take into account that a walk of length $r-1$ in the multilayer network corresponds to a walk of length r in the original temporal graph, and thus to weight such walks as $c_r\alpha^{r-1}$ (as opposed to $c_{r-1}\alpha^{r-1}$, which arises when f is applied instead of ∂f). To recover the required weighting, we must then multiply everything by α. Finally, we add[5] a term $c_0 I$ since walks of length zero in the original time-evolving graph do not have any correspondence in the graph associated to M. Observe that in the special case of Katz centrality $\partial f(z) = f(z) = (1-z)^{-1}$, and therefore the importance of applying the operator ∂ is not manifest.

[5] Of course, adding such a term does not change the ranking associated with the corresponding f-centrality, and therefore it is not necessary in a practical implementation of an algorithm to compute it. We incorporate it to obtain the correct combinatorial expressions.

Example 1. Let us consider $f(z) = e^z$, so that

$$\partial f(z) = \psi_1(z) = \sum_{r=0}^{\infty} \frac{z^r}{(r+1)!},$$

in the case of three time frames. Then, the exponential subgraph centrality for all $\beta > 0$ can be computed as the diagonal entries of

$$I + \beta \mathcal{L}^T \psi_1 \left(\beta \begin{bmatrix} W^{[1]} & W^{[1,2]} & W^{[1,3]} \\ 0 & W^{[2]} & W^{[2,3]} \\ 0 & 0 & W^{[3]} \end{bmatrix} \right) \mathcal{R} \tag{14}$$

while the total communicability vector is obtained by multiplying (14) by $\mathbf{1}$. We emphasize that the generating function (14) is generally *not* equal to $e^{\beta A^{[1]}} e^{\beta A^{[2]}} e^{\beta A^{[3]}}$.

Indeed, consider for example the temporal graph $\mathcal{G}$ represented by the following adjacency matrices

$$A^{[1]} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \; A^{[2]} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \text{ and } A^{[3]} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Clearly, all the admissible walks in this temporal graph are

- walks of length one, weighted by β:

$$1 \xrightarrow{t_1} 2, \; 2 \xrightarrow{t_2} 3, \quad \text{and} \quad 3 \xrightarrow{t_3} 4;$$

- walks of length two, weighted by $\frac{\beta^2}{2}$:

$$1 \xrightarrow{t_1} 2 \xrightarrow{t_2} 3 \text{ and } 2 \xrightarrow{t_2} 3 \xrightarrow{t_3} 4;$$

  and finally,
- one walk of length three, weighted by a factor $\frac{\beta^3}{3!}$

$$1 \xrightarrow{t_1} 2 \xrightarrow{t_2} 3 \xrightarrow{t_3} 4.$$

Since these are the only admissible walks, together with walks of length zero, weighted by 1, we expect the entries of the 4×4 matrix (14) to encode these weights in the appropriate entries; for example, in the entry $(1,3)$ we expect to read the weight $\frac{\beta^2}{2}$ since the only walk in the network originating at node 1 and terminating at node 3 is of length two.

It is easy to verify that, up to permutation similarity,

$$M = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

which is nilpotent, and hence

$$\psi_1(\beta M) = I_3 + \frac{\beta}{2}M + \frac{\beta^2}{3!}M^2 = \begin{bmatrix} 1 & \frac{\beta}{2} & \frac{\beta^2}{3!} \\ 0 & 1 & \frac{\beta}{2} \\ 0 & 0 & 1 \end{bmatrix}.$$

With the labeling of edges induced by M above it holds that

$$\mathcal{L} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \mathcal{R} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

It immediately follows that the matrix in (14) is

$$I_4 + \beta \mathcal{L}^T \psi_1(\beta M)\mathcal{R} = \begin{bmatrix} 1 & \beta & \frac{\beta^2}{2} & \frac{\beta^3}{3!} \\ 0 & 1 & \beta & \frac{\beta^2}{2} \\ 0 & 0 & 1 & \beta \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

which encodes in its entries exactly the required weights. On the other hand, multiplying the exponentials of the adjacency matrices gives

$$e^{\beta A^{[1]}} e^{\beta A^{[2]}} e^{\beta A^{[3}} = \begin{bmatrix} 1 & \beta & \beta^2 & \beta^3 \\ 0 & 1 & \beta & \beta^2 \\ 0 & 0 & 1 & \beta \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

where we have used $(A^{[\tau]})^r = 0$ for all $r \geq 2$ and $A^{[1]}A^{[3]} = 0$. This matrix fails to correctly weight walks of length two and three in a combinatoric sense.

In the next section we move on to the problem of generalizing the results obtained so far to the non-backtracking setting, where backtracking is disallowed within time frames or across time frames. The construction presented mirrors the one described above and will build on modified versions of the global temporal transition matrix M.

6. Non-backtracking walks

Non-backtracking walks, as defined in Definition 2, may be studied using the *Hashimoto matrix*; see [18]. We also note that the Hashimoto matrix plays a key role in related studies of *random* NBT walks [14].

Definition 11. The Hashimoto matrix associated with a graph $G = (V, E)$ with nodes $V = \{1, 2, \dots, n\}$ and m edges is the matrix $B \in \mathbb{R}^{m\times m}$ defined as

$$B_{i\to j,k\to\ell} = \delta_{jk}(1 - \delta_{i\ell})$$

for all $i \to j, k \to \ell \in E$.

It is easily verified that

$$B = W - W \circ W^T$$

where $\circ$ denotes the Schur (or entrywise) product and W is the adjacency matrix of the line graph of G. In words, rows and columns of B correspond to edges in G, and the nonzero entries record pairs of edges that form a NBT walk of length two in G.

Taking powers of this matrix and then projecting back to the node space using the source and target matrices allows us to count NBT walks taking place in G. Specifically,

$$(L^T B^{r-1} R)_{ij} = (p_r(A))_{ij} \tag{15}$$

is the number of NBT walks of length r originating at node i and ending at node j; see [4]. Here and in the following we denote by $p_r(A) \in \mathbb{R}^{n\times n}$ the matrix whose entries record the number of NBT walks of length r between any two nodes in the network with adjacency matrix A. These matrices satisfy a four-term recurrence that allows the computation of the number of NBT walks of any length in the network. We refer the interested reader to [2,16] and references therein.

6.1. Non-backtracking walk-based centrality measure

A NBT version of Katz centrality was proposed and studied in [2,16]. Generalization to other f-centrality measures was presented in [3]. Later, in [4] it was shown how NBT Katz centrality, as well as other NBT versions of f-subgraph centrality and f-total communicability, could also be derived via the Hashimoto matrix.

We may define the NBT Katz centrality by changing (1) to

$$\widehat{\mathbf{y}}(\alpha) = \sum_{r=0}^{\infty} \alpha^r p_r(A)\mathbf{1}.$$

As shown in [4], we may also obtain $\widehat{\mathbf{y}}(\alpha)$ by computing Katz centrality for the graph of the Hashimoto matrix and then projecting via the source and target matrices; that is,

$$\widehat{\mathbf{y}}(\alpha) = \left(I + \alpha L^T (I - \alpha B)^{-1} R\right)\mathbf{1},$$

for $\alpha < 1/\rho(B)$. Similarly, NBT f-total communicability is obtained by computing ∂f-total communicability for the Hashimoto matrix and then projecting, where ∂ is the operator defined in (11), that is,

$$\widehat{\mathbf{y}}(\alpha) = \big(f(0)I + \alpha L^T \partial f(\alpha B) R\big)\,\mathbf{1}.$$

NBT versions of f-subgraph centrality can also be defined analogously using the diagonal elements of $f(0)I + \alpha L^T \partial f(\alpha B)R$.

6.2. Temporal NBT centrality measures

In the remainder of this section we carry through concepts and results from sections 4 and 5 to the NBT setting. This produces, for the first time, definitions and computable expressions for temporal NBT centrality measures. We first notice that there is not just one type of backtracking for temporal networks; indeed, there are three:

- Backtracking happens within a certain time frame; we will refer to this as *backtracking in space*.
- Backtracking happens across time frames; we will refer to this as *backtracking in time*.
- Backtracking happens both within a time frame and across time frames (not necessarily in that order); we will refer to this as *backtracking in time and space*.

To explain these different types, consider the temporal graph $\mathcal{G}$ in Fig. 1. The walks $1 \xrightarrow{t_3} 4 \xrightarrow{t_3} 1$ and $2 \xrightarrow{t_1} 3 \xrightarrow{t_2} 2$ showcase two different types of backtracking: the first is backtracking in space and the second is backtracking in time; additionally, the walk $4 \xrightarrow{t_1} 1 \xrightarrow{t_3} 4$ provides an example of a walk that backtracks in both space *and* time.

6.2.1. Non-backtracking Katz centrality for time-evolving networks: the case of 2 time frames

As in section 5, we begin by considering the case of $\mathcal{G} = (G^{[1]}, G^{[2]})$ at times $t_1 < t_2$. In the following, we make use of the notation $B^{[1,2]} := W^{[1,2]} - W^{[1,2]} \circ {W^{[2,1]}}^T$.

Remark 5. Recall that the matrix $W^{[1,2]} = R^{[1]}(L^{[2]})^T \in \mathbb{R}^{m_1 \times m_2}$ is a possibly rectangular matrix that encodes in its entries whether two edges, one appearing at time $t = t_1$ and a second appearing at time $t = t_2$, can be concatenated; see Definition 7 and Proposition 2. Analogously, the matrix $B^{[1,2]} \in \mathbb{R}^{m_1 \times m_2}$ records whether a walk of length two that occurs across time frames t_1 and t_2 is non-backtracking, since we have

$$(B^{[1,2]})_{i \to j, k \to \ell} = \delta_{jk}(1 - \delta_{i\ell})$$

for all $i \to j \in E^{[1]}$ and for all $k \to \ell \in E^{[2]}$. We will formalize this concept in Definition 12 and Proposition 5 below.

With consideration to the previous interpretation of the terms appearing in (8), if one wants to forbid backtracking, in full or in part, it is appropriate to generalize the expression (8) in three possible ways, depending on the type of backtracking behavior that we want to forbid.

- Backtracking in space forbidden: we replace the $W^{[\tau]}$ with the Hashimoto matrix $B^{[\tau]}$ for $\tau = 1, 2$, giving

$$I_n + \alpha \left(\sum_{\tau=1}^{2} (L^{[\tau]})^T (I_m - \alpha B^{[\tau]})^{-1} R^{[\tau]} \right) + \alpha^2 (L^{[1]})^T (I_m - \alpha B^{[1]})^{-1} W^{[1,2]} (I_m - \alpha B^{[2]})^{-1} R^{[2]}. \tag{16}$$

- Backtracking in time forbidden: we replace $W^{[1,2]}$ with $B^{[1,2]}$, giving

$$I_n + \alpha \left(\sum_{\tau=1}^{2} (L^{[\tau]})^T (I_m - \alpha W^{[\tau]})^{-1} R^{[\tau]} \right) + \alpha^2 (L^{[1]})^T (I_m - \alpha W^{[1]})^{-1} B^{[1,2]} (I_m - \alpha W^{[2]})^{-1} R^{[2]}. \tag{17}$$

- Backtracking in time and space both forbidden: we perform both replacements, giving

$$I_n + \alpha \left(\sum_{\tau=1}^{2} (L^{[\tau]})^T (I_m - \alpha B^{[\tau]})^{-1} R^{[\tau]} \right) + \alpha^2 (L^{[1]})^T (I_m - \alpha B^{[1]})^{-1} B^{[1,2]} (I_m - \alpha B^{[2]})^{-1} R^{[2]}. \tag{18}$$

In the case of (16), we observe that for $\tau = 1, 2$

$$\alpha (L^{[\tau]})^T (I_m - \alpha B^{[\tau]})^{-1} R^{[\tau]} = \alpha \sum_{r=0}^{\infty} \alpha^r p_{r+1}(A^{[\tau]}),$$

where we have used (15). Moreover, for small enough values of α,

$$\sum_{r=0}^{\infty} \alpha^r p_r(A^{[\tau]}) = (1 - \alpha^2)[I - \alpha A^{[\tau]} + \alpha^2 (D^{[\tau]} - I) + \alpha^3 (A^{[\tau]} - S^{[\tau]})]^{-1},$$

where

$$D^{[\tau]} = \operatorname{diag}\operatorname{diag}({A^{[\tau]}}^2), \qquad S^{[\tau]} = A^{[\tau]} \circ (A^{[\tau]})^T \tag{19}$$

with $\operatorname{diag}\operatorname{diag}({A^{[\tau]}}^2)$ denoting the diagonal matrix whose diagonal entries are equal to the diagonal elements of ${A^{[\tau]}}^2$. (Note that both of the above formulae are proved in the existing literature [2,4]). Hence, all the terms appearing in (16) can be reformulated in terms of matrices of order n, thus obtaining a *non-backtracking (in space only) dynamic communicability matrix*:

$$\mathcal{Q} = (1-\alpha^2)^2 \prod_{\tau=1}^{2} [I - \alpha A^{[\tau]} + \alpha^2 (D^{[\tau]} - I) + \alpha^3 (A^{[\tau]} - S^{[\tau]})]^{-1}.$$

When possible, it is clearly preferable to work at node-level, since for large values of n it may easily happen that $n \ll m$. We observe that this may be true even if, individually, each graph has $O(n)$ edges, since in total there may be up to $O(Nn)$ edges. However, a direct node-level formulation appears to be infeasible when backtracking is also forbidden in time, due to the fact that a memory of the last traveled edge in a given time frame is necessary. Thus, below we will focus on developing further the edge level formulations (16)–(18).

Our goal is to generalize these formulae to the case of $N > 2$ time frames. When doing so, one issue that arises is that the above formulae for the dynamic communicability matrices become unwieldy. The solution we propose builds on the fact that (16)–(18) can be rewritten using block matrices, just like we did with (8). Indeed, depending on what type of backtracking is forbidden, one can generalize (9) as follows:

$$M^{[1,2]} = \begin{bmatrix} C^{[1]} & C^{[1,2]} \\ 0 & C^{[2]} \end{bmatrix}, \tag{20}$$

where

- $C^{[\tau]} = B^{[\tau]}$ for $\tau = 1, 2$ and $C^{[1,2]} = W^{[1,2]}$, if one wants to recover (16), i.e., avoid backtracking in space but not in time;
- $C^{[\tau]} = W^{[\tau]}$ for $\tau = 1, 2$ and $C^{[1,2]} = B^{[1,2]}$, if one wants to recover (17), i.e., avoid backtracking in time but not in space; and
- $C^{[\tau]} = B^{[\tau]}$ for $\tau = 1, 2$ and $C^{[1,2]} = B^{[1,2]}$, if one wants to recover (18), i.e., avoid backtracking in space and time.

The following result then holds.

Proposition 4. *Suppose $M^{[1,2]}$ is defined as in (20). Then, within the radius of convergence,*

$$(I_m - \alpha M^{[1,2]})^{-1} = \begin{bmatrix} (I_m - \alpha C^{[1]})^{-1} & (I_m - \alpha C^{[1]})^{-1} \alpha C^{[1,2]} (I_m - \alpha C^{[2]})^{-1} \\ 0 & (I_m - \alpha C^{[2]})^{-1} \end{bmatrix}.$$

Our proof of this result mirrors the proof of Proposition 1 and is therefore omitted.

By using the above proposition and the fact that

$$(I_m - \alpha M^{[1,2]})^{-1} = I_m + \sum_{r=1}^{\infty} \alpha^r {M^{[1,2]}}^r,$$

we can easily recover (16)–(18) by projecting back to the node-level, multiplying by α to account for the fact that a walk on the edge level is one step shorter than its equivalent on the node level, and adding back the identity matrix I_n; such a projection is achieved by the global source and target matrices associated with $\mathcal{G}$:

$$I_n + \alpha {\mathcal{L}^{[1,2]}}^T (I_m - \alpha M^{[1,2]})^{-1} \mathcal{R}^{[1,2]}.$$

We now move to the goal of extending this line-graph interpretation of Katz centrality for evolving networks to possibly more than two time frames. In doing so, we will allow for backtracking to be forbidden (in time or space or both). We adopt the same strategy used in sections 4 and 5.

6.2.2. Non-backtracking Katz centrality for time-evolving networks: more than 2 *time frames*

We begin by extending Definition 7 and Definition 8 to the NBT framework. The latter may be reformulated in different ways, depending on the type of backtracking that one wants to avoid.

Definition 12. Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with N time frames. Let moreover $G^{[\tau]} = (\mathcal{V}, E^{[\tau]})$ for all $\tau = 1, 2, \ldots, N$. The non-backtracking transition matrix $B^{[\tau_1,\tau_2]}$ representing walks of length two that traverse the first edge at time t_{τ_1} and the second at time t_{τ_2}, $\tau_1 < \tau_2$, is defined entry-wise as follows:

$$(B^{[\tau_1,\tau_2]})_{i\to j,k\to\ell} = \delta_{jk}(1 - \delta_{i\ell})$$

for all $i \to j \in E^{[\tau_1]}$ and $k \to \ell \in E^{[\tau_2]}$.

These matrices, which are generally non-square, record information about NBT walks of length two where the first edge is traversed at time τ_1 and the second is traversed at time τ_2 (after staying idle for some time, in the case where $\tau_2 > \tau_1 + 1$). The next result extends Proposition 2.

Proposition 5. *Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network. Let moreover $L^{[\tau]}$ and $R^{[\tau]}$ be the source and target matrices associated with graph $G^{[\tau]}$. Then for all $1 \le \tau_1 < \tau_2 \le N$ we have*

$$B^{[\tau_1,\tau_2]} = W^{[\tau_1,\tau_2]} - W^{[\tau_1,\tau_2]} \circ {W^{[\tau_2,\tau_1]}}^T = R^{[\tau_1]}(L^{[\tau_2]})^T - (R^{[\tau_1]} {L^{[\tau_2]}}^T) \circ (L^{[\tau_1]} {R^{[\tau_2]}}^T).$$

Proof. We proceed entrywise. Let $i \to j \in E^{[\tau_1]}$ and $k \to \ell \in E^{[\tau_2]}$ be two edges in $\mathcal{G}$. Then

$$(R^{[\tau_1]} {L^{[\tau_2]}}^T)_{i\to j,k\to\ell} = \sum_{h=1}^{n} (R^{[\tau_1]})_{i\to j,h} (L^{[\tau_2]})_{k\to\ell,h} = \delta_{jk}.$$

Similarly,

$$(L^{[\tau_1]}R^{[\tau_2]^T})_{i\to j,k\to \ell} = \sum_{h=1}^{n}(L^{[\tau_1]})_{i\to j,h}(R^{[\tau_2]})_{k\to \ell,h} = \delta_{i\ell}.$$

The conclusion then follows from Definition 12 and Proposition 2. □

An advantage of the block-matrix approach is that it is readily expanded to deal with N time frames. This is done by defining $M^{[1,\ldots,N]}$ as one of the following block upper triangular block matrices.

Definition 13. Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with N time frames. The NBT global temporal transition matrix associated with $\mathcal{G}$ is the $m \times m$ block matrix

$$M = M^{[1,\ldots,N]} = \begin{bmatrix} C^{[1]} & C^{[1,2]} & C^{[1,3]} & \ldots & C^{[1,N]} \\ 0 & C^{[2]} & C^{[2,3]} & \ldots & C^{[2,N]} \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \ldots & \ldots & 0 & C^{[N]} \end{bmatrix}, \tag{21}$$

where

(i) $C^{[\tau_1]} = B^{[\tau_1]}$ and $C^{[\tau_1,\tau_2]} = W^{[\tau_1,\tau_2]}$ for all $\tau_1, \tau_2 = 1, 2, \ldots, N$ $(\tau_1 < \tau_2)$ if backtracking in space is forbidden;
(ii) $C^{[\tau_1]} = W^{[\tau_1]}$ and $C^{[\tau_1,\tau_2]} = B^{[\tau_1,\tau_2]}$ for all $\tau_1, \tau_2 = 1, 2, \ldots, N$ $(\tau_1 < \tau_2)$ if backtracking in time is forbidden; and
(iii) $C^{[\tau_1]} = B^{[\tau_1]}$ and $C^{[\tau_1,\tau_2]} = B^{[\tau_1,\tau_2]}$ for all $\tau_1, \tau_2 = 1, 2, \ldots, N$ $(\tau_1 < \tau_2)$ if backtracking in both time and space is forbidden.

Such a formulation allows for non-backtracking across multiple graphs to be calculated.

Remark 6. In the third case, one can calculate M from the global source and target matrices as $\mathcal{R}\mathcal{L}^T - \mathcal{R}\mathcal{L}^T \circ \mathcal{L}\mathcal{R}^T$ by setting all elements below the block diagonal to zero.

We can now define Katz centrality on a time-evolving network with NBT global temporal transition matrix $M = M^{[1,\ldots,N]}$ equal to any of the three options in Definition 13 (depending on the type of backtracking allowed) as

$$\widehat{\boldsymbol{y}}(\alpha) = \sum_{r=0}^{\infty}(\alpha M)^r \mathbf{1}.$$

The following result gives an upper bound for the possible choices of $\alpha > 0$.

Proposition 6. *Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with adjacency matrices $A^{[1]}, A^{[2]}, \ldots, A^{[N]}$ and let $M = M^{[1,\ldots,N]}$ be defined as in Definition 13. Moreover, let $\rho = \max_\tau \rho(A^{[\tau]})$ and $\lambda = \min_\tau \lambda_\tau$, where λ_τ is the smallest eigenvalue of the matrix polynomial $P^{[\tau]}(z) = I - A^{[\tau]}z + (D^{[\tau]} - I)z^2 + (A^{[\tau]} - S^{[\tau]})z^3$, for all $\tau = 1, 2, \ldots, N$, where $D^{[\tau]}$ and $S^{[\tau]}$ are as in (19).*

Then, the series $\sum_{r=0}^{\infty}(\alpha M)^r$ converges and moreover

$$\sum_{r=0}^{\infty}(\alpha M^{[1,\ldots,N]})^r = (I_m - \alpha M^{[1,\ldots,N]})^{-1}$$

for all $\alpha \in (0, \ell)$, where

- *$\ell = \lambda$, if M is as in (i) or (iii) from Definition 13;*
- *$\ell = \rho^{-1}$, if M is as in (ii) from Definition 13.*

Proof. The rightmost endpoint of the interval of allowed values for α is the radius of convergence of $\sum_{r=0}^{\infty} M^r$, which is equal to the inverse of the spectral radius of M. Since the latter is a block triangular matrix, its spectral radius is equal to the maximum of the spectral radii of the diagonal blocks. It follows by the analysis in [2,4,16] that the spectral radius of $B^{[i]}$ is λ_i^{-1}, while by Flanders' theorem the spectral radius of $W^{[i]} = R^{[i]}(L^{[i]})^T$ is equal to the spectral radius of $A^{[i]} = (L^{[i]})^T R^{[i]}$, which is ρ_i. $\square$

This convergence result allows us to thus define NBT Katz centrality for temporal networks as follows.

Definition 14. Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \ldots, G^{[N]})$ be a temporal network with N time frames. Let M be defined as in Definition 13 and let $\alpha \in (0, \ell)$, where ℓ is defined according to Proposition 6. We define NBT temporal Katz centrality as the vector

$$\widehat{\boldsymbol{y}}(\alpha) = \sum_{r=0}^{\infty}(\alpha M)^r \mathbf{1} = (I_n + \alpha(\mathcal{L}^T(I_m - \alpha M)^{-1}\mathcal{R})\mathbf{1}_n.$$

Remark 7. Note that, since $\mathcal{R}\mathbf{1}_n = \mathbf{1}_m$, Katz centrality is also equal to

$$\widehat{\boldsymbol{y}}(\alpha) = \mathbf{1}_n + \alpha\mathcal{L}^T(I - \alpha M)^{-1}\mathbf{1}_m.$$

Remark 8. One may also define subgraph centrality indices by considering the diagonal entries of the matrix under study:

$$\widehat{\boldsymbol{x}}(\alpha)_i = 1 + \alpha(\mathcal{L}^T(I_m - \alpha M)^{-1}\mathcal{R})_{ii}.$$

The results presented so far for the matrix resolvent can also be extended to treat other analytic matrix functions. Indeed, the following result is an analogue of Proposition 3 in the non-backtracking framework.

Proposition 7. *If the power series $f(z) = \sum_{r=0}^{\infty} c_r z^r$ converges with radius of convergence R, then the series $\sum_{r=0}^{\infty} c_r \alpha^r M^r$ also converges for all $\alpha \in [0, R/\ell)$, with M is as in Definition 13 and ℓ is as in Proposition 6. Moreover,*

$$\sum_{r=0}^{\infty} c_r \alpha^r M^r = \partial f(\alpha M),$$

where ∂ is the functional operator defined in (11).

Using this result, Definition 14 can straightforwardly be generalized to describe centrality indices that avoid different types of backtracking, according to how the matrix M in (21) is selected.

Definition 15. Let $\mathcal{G}$ be a temporal network and let $M = M^{[1,\ldots,N]}$ be defined as in Definition 13 Let f be a function which is analytic in a neighborhood of zero with Maclaurin series $f(z) = \sum_{r=0}^{\infty} c_r z^r$, such that $c_r \geq 0$ for all r, and let $\alpha \in (0, \ell)$, where ℓ is as in Proposition 6. Moreover, let ∂ be the functional operator defined in (11). The NBT temporal f-subgraph centrality of node i is defined as

$$\widehat{\boldsymbol{x}}(\alpha)_i = \left(c_0 I + \alpha \mathcal{L}^T \partial f(\alpha M) \mathcal{R}\right)_{ii}. \tag{22}$$

Additionally, the NBT temporal f-total communicability of node i is defined as the ith entry of the following vector:

$$\widehat{\boldsymbol{y}}(\alpha) = c_0 \mathbf{1}_n + \alpha \mathcal{L}^T \partial f(\alpha M) \mathbf{1}_m, \tag{23}$$

where $\mathcal{L}$ and $\mathcal{R}$ be defined as in Definition 9.

7. Conclusions

Our aim in this work was to study walk-based centrality measures for temporal networks. This required us to extend existing work involving matrix functions applied to (a) the adjacency matrix of a network, (b) the adjacency matrix of the line graph, and (c) the Hashimoto matrix. For the Katz, or matrix resolvent, case, it is known from [17] that dynamic centrality may be computed at the node level; that is, by using n by n matrices, where n is the number of nodes. Here, we proved that any other matrix function-based measure does not have such a straightforward representation, but can be expressed in terms of a higher dimensional edge-level formula. In the case of non-backtracking temporal centrality, we identified three types of constraint and showed how these may be dealt with using block matrix extensions of the Hashimoto construction.

Declaration of competing interest

There is no competing interest.

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