WEIGHTED ENUMERATION OF NONBACKTRACKING WALKS 2 **ON WEIGHTED GRAPHS ***

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5 Abstract. We extend the notion of nonbacktracking walks from unweighted graphs to graphs 6 whose edges have a nonnegative weight. Here the weight associated with a walk is taken to be 7 the product over the weights along the individual edges. We give two ways to compute the associated generating function, and corresponding node centrality measures. One method works directly 8 9 on the original graph and one uses a line graph construction followed by a projection. The first method is more efficient, but the second has the advantage of extending naturally to time-evolving 10 11 graphs. Based on these generating functions, we define and study corresponding centrality measures. Illustrative computational results are also provided. 12

13 Key words. Complex network, matrix function, generating function, line graph, combinatorics, evolving graph, temporal network, centrality measure, Katz centrality. 14

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1. Introduction. Complex network analysis is an expanding scientific discipline that has recently been producing many research challenges, with applications across 17 several fields of science and engineering [11, 24]. One important question is that of 18ranking the nodes of a graph by importance, or, in more mathematical terms, defining 19 and studying an appropriate *centrality measure*. Those centrality measures that can 20 be formulated and computed via combinatorial properties of walks on the underlying 21 22 graph have received special attention [7, 12, 13, 19, 23] because they have convenient formulations in terms of linear algebra that lead to efficient computational methods. 23 In recent years, this paradigm has been refined by studying centrality measures that 24 are based on counting not all walks but only some of them, namely, walks that do not 25backtrack [1, 2, 5, 14, 28–30] or more generally do not cycle [5]. Nonbacktracking walks 26are known to be linked to zeta functions of graphs [18, 21, 22, 26]. Their associated 27 centrality measures have been shown to possess attractive computational properties 28[1, 2, 4, 14] and have been studied both for undirected and directed graphs, and more 29 recently for time evolving graphs [3]. However, in the context of the combinatorics 30 of nonbacktracking walks, so far only unweighted graphs have been studied. We mention that nonbacktracking random walks were previously considered in [20], but 32 the problems studied there are different to the ones analyzed in the present paper. Moreover, [20] focuses only on the special case where the nodes are given themselves a 34 positive weight $\varphi(i)$, and the weight of the edge (i, j) is defined as $\omega((i, j)) = \varphi(i)\varphi(j)$. 35

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Instead, we do not impose any restriction on the edges' weights. In the theory of graph 36

37 zeta functions, weighted graphs have been considered by defining the weight of a walk

to be the sum (and not the product, as in this paper) of the weights of its edges [18]. 38

We discuss this issue further in section 2. 39

The main purpose of the present paper is to extend the combinatorial theory of 40 nonbacktracking walks, and corresponding centrality measures, to graphs whose edges 41 carry a positive *weight*. These graphs are associated with generic nonnegative adja-42 cency matrices, in contrast to unweighted graphs that correspond to binary adjacency 43 matrices. While for unweighted graphs one may be interested in the enumeration of 44 walks of a given length, for weighted graphs the combinatorial problem is more so-45phisticated due to the presence of weights. The edge weights naturally give rise to 4647 an overall weight for each walk, a concept that can be used alongside the length (i.e., the number of edges traversed). 48

The structure of the paper is as follows. In Section 2 we introduce some relevant 49 notation and core concepts. Section 3 sets up and studies the issue of characterizing 50the classical generating function associated with nonbacktracking weighted walks and using it to compute a centrality measure. In section 4 we introduce an alternative 53 formulation that applies to a wider class of generating functions and centrality measures. Section 5 shows how these ideas can be extended to the case of evolving graphs. 54Numerical experiments are conducted in Section 6. We finish in Section 7 with a brief discussion. 56

57 2. Background and Notation. In this paper, we consider finite graphs. A finite graph is a triple $G = (V, E, \Omega)$ where V = [n] is the set of the nodes (or 58 vertices), $E \subset V \times V$ is the set of (directed) edges, and $\Omega: E \to (0, \infty)$ is a weight function that associates to each edge a positive weight. If $\Omega(e) = 1$ for all $e \in E$, 60 then the graph is said to be *unweighted*; if for any pair $i \neq j$, with $i, j \in V$ we have 61 that $(i, j) \in E \Leftrightarrow (j, i) \in E$ and that $\Omega((i, j)) = \Omega((j, i))$ then the graph is said to be 62 *undirected*; and if, for every $i \in V$, we have that $(i, i) \notin E$ then the graph is said to be 63 without loops. Graphs that are not unweighted are usually called *weighted* and graphs 64 65 that are not undirected are usually called *directed*. It is, however, convenient (and we will do so within this work) to relax the terminology so that the set of directed 66 (resp., weighted) graphs contains as special cases also undirected (resp., unweighted) 67 graphs, further we will assume that all graphs are without loops. 68

A walk of length ℓ on the graph G is a sequence of nodes $i_1, i_2, \ldots, i_{\ell+1}$ such that 69 $(i_j, i_{j+1}) \in E$ for all $1 \leq j \leq \ell$. Equivalently, it can be seen as a sequence of edges 70 e_1, \ldots, e_ℓ such that $e_j \in E$ for all $j = 1, \ldots, \ell - 1$ and the end node of e_j coincides 71with the starting node of e_{i+1} . 72

DEFINITION 2.1. Let $G = (V, E, \Omega)$ be a weighted graph. The weight of the walk 73 74 e_1,\ldots,e_ℓ is

$$\prod_{k=1}^{\ell} \Omega(e_k)$$

where $\Omega(e_k)$ is the weight of the edge $e_k \in E$. 76

77 REMARK 2.2. When $\Omega: E \to \{1\}$ is the weight function associated with an unweighted graph, then the weight of all walks in the network is one, regardless of their 78length. 79

In the context of mainstream graph theory, the *weight* (or *length* or *cost*) of a walk is 80

sometimes defined as the *sum*, rather than the product, of the weights of its edges. In 81 2

that scenario, zeta functions of graphs (which are closely related to the enumeration of nonbacktracking walks) have been studied [18]. However, we argue that within complex network analysis Definition 2.1 has several useful applications. For example, consider a road network where nodes represent towns and a nonnegative integer edge weight A_{ij} records the number of distinct roads connecting town i and town j. Then, the number of distinct routes from i to j that pass through one intermediate town is equal to

$$\sum_{k=1}^{n} A_{ik} A_{kj},$$

90 that is, the weighted sum of walks of length two, where the weight is the *product* of the 91 weights of its edges. Similarly, in a model where edges represent independent prob-92 abilistic events and their weights are their probabilities, as discussed in the original 93 work of Katz [19], it is natural to postulate that the weight of a walk is the product 94 of the weight of its edges, in agreement with the fact that the joint probability of a 95 sequence of independent events is the product of the individual probabilities.

Given a node ordering, the corresponding adjacency matrix of a graph is the matrix $A \in \mathbb{R}^{n \times n}$ entrywise defined as:

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$$A_{ij} = \begin{cases} 0 & \text{if } (i,j) \notin E; \\ \Omega((i,j)) & \text{if } (i,j) \in E. \end{cases}$$

Note that a graph is undirected if and only if its adjacency matrix is symmetric; it is without loops if and only if its adjacency matrix has zero diagonal; and it is unweighted if and only if its adjacency matrix has entries all lying in $\{0, 1\}$.

The problems of enumerating walks in unweighted graphs and enumerating weighted walks in weighted graphs may both be solved by considering powers of the adjacency matrix: indeed, the (i, j) entry of A^k is equal to, respectively, the number of walks of length k from node i to node j (when the graph is unweighted) or the weighted sum of walks of length k from node i to node j (when the graph is weighted). As a consequence, the generating function for the (possibly weighted) enumeration of walks is given by

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$$I + tA + t^2A^2 + \dots = \sum_{k=0}^{\infty} t^k A^k = (I - tA)^{-1},$$

where we adopt the standard convention that the (weighted) sum of walks of length 110 zero from i to j is 1 if i = j and 0 otherwise. Here, t is a real parameter small enough 111 to ensure convergence of the series which scales by t^k the count for walks of length k. 112A walk can also be seen as a sequence of nodes. If the sequence does not contain 113a subsequence of the form iji for some nodes i and j, then the walk is said to be 114 nonbacktracking (NBT). We define $p_k(A)$ to be the matrix whose (i, j) entry contains 115 the sum of the weights of all nonbacktracking walks of length k from node i to node j. 116By convention, $p_0(A) = I$. Note that, by definition, $p_k(A) \leq A^k$ elementwise. Combi-117 natorially, the problem of computing the (weighted) enumeration of nonbacktracking 118walks is equivalent to finding an explicit expression for the generating function 119

120 (2.1)
$$\Phi(t) = \sum_{k=0}^{\infty} t^k p_k(A)$$

121 for suitable values of the parameter t > 0.

This problem was addressed in [14] for unweighted undirected graphs, and later in [1] for unweighted directed graphs. In [2], the solution was extended to the more general generating function

125 (2.2)
$$\kappa(t) = \sum_{k=0}^{\infty} c_k t^k p_k(A),$$

where $(c_k)_k \subset [0, \infty)$ is an arbitrary sequence. In [3], the theory was further extended to consider time evolving graphs. However, so far, the quantities (2.1) and (2.2) have not yet been studied for weighted graphs. Their characterization is the main contribution of this paper.

A corollary of obtaining such computable expressions is a numerical recipe for associated nonbacktracking centralities. Indeed, beyond its algebraic interpretation as a generating function, (2.2) can be interpreted analytically as a function that will converge for sufficiently small values of the variable t. Choosing one such value for t allows us to define a centrality measure based on the weighted sum of edges. For example, if **1** is the vector of all ones, then the *i*-th component of the vector

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$$\left(\sum_{k=0}^{\infty} c_k t^k p_k(A)\right) \mathbf{1}$$

computes a nonbacktracking version of Katz centrality [19]. The latter is defined as the doubly weighted sum of all the walks departing from node i, where the weight of each walk within the sum is the product of the weight of the walk itself and t^k , where k is the walk length. Similarly, for the *subgraph centrality* version of nonbacktracking Katz, the doubly weighted sum of all the walks that start and end on node i is given by

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$$\left(\sum_{k=0}^{\infty} c_k t^k p_k(A)\right)_{ii}$$

As a consequence, two additional questions that we address in this paper are to describe the radius of convergence of (2.2) and to derive computable expressions for the associated centrality measures. We refer to [1, 2, 14], and the references therein, for details of the benefits of nonbacktracking in the centrality context.

We consider two approaches to bridge the gap between weighted graphs and 148 149current results on the combinatorics of nonbacktracking walks. The first is specialized to the case $c_k \equiv 1$, i.e., to compute (2.1); it leads directly to an expression that has 150computational advantages as it does not require to go through the edge-level and, 151thus, it requires the construction of a potentially much smaller matrix than the second 152approach. The second is based on a technique, described in [3, 5], of forming the line 153graph, obtaining a generating function there, and finally projecting back to compute 154155(2.2). While, potentially, the second approach may be computationally less efficient, it has the advantages that (i) it is able to solve the more general problem (2.2), (ii) 156it can be generalized to the setting of time evolving graphs, and (iii) it allows us to 157easily estimate the convergence radius of (2.2) (including the special case of (2.1)). 158

3. The generating function of nonbacktracking walks on a weighted graph. In this section, we assume that G is a finite directed weighted graph with n nodes, without loops, and having adjacency matrix A. The directed edge from node i to node j has weight $A_{ij} > 0$. Following Definition 2.1, to the walk $i_1i_2i_3...i_{\ell+1}$ 163 of length ℓ we assign the weight $A_{i_1i_2}A_{i_2i_3}\cdots A_{i_\ell i_{\ell+1}}$. We note the distinction here 164 between the *length* and the *weight* of a walk.

165 The goal of this section is to obtain a convenient formula for the generating 166 function $\Phi(t)$ in (2.1). We note that this generalizes the version previously studied 167 for an unweighted graph [1], and the expression $\Phi(t)\mathbf{1}$ is then a natural candidate for 168 a node centrality measure.

3.1. Describing the matrices $p_k(A)$ via a recurrence relation. Let us first 169set up some further notation: given two square matrices $X, Y \in \mathbb{R}^{n \times n}$ we distinguish 170between matrix multiplication, XY, and elementwise multiplication, $X \circ Y$, where 171 $(X \circ Y)_{ij} = X_{ij}Y_{ij}$. Similarly, we differentiate between the k-th linear algebraic power X^k and the k-th elementwise power, $X^{\circ k}$, so $(X^{\circ k})_{ij} = (X_{ij})^k$. Moreover, 172173174following Matlab notation, dd(X) := diag(diag(X)) will denote the diagonal matrix whose diagonal entries are equal to the diagonal entries of X. We first prove the 175following k-term recurrence, which generalizes previous results that have been derived 176 177independently for the unweighted [10, 27] and undirected [26] cases.

178 THEOREM 3.1. For all $k \geq 1$,

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$$p_k(A) = \sum_{\substack{\ell = 2h+1 \text{ odd} \\ 1 \le \ell \le k}} (A^{\circ(h+1)} \circ (A^T)^{\circ h}) p_{k-\ell}(A) - \sum_{\substack{\ell = 2h \text{ even} \\ 2 \le \ell \le k}} \mathrm{dd}((A^{\circ h})^2) p_{k-\ell}(A).$$

180 Proof. For the base case of k = 1, the statement reduces to $p_1(A) = (A \circ \mathbf{11}^T)p_0(A)$. Since $A \circ \mathbf{11}^T = A$ and $p_0(A) = I$, in turn this yields $p_1(A) = A$, 182 which is manifestly true since any walk of length one is nonbacktracking. Let us now 183 give a proof by induction.

We start by considering $Ap_{k-1}(A)$, whose (i, j) entry is equal to the sum of the 184weights of all walks of length k from i to j that are nonbacktracking if the first step is 185 removed. This value is equal to $p_k(A)_{ij}$ plus the sum of the weights of all backtracking 186 walks of length k from i to j that are nonbacktracking if the first step is removed. 187 Such walks must be of the form $iai \dots j$: the weight of one such walk is $A_{ia}A_{ai}$ times 188 the weight of a certain NBT walk of length k-2 from i to j. Summing over all a 189 adjacent to i yields $dd(A^2)p_{k-2}(A)$. However, we have subtracted too much, because 190any such walk of the form $iaia \dots j$, being backtracking after removing the first step, 191 was not present in $(Ap_{k-1}(A))_{ij}$. The weight of one such walk is $A_{ia}A_{ai}A_{ia} = A_{ia}^2A_{ai}$ 192 times the weight of a certain NBT walk of length k-3 from a to j. We can sum again 193over all a adjacent to i, to obtain $((A^{\circ 2} \circ A^T)p_{k-3}(A))_{ij}$. We should sum this value 194back, but again we are adding a bit too much, because walks satisfying the previous 195196 requirements and being of the form $iaiai \dots i$ should not be there.

197 It is clear that this sequence of corrections goes on until we exhaust the length 198 of the walk and the statement of the theorem is a consequence of the two following 199 facts, both true for all $h \ge 0$.

200 201 202 1. The total weight of walks of length k from i to j of the form $i(ai)^h a \dots j$, such that the final subwalk (of length k - (2h+1)) from a to j is not backtracking, is equal to

$$\sum_{a:(i,a)\in E} (A_{ia})^{h+1} (A_{ai})^h p_{k-2h-1}(A)_{aj} = \left((A^{\circ(h+1)} \circ (A^T)^{\circ h}) p_{k-2h-1}(A) \right)_{ij}.$$

204 205 2. The total weight of walks of length k from i to j of the form $(ia)^{2h}i \dots j$, such that the final subwalk (of length k - 2h) from i to j is not backtracking, is

206 equal to

$$\sum_{a:(i,a)\in E} (A_{ia})^h (A_{ai})^h p_{k-2h}(A)_{ij} = \left(\mathrm{dd}((A^{\circ h})^2) p_{k-2h-1}(A) \right)_{ij}.$$

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3.2. Solving the recurrence relation. Let us continue by giving a combinatorial result in Proposition 3.2. Its statement expresses the generating function of a sequence satisfying a growing recurrence relation in terms of two individual generating functions.

PROPOSITION 3.2. Let $(\mathcal{P}_k)_k$ and $(\mathcal{C}_\ell)_\ell$ be two sequences in some (possibly noncommutative) ring, and suppose that $(\mathcal{P}_k)_k$ satisfies the growing recurrence

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$$\sum_{\ell=0}^{k} \mathcal{C}_{\ell} \mathcal{P}_{k-\ell} = 0$$

for all $k \ge 1$. Then, the (formal) generating functions $\Phi(t) = \sum_{k=0}^{\infty} \mathcal{P}_k t^k$ and $\Psi(t) = \sum_{\ell=0}^{\infty} \mathcal{C}_{\ell} t^{\ell}$ are related by the formula $\Psi(t) \Phi(t) = \mathcal{C}_0 \mathcal{P}_0$.

217 *Proof.* Observe that, using the recurrence,

$$\Psi(t)\Phi(t) = \sum_{k=0}^{\infty} t^k \sum_{\ell=0}^{\infty} \mathcal{C}_{\ell} \mathcal{P}_{k-\ell} = \mathcal{C}_0 \mathcal{P}_0.$$

We can now apply the general technique of Proposition 3.2 to the special case of the generating function (2.1), whose coefficients satisfy the recurrence described in Theorem 3.1. In other words, we specialize Proposition 3.2 to sequences in the ring $\mathbb{R}^{n \times n}$ where $\mathcal{P}_k = p_k(A)$ and

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$$C_{\ell} = \begin{cases} I & \text{if } \ell = 0; \\ -[A^{\circ(h+1)} \circ (A^{T})^{\circ h}] & \text{if } \ell = 2h + 1; \\ \mathrm{dd}((A^{\circ h})^{2}) & \text{if } \ell = 2h > 0 \end{cases}$$

In particular, $C_0 = \mathcal{P}_0 = I$, and hence by Proposition 3.2 $\Phi(t) = \Psi(t)^{-1}$. In turn, we can write $\Psi(t) = \Psi_e(t) - \Psi_o(t)$ by splitting even and odd terms and by extracting the minus sign appearing in the odd terms of $(\mathcal{C}_\ell)_\ell$. It is easy to see that $\Psi_e(t)$ is diagonal while $\Psi_o(t)$ is the off-diagonal part of $\Psi(t)$, since we assume G to be without loops. Moreover,

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$$(\Psi_o(t))_{ij} = \sum_{h=0}^{\infty} t^{2h+1} A_{ij}^{h+1} A_{ji}^h = \frac{tA_{ij}}{1 - t^2 A_{ij} A_{ji}}$$

230 Similarly,

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$$(\Psi_e(t))_{ii} = 1 + \sum_{h=1}^{\infty} t^{2h} \sum_{j=1}^n A^h_{ij} A^h_{ji} = 1 + \sum_{j=1}^n \frac{t^2 A_{ij} A_{ji}}{1 - t^2 A_{ij} A_{ji}}.$$

232 Let $S = A \circ A^T$, let $Q = S^{\circ 1/2}$, let

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$$f_1(x) = \frac{x}{1-x}, \quad f_2(x) = \frac{x}{1+x},$$

and let $f_i(\circ tX)$ denote the *elementwise* application of f_i to the matrix tX, for i = 1, 2. Then, if we denote by \circ / the elementwise application of /, we can write

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$$\Psi_e(t) = I + \mathrm{dd}(f_1(\circ tQ)f_2(\circ tQ)), \qquad \Psi_o(t) = tA \circ /(\mathbf{1}\mathbf{1}^T - t^2S)$$

and hence $\Psi(t) = I + \mathrm{dd}(f_1(\circ tQ)f_2(\circ tQ)) - tA \circ /(\mathbf{11}^T - t^2S).$ We can state this more formally as a theorem.

THEOREM 3.3. In the notation above, for all values of t such that (2.1) converges, we have

241 (3.1)
$$\Phi(t) = (I + \mathrm{dd}[f_1(\circ tQ)f_2(\circ tQ)] - tA \circ / (\mathbf{1}\mathbf{1}^T - t^2S))^{-1}.$$

As a sanity check, let us see what happens in three distinct interesting limiting cases that have been addressed previously in the literature.

• First, let us verify that in the limit of an unweighted graph we recover [1, equation (3.3)]. In this case, $(A_{ij})^h = A_{ij} \in \{0,1\}$ for all $h \ge 1$. As a result, if $D = dd(A^2)$,

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$$(\Psi_e(t))_{ii} = 1 + \sum_{h=1}^{\infty} t^{2h} \sum_{j=1}^{n} A_{ij} A_{ji} = 1 + D_{ii} \frac{t^2}{1 - t^2} \Rightarrow \Psi_e(t) = \frac{I - t^2 I + t^2 D}{1 - t^2}$$

248 and

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$$(\Psi_o(t))_{ij} = tA_{ij} + \sum_{h=1}^{\infty} t^{2h+1} A_{ij} A_{ji} = tA_{ij} + \frac{t^3 S_{ij}}{1 - t^2} \Rightarrow \Psi_o(t) = \frac{tA - t^3(A - S)}{1 - t^2}$$

250 which imply the known $\Phi(t) = (1 - t^2)(I - tA + t^2(D - I) + t^3(A - S))^{-1}$ 251 from [1, Equation (3.3)].

- Next, let us observe that if no edge is reciprocated, that is, if there is no $(i, j) \in E$ 253 E such that $(j, i) \in E$, then S = Q = 0. Hence, we recover the generating 254 function associated with classical Katz centrality, i.e., $\Phi(t) = (I - tA)^{-1}$, 255 which is consistent with the fact that every walk is nonbacktracking under 256 this assumption.
 - Finally, if the graph is undirected then $S = A^{\circ 2}$ and Q = A. Hence, the formulae simplify to

$$\Psi_e(t) = I + dd[f_1(\circ tA)f_2(\circ tA)], \qquad \Psi_o(t) = tA \circ /(\mathbf{1}\mathbf{1}^T - t^2A^{\circ 2})$$

260 yielding in particular

$$\Phi(t) = (I + dd[f_1(\circ tA)f_2(\circ tA)] - tA \circ /(\mathbf{11}^T - t^2A^{\circ 2}))^{-1}$$

If we additionally assume that the graph is unweighted, we further reduce to $\Phi(t) = (1 - t^2)(I - At + t^2(D - I))^{-1}$ in agreement with [14, Equation (5.3)].

We now briefly comment on the convergence of $\Phi(t) = \sum_k p_k(A)t^k$ to the righthand-side of (3.1). Since the series converges to a rational function, its radius of convergence is equal to the smallest of its poles. One way to compute the radius is therefore via the eigenvalues of the rational function $\Psi(t) = \Phi(t)^{-1}$. A more straightforward method (albeit possibly less efficient) to estimate the radius of convergence is available when computing $\Phi(t)$ with a different method. This is described in more detail in Section 3 and, in particular, within Corollary 4.8. In spite of the somewhat awkward notation, (3.1) is in fact quite straightforward to compute given A, by composing elementwise functions and matrix addition and multiplications.

We conclude this section by recalling that we can define a nonbacktracking version of Katz centrality on weighted graphs by summing the value of the generating function over all possible ending nodes, which can be expressed as the linear algebraic matrixvector multiplication $\Phi(t)\mathbf{1}$.

The following corollary is then an immediate consequence of Theorem 3.1.

COROLLARY 3.4. For all values of t such that (2.1) converges, consider the centrality measure where node i is assigned the value x_i according to $\mathbf{x} = \Phi(1)\mathbf{1}$. Then \mathbf{x} may be found by solving the linear system

281 (3.2) $(I + dd[f_1(\circ tQ)f_2(\circ tQ)] - tA \circ /(\mathbf{11}^T - t^2S))\mathbf{x} = \mathbf{1}.$

Corollary 3.4 shows in particular that the centrality measure can be found without explicitly computing the inverse in (3.1). We can instead compute the vector of nonbacktracking centralities \mathbf{x} by solving the linear system (3.2). We note that the coefficient matrix in (3.2) is no less sparse than I - tA; hence the computational complexity of solving such a linear system is the same as for classical Katz centrality, and the task is feasible with standard tools for sparse linear systems for very large, sparse networks.

4. Generating function by constructing the line graph and projecting back. In this section, we derive an alternative computable expression for the generating function $\Phi(t)$. Although generally this second method is less computationally efficient, it offers three main advantages: (i) it can be extended to nonbacktracking centrality measures other than Katz (for example, based the exponential rather than the resolvent); (ii) it allows for a simple characterization of the radius of convergence of the generating function; and (iii) it can be extended to time evolving graphs.

As before, we consider a finite weighted graph with n nodes. We also assume (directed) edges have been labelled from 1 to m in an arbitrary, but fixed, manner. We may then define the *source matrix* $L \in \mathbb{R}^{m \times n}$ and *target* (or *terminal*) *matrix* $R \in \mathbb{R}^{m \times n}$ as follows [31]:

$$L_{ej} = \begin{cases} 1 & \text{if edge } e \text{ starts from node } j \\ 0 & \text{otherwise} \end{cases} \qquad \qquad R_{ej} = \begin{cases} 1 & \text{if edge } e \text{ ends on node } j \\ 0 & \text{otherwise.} \end{cases}$$

Moreover, we let Z be an $m \times m$ diagonal matrix such that $Z_{ee} = A_{ij}$, where (in the chosen labelling of the edges) the *e*-th edge is precisely (i, j).¹ Then, we have the following relationship.

299 PROPOSITION 4.1. We have $A = L^T Z R$.

Proof. Since Z is diagonal, $(L^T Z R)_{ij} = \sum_{e=1}^m L_{ei} Z_{ee} R_{ej}$. But there is at most one value of e such that $L_{ei} R_{ej} \neq 0$, and that is precisely the value identifying the edge $i \rightarrow j$, if this is an edge of the graph. If such an edge does not exist then the summation yields 0, as desired. If such an edge exists, then, for that $e, Z_{ee} = A_{ij}$ which concludes the proof.

Now let W be the weighted matrix of the dual graph (or line graph), i.e., the graph whose nodes correspond to the original (directed) edges, and whose edges are

¹For clarity, we will sometimes use the notation $i \to j$ to denote the edge $(i, j) \in E$.

pairs of edges from the original graph that can form a walk. The pair $(i \rightarrow j, j \rightarrow k)$ represents a walk that has weight equal to the product of the original edge weights; that is, $A_{ij}A_{jk}$. These values are recorded in the entries of W, with $W_{ef} = A_{ij}A_{jk}$ if *e* is the label of edge $i \rightarrow j$ and *f* is the label of edge $j \rightarrow k$.

311 THEOREM 4.2. We have $W = ZRL^TZ$.

Proof. We proceed entrywise. Suppose for concreteness that edge e is $i \to j$ and edge f is $k \to \ell$, where $i \neq j$, $k \neq \ell$ are (possibly, but not necessarily, all distinct) nodes. Note for a start that $W_{ef} = A_{ij}A_{j\ell}$ if j = k and $W_{ef} = 0$ if $j \neq k$. Now, since Z is diagonal,

$$(ZRL^TZ)_{ef} = Z_{ee}Z_{ff}\sum_{h=1}^n R_{eh}L_{fh} = A_{ij}A_{k\ell}\sum_{h=1}^n R_{eh}L_{fh}.$$

Suppose $j \neq k$; then there is no h such that $R_{eh}L_{fh} \neq 0$, so the summation above is 0 = W_{ef} . On the other hand, if j = k then the summation over h yields 1 so that (ZRL^TZ)_{ef} = $A_{ij}A_{j\ell} = W_{ef}$.

In the unweighted case, we have a projection relation $L^T W^k R = A^{k+1}$ [5, Propo-315 sition 2.4]. However, for weighted graphs, entries of W^k count walks of length k+1, 316but with incorrect weights. For example, the walk $1 \rightarrow 2 \rightarrow 3 \rightarrow 4$ would be weighted 317 $A_{12}A_{23}^2A_{34}$ rather than $A_{12}A_{23}A_{34}$. We now exhibit a trick that corrects this prob-318 lem. Coherently with the notation of the previous section, below $M^{\circ 1/2}$ denotes the 319 elementwise nonnegative square root of a nonnegative matrix M; note that generally this does not correspond to the classical matrix square root \sqrt{M} (i.e., the matrix X 321 such that $X^2 = M$, a notable exception being the case of a diagonal square matrix 322 with nonnegative diagonal. We note that Z falls in this latter category, hence the 323 notation in the following result. 324

THEOREM 4.3. Let $0 < k \in \mathbb{N}$. The (e, f) element of $\sqrt{Z}(W^{\circ 1/2})^k \sqrt{Z}$ counts, with weights, all walks of length k + 1 from edge e to edge f.

Proof. The crucial observation is that $W^{\circ 1/2} = \sqrt{Z}RL^T\sqrt{Z}$, which is clear by a minor modification of the proof of Theorem 4.2. We now proceed by induction on k. For the base case k = 1, it suffices to observe that $\sqrt{Z}W^{\circ 1/2}\sqrt{Z} = ZRL^TZ = W$. Suppose now that the statement holds for k - 1. Then,

$$\sqrt{Z} (W^{\circ 1/2})^k \sqrt{Z} = \sqrt{Z} (W^{\circ 1/2})^{k-1} \sqrt{Z} (Z^{-1/2}) W^{\circ 1/2} \sqrt{Z}$$

Define for notational simplicity $U := \sqrt{Z} (W^{\circ 1/2})^{k-1} \sqrt{Z}$, $X := Z^{-1/2}$, $Y := W^{\circ 1/2}$, $\Sigma := \sqrt{Z}$. Then, since X and Σ are diagonal,

$$(UXY\Sigma)_{ef} = \sum_{g \in E} U_{eg} X_{gg} Y_{gf} \Sigma_{ff}.$$

Suppose now that edge e is $i \to j$ and edge f is $h \to \ell$; then edges g must be of the form $x \to h$ for some node x. Indeed, $Y_{gf} = 0$ unless the end node of edge g coincides with the start node of edge f, i.e., unless gf is a walk of length two. Hence, in this notation,

$$(UXY\Sigma)_{ef} = \sum_{x:A_{xh}>0} U_{e,x\to h} \sqrt{A_{h\ell}A_{xh}} \sqrt{\frac{A_{h\ell}}{A_{xh}}} = A_{h\ell} \sum_{x:A_{xh}>0} U_{e,x\to h},$$

where $\sum_{x:A_{xh}>0} U_{e,x\to h}$ is, by the inductive assumption, the count (with weights) of all walks of length k-1 from edge e to all edges of the form $x \to h$, i.e., the weighted enumeration of all walks of length k-1 from edge e to node h. However, the count with weights of all walks of length k from edge e to edge f is precisely the count with weights of all walks of length k from edge e to node ℓ with node h as the penultimate node, i.e., the right hand side in the latter displayed equation.

- We have the following consequence of Theorem 4.3.
- 334 COROLLARY 4.4. For all $k \in \mathbb{N}$, $L^T \sqrt{Z} (W^{\circ 1/2})^k \sqrt{Z} R = A^{k+1}$.
- 335 Proof. The result follows from Proposition 4.1, if k = 0, and from Theorem 4.3, 336 if k > 0.

Now let $B \in \mathbb{R}^{m \times m}$ be the nonbacktracking version of W, i.e., $B_{ef} = 0$ if WefWfe $\neq 0$ and $B_{ef} = W_{ef}$ otherwise. This matrix is often referred to as the Hashimoto matrix [16]. Recall, moreover, that $p_k(A) \in \mathbb{R}^{n \times n}$ is the matrix counting all NBT walks of length k (from i to j in its (i, j) element). Now we can observe that all the proofs above hold for B as well, modulo substituting walks with nonbacktracking walks. Hence, the projection relation still holds.

343 THEOREM 4.5. For all
$$k \in \mathbb{N}$$
, we have $L^T \sqrt{Z} (B^{\circ 1/2})^k \sqrt{Z} R = p_{k+1}(A)$.

Proof. We have $p_1(A) = A = L^T Z R$, and when k > 0 the result follows from a minor modification of the arguments used to prove Corollary 4.4.

Suppose now that $(c_k)_k \subset [0,\infty)$ is a sequence and t is such that

$$\kappa(t,A) = \sum_{k=0}^{\infty} c_k t^k p_k(A)$$

346 as in (2.2) converges; we are interested in the centrality measure

347 (4.1)
$$\boldsymbol{v}(t,A) = \kappa(t,A)\mathbf{1}.$$

We now derive formulae for $\kappa(t, A)$ and $\boldsymbol{v}(t, A)$. To this end, we introduce the following notation. Given a real-analytic scalar function

$$f(x) = \sum_{k=0}^{\infty} c_k x^k$$

consider the operator

$$\partial f(x) = \sum_{k=0}^{\infty} c_{k+1} x^k = \frac{f(x) - c_0}{x}$$

348 We then have the following.

349 THEOREM 4.6. It holds that

350
$$\sum_{k=0}^{\infty} c_k t^k p_k(A) = c_0 I + t L^T \sqrt{Z} \partial f(tV) \sqrt{Z} R,$$

for $V = B^{\circ 1/2}$ and $|t| < r/\rho(V)$, where $\rho(V)$ is the spectral radius of V and r is the radius of convergence of the scalar function $f(x) = \sum_{k=0}^{\infty} c_k t^k$.

Hence, for the centrality associated with f(x) and t small enough to give convergence in the matrix power series, in (4.1) we have

$$\boldsymbol{v}(t,A) = c_0 \mathbf{1} + t L^T \sqrt{Z} \partial f(tV) \sqrt{Z} \mathbf{1}.$$
10

Proof. By Theorem 4.5 we easily see that

$$\kappa(t,A) = c_0 I + t L^T \sqrt{Z} \left(\sum_{k=0}^{\infty} c_{k+1} t^k (B^{\circ 1/2})^k \right) \sqrt{Z} R$$

As a consequence,

$$\boldsymbol{v}(t,A) = c_0 \mathbf{1} + t L^T \sqrt{Z} \left(\sum_{k=0}^{\infty} c_{k+1} t^k (B^{\circ 1/2})^k \right) \sqrt{Z} \mathbf{1}$$

Observing that the resolvent is an eigenfunction (with eigenvalue 1) of ∂ , we note in particular that for Katz centrality, i.e., $c_k = 1$ for all k, $\partial f(x) = f(x) = (1-x)^{-1}$. Hence, we have the following special case.

COROLLARY 4.7. In the notation of Theorem 4.6, we have that the generating function $\Phi(t)$ defined in (2.1) can be expressed as

358 (4.2)
$$\Phi(t) = I + tL^T \sqrt{Z} (I - tV)^{-1} \sqrt{Z} R.$$

This analysis in particular yields a lower bound for the radius of convergence for (2.1).

361 COROLLARY 4.8. If $|t| < \rho(V)^{-1}$, where $V = B^{\circ 1/2}$, then the sequence $\Phi(t) = \sum_{k=0}^{\infty} p_k(A) t^k$ converges.

363 REMARK 4.9. Letting r denote the radius of convergence of (2.1), Corollary 4.8 364 shows that $r \ge \rho(V)^{-1}$. It is possible to strengthen this result and prove that r =365 $\rho(V)^{-1}$. A proof of this fact, which is beyond the scope of the present article, appears 366 in [25, Theorem 5.2].

5. Nonbacktracking centralities for evolving weighted graphs. In Sec-367 tions 3 and 4, we obtained formulae for the generating function $\Phi(t)$ in (2.1) by 368 working, respectively, at node and edge level. For a static network, i.e., one which 369 does not evolve in time, working at the node level is clearly preferable as, for large n, 370 we may have that $n \ll m$. However, a significant advantage of the latter, edge-level, 371 372 formula is that it easily extends to the case of temporal networks in all backtracking regimes, whereas a direct node-level formula which forbids backtracking in time is 373 generally unavailable [3]. Let us first generalize the definition of graph, walk, and 374 NBT walk to the dynamic case. 375

376 DEFINITION 5.1. A finite time-evolving graph \mathcal{G} is a finite collection of graphs 377 $(G^{[1]}, \ldots, G^{[N]})$, associated with the non-decreasing time stamps $(t_1, \ldots, t_N) \in \mathbb{R}^N$, 378 such that the set of nodes of $G^{[i]}$ does not depend on i and when observed at time t_i 379 the structure of \mathcal{G} is identical to that of $G^{[i]}$.

We remark that the concept of a graph can be extended to the dynamic setting in a number of ways [17]. The discrete-time framework of Definition 5.1 covers a range of realistic scenarios where interactions take place, or are recorded, at specific points in time. For example, in an on-line social media platform, an edge may represent a form of communication between users, and $G^{[i]}$ may count the number of interactions between each pair of individuals over time $(t_{i-1}, t_i]$.

The definition of walk across a network can be extended to the setting of temporal graphs as follows. BEFINITION 5.2. A walk of length ℓ across a temporal network is defined as an ordered sequence of ℓ edges $e_1e_2 \dots e_\ell$ such that for all $k = 1, \dots, \ell - 1$ the end node of e_k coincides with the start node of e_{k+1} and, moreover, that $e_k \in E^{[\tau_1]}, e_{k+1} \in E^{[\tau_2]}$ for some $1 \leq \tau_1 \leq \tau_2 \leq N$, where $E^{[\tau_i]}$ denotes the set of edges of the graph $G^{[\tau_i]}$.

392 It is useful to make an equivalent definition.

BEFINITION 5.3. A walk of length ℓ across a temporal network is defined as an ordered sequence of $\ell + 1$ nodes $i_1 i_2 \dots i_{\ell+1}$ such that for all $k = 2, \dots, \ell$ it holds that $i_{k-1} \to i_k \in E^{[\tau_1]}$ and $i_k \to i_{k+1} \in E^{[\tau_2]}$ for some $1 \le \tau_1 \le \tau_2 \le N$.

We want to stress that multiple edges can be crossed at one given time stamp and, moreover, that a walk is allowed to remain inactive for some of the time stamps. We also recall here that there is not just one definition of backtracking for temporal networks; indeed, three arise naturally [3]:

- backtracking happens within a certain time-stamp; we will refer to this as
 backtracking in space,
- backtracking happens across time-stamps; we will refer to this as *backtracking in time*,
- backtracking happens both within a time-stamp and across time-stamps (not necessarily in this order); we will refer to this as *backtracking in time and space*.

Given any finite time-evolving graph \mathcal{G} , we can associate with it a matrix M called the global temporal transition matrix which was defined in [3] for unweighted graphs. Definition 5.4 below generalizes the definition of the global temporal transition matrix to the weighted case.

411 DEFINITION 5.4. Let $\mathcal{G} = (G^{[1]}, G^{[2]}, \dots, G^{[N]})$ be a time-evolving graph with N 412 time stamps. The weighted global temporal transition matrix associated with \mathcal{G} is the 413 $m \times m$ block matrix

414 (5.1)
$$M = M^{[1,\dots,N]} = \begin{bmatrix} C^{[1]} & C^{[1,2]} & C^{[1,3]} & \dots & C^{[1,N]} \\ 0 & C^{[2]} & C^{[2,3]} & \dots & C^{[2,N]} \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & & \vdots \\ 0 & \dots & \dots & 0 & C^{[N]} \end{bmatrix}^{\circ 1/2}$$

⁴¹⁵ where the definition of the blocks depends on the chosen backtracking regime in the ⁴¹⁶ following way:

417 (i) $C^{[\tau_1]} = W^{[\tau_1]}$ and $C^{[\tau_1,\tau_2]} = W^{[\tau_1,\tau_2]} := S^{[\tau_1]}R^{[\tau_1]}(L^{[\tau_2]})^T S^{[\tau_2]}$ for all $\tau_1, \tau_2 = 1, 2, \dots, N$ ($\tau_1 < \tau_2$) if backtracking in both space and time is permitted;

- 419 (ii) $C^{[\tau_1]} = B^{[\tau_1]}$ and $C^{[\tau_1,\tau_2]} = W^{[\tau_1,\tau_2]}$ for all $\tau_1, \tau_2 = 1, 2, ..., N$ ($\tau_1 < \tau_2$) if 420 backtracking in space is forbidden but backtracking in time is permitted;
- $\begin{array}{ll} 421 \\ 421 \\ 422 \\ 422 \\ 423 \end{array} \begin{array}{l} (iii) \ C^{[\tau_1]} = W^{[\tau_1]} \ and \ C^{[\tau_1,\tau_2]} = B^{[\tau_1,\tau_2]} := W^{[\tau_1,\tau_2]} (W^{[\tau_1,\tau_2]} \circ W^{[\tau_2,\tau_1]}{}^T)^{\circ 1/2} \\ for \ all \ \tau_1,\tau_2 = 1,2,\ldots,N \ (\tau_1 < \tau_2) \ if \ backtracking \ in \ time \ is \ forbidden \ but \\ backtracking \ in \ space \ is \ permitted; \ and \end{array}$
- 424 (iv) $C^{[\tau_1]} = B^{[\tau_1]}$ and $C^{[\tau_1,\tau_2]} = B^{[\tau_1,\tau_2]}$ for all $\tau_1, \tau_2 = 1, 2, ..., N$ ($\tau_1 < \tau_2$) if 425 backtracking in both time and space is forbidden.

It was further shown in [3] that the global temporal transition matrix provides an accurate way of counting walks in all backtracking regimes across a finite unweighted time-evolving graph and thereby allows for the computation of the (nonbacktracking) 429 Katz centrality \boldsymbol{v} via the formula:

430 (5.2)
$$\boldsymbol{v}(t) = (I + t\mathcal{L}^T (I - tM)^{-1} \mathcal{R}) \mathbf{1},$$

431 where \mathcal{L}, \mathcal{R} are the global source and target matrices respectively as defined in [3, 432 Definition 4.4].

To handle the weighted case, we may extend Theorem 4.5 naturally to the global temporal transition matrix M in the following way.

435 THEOREM 5.5. For a finite time-evolving graph with N-many time frames, let the 436 global weight matrix Z be defined block-wise as

$$Z := Z^{[1,2,\ldots,N]} = \operatorname{diag}(Z^{[1]}, Z^{[2]}, \ldots, Z^{[N]}),$$

438 where $Z^{[\tau_i]}$ is the diagonal matrix associated with time stamp $1 \leq \tau_i \leq N$. For each of 439 these matrices, their diagonal entries are given by $Z_{ee}^{[\tau_i]} = w_e^{[\tau_i]}$, with $w_e^{[\tau_i]}$ being the 440 weight of edge e at time stamp τ_i . Further let the backtracking regime be fixed such 441 that the weighted global temporal transition matrix M is fixed. Then, for $0 < k \in \mathbb{N}$, 442 the (e, f)-th entry of $\sqrt{Z}M^k\sqrt{Z}$ counts, with weights, all permitted walks of length 443 k + 1 from edge e to edge f across the time evolving graph given the backtracking 444 regime.

445 Proof. Suppose the backtracking regime is given such that the structure of M is 446 fixed as specified in Definition 5.4. We prove the theorem by induction on the length 447 of permitted walks $k \in \mathbb{N}$. Consider the basis case k = 1:

$$\sqrt{Z}M\sqrt{Z} = \sqrt{Z} \begin{bmatrix} C^{[1]} & C^{[1,2]} & C^{[1,3]} & \dots & C^{[1,N]} \\ 0 & C^{[2]} & C^{[2,3]} & \dots & C^{[2,N]} \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \dots & \dots & 0 & C^{[N]} \end{bmatrix}^{\circ 1/2} \sqrt{Z}.$$

The (e, f)-th element of this matrix correctly counts the unique walk of length two with weights from edge e to edge f. In the following we will omit the temporal superscript, since the indices e and f also uniquely determine the time frame. With this convention:

453
$$\left(\sqrt{Z}M\sqrt{Z}\right)_{ef} = \sum_{r,s} \sqrt{Z}_{er}M_{rs}\sqrt{Z}_{sf}$$

454

448

437

$$= (\sqrt{Z})_{ee} (\sqrt{Z})_{ff} M_{ef}$$

455 456

 $= \begin{cases} \sqrt{w_e}\sqrt{w_f}\sqrt{w_ew_f} = w_ew_f & ef \text{ is a permitted walk of length two} \\ 0 & \text{otherwise.} \end{cases}$

457 where we have used the fact that, if ef is an admissible walk of length two, then 458 $(M)_{ef} = \sqrt{w_e w_f}$.

Suppose now that the result holds for k-1 and for brevity denote by P the matrix $\sqrt{Z}M^{k-1}\sqrt{Z}$, which, by the inductive assumption, correctly counts in its entries the number of weighted temporal walks of length k. Then, using the fact that Z is

diagonal, 462

$$= \sum_{r} P_{er} (Z^{-1/2})_{rr} M_{rf} (\sqrt{Z})_{ff}$$

465
466
$$= \begin{cases} w_f \sum_r P_{er} & e \dots rf \text{ is a permitted walk of length } k+1\\ 0 & \text{otherwise.} \end{cases}$$

 $(\sqrt{Z}M^k\sqrt{Z})_{ef} = \sum_{r.s.t} \left(\sqrt{Z}M^{k-1}\sqrt{Z}\right)_{er} (Z^{-1/2})_{rs} M_{st}(\sqrt{Z})_{tf}$

By the inductive assumption P_{er} counts the permitted weighted walks of length 467 k from edge e to edge r. Therefore the above formula does indeed count the weighted 468 permitted walks beginning with edge e and ending on edge f with length k + 1469П correctly. 470

THEOREM 5.6. Given global source, target and weight matrices, \mathcal{L} , \mathcal{R} and Z re-471 spectively, we can compute M when backtracking is entirely forbidden in two steps: 4721. $\widehat{M} = \left(\sqrt{Z}(\mathcal{R}\mathcal{L}^T - \mathcal{R}\mathcal{L}^T \circ \mathcal{L}\mathcal{R}^T)\sqrt{Z}\right);$ 473

2. Obtain M from \widehat{M} by setting all entries below the block diagonal to 0. 474

Proof. The above theorem is easy to prove by observing that the (i, j)-th block of 475the matrix \mathcal{RL}^T is equal to $R^{[i]}L^{[j]T}$, whereas the (i, j)-th block of the matrix \mathcal{LR}^T 476 is equal to $L^{[i]}R^{[j]T} = (R^{[j]}L^{[i]T})^T$; whereupon the (i, j)-th block of the matrix \widehat{M} 477 becomes 478

479
480
$$\widehat{M}_{ij} = \sqrt{Z^{[i]}} \left(R^{[i]} L^{[j]T} - R^{[i]} L^{[j]T} \circ (R^{[j]} L^{[i]T})^T \right) \sqrt{Z^{[j]}}.$$

The central term here in brackets can be seen as the binarized $B^{[i,j]}$, i.e., $B^{[i,j]}$ where 481 all non-zero weights are uniformly equal to 1, thus the presence of a non-zero entry 482 $(B^{[i,j]})_{ef}$ simply reflects whether or not the concatenation of edges e and f forms a 483 non-backtracking walk of length two. Matrix multiplication from the left by $\sqrt{Z^{[i]}}$ 484and on the right by $\sqrt{Z^{[j]}}$ then provides the appropriate weighting for the (e, f)-th 485 entry, namely $\sqrt{w_e}\sqrt{w_f}$, as required. Finally, the second step of setting all blocks 486 below the block diagonal, i.e., \widehat{M}_{ij} with i > j, to zero reflects the requirement that 487 walks may not move back in time. 488 Π

We can also compute the *f*-total communicability of the time-evolving graph with 489weights by using the global temporal transition matrix M. 490

THEOREM 5.7. Given a function f with series expansion $f(t) = \sum_{k=0}^{\infty} c_k t^k$ having 491 radius of convergence r, and some fixed backtracking regime, the f-total communica-bility $\boldsymbol{v}_f(t)$ of the time-evolving graph $\mathcal{G} = (G^{[1]}, \ldots, G^{[N]})$ with N time stamps is 492 493given by the formula: 494

495 (5.3)
$$\boldsymbol{v}_f(t) = (c_0 I + t \partial \mathcal{L}^T \sqrt{Z} f(tM) \sqrt{Z} \mathcal{R}) \mathbf{1}$$

for $0 < |t| < r / \max_{i=1,\dots,N} \{ \rho(C^{[\tau_i]}) \}.$ 496

Proof. By Proposition 5.5, we have that $\sqrt{Z}M^k\sqrt{Z}$ counts with weights all walks 497 of length k + 1, thus 498

499
$$\boldsymbol{v}_f(t) = (c_0 I + t\partial \mathcal{L}^T \sqrt{Z} f(tM) \sqrt{Z} \mathcal{R}) \mathbf{1} = c_0 I + t \sum_{k=0}^{\infty} c_{k+1} t^k \mathcal{L}^T \sqrt{Z} M^k \sqrt{Z} \mathcal{R} \mathbf{1}.$$

_

Non-binarized graph $\rho(B^{\circ 1/2})$	926.9
Binarized graph $\rho(B)$	48.61
Non-binarized nonbacktracking permitted range of t	$t \in [0, 1.079 \cdot 10^{-3})$
Binarized nonbacktracking permitted range of \boldsymbol{t}	$t \in [0, 2.057 \cdot 10^{-2}]$
Non-binarized $\rho(A)$	1038
Binarized $\rho(A)$	51.26
Non-binarized backtracking permitted range of t	$t \in [0, 9.635 \cdot 10^{-4})$
Binarized backtracking permitted range of t	$t \in [0, 1.951 \cdot 10^{-2}]$

Table 6.1: Static network convergence information.

In the above formula we see the number of walks of length k + 1 correctly counted with weights that are further weighted by the coefficient $c_{k+1}t^{k+1}$, which is provided by the series expansion of f(x).

6. Numerical Experiments. In this section we show how the formulae for 503 504nonbacktracking Katz centrality from sections 3, 4 and 5 may produce significantly different node-rankings for real-world social networks when compared with Katz cen-505trality which permits backtracking walks. We further examine the effect of weighting 506edges on the rankings produced by both centrality measures. To this end, we consider 507 the Katz centrality formula (5.2) as applied to one static network and one temporal 508network, both derived from the same data set (Fauci's email release [6])². The origi-509nal dataset is a collection of over 3000 pages of emails involving Anthony Fauci and his 510staff during the COVID-19 pandemic. Data includes sender and receivers (including 511CC'd) of emails, as well as time stamps of when the emails were sent. Both networks used in the following were presented in [6]. 513

6.1. Analysis on Static Networks. In this section, we analyze a static network produced by [6] which is both undirected and weighted. We have an edge (i, j) if there exists an email which involves both nodes i and j as any combination of sender and recipient (including CC'd recipients). The weight assigned to such an edge, $\Omega((i, j))$, is a positive integer equal to the number of such emails that were sent.

In our analysis, we apply Corollary 3.4 to obtain the NBT Katz centrality vector 519 for our network, which is then contrasted with the classical Katz centrality vector 520for attenuation factor values $t = 0.5/\rho$ and $t = 0.95/\rho$, where $1/\rho$ is the radius of 521convergence for the respective centrality measure. In particular $1/\rho$ is equal to $1/\rho(A)$, 522 where A is the adjacency matrix of the graph in the case of classical Katz centrality; 523 whereas $1/\rho = 1/\rho(B^{\circ 1/2})$ in the case of weighted nonbacktracking Katz centrality [25, 524Theorem 5.2], where B is the Hashimoto matrix associated to the graph. These values 526 are given in Table 6.1. We also analyze the binarized graph which is produced from the static graph by setting all edge weights to 1. In the context of the binarized 527 528 network $1/\rho$ equals $1/\rho(A)$ in the case of classical Katz centrality, and $1/\rho(B)$ for nonbacktracking Katz centrality, where A and B are the adjacency and Hashimoto 529matrices associated with the binarized network, respectively. 530

531 The results are visualised in Figures 6.1, 6.2 and 6.3. Figure 6.1 shows that 532 NBT Katz centrality emphasizes a clique not containing the node corresponding to 533 Antony Fauci, and that for large values of the attenuation factor this clique begins to

²The code used in the following analysis can be found at https://github.com/rwood12347/ Weighted-enumeration-of-nonbacktracking-walks-on-weighted-graphs



NBT Katz centrality $t = 0.5/\rho(B^{\circ 1/2})$

NBT Katz centrality $t = 0.95/\rho(B^{\circ 1/2})$

Fig. 6.1: Visualizations of classical (top/red) and NBT Katz (bottom/blue) across the static email network with large node size and dark colour indicating large centrality values; darker edges indicate a larger weight.



Fig. 6.2: Classical and nonbacktracking Katz centrality vector values for backtracking fully forbidden with attenuation factor $t = 0.5/\rho$ and $t = 0.95/\rho$, respectively. In each plot we display the union of the 10 most central nodes according to each centrality measure.

dominate the ranking to such an extent that the node corresponding to Anthony Fauci, 534which occupies the central position in the network visualisation, is no longer counted among the 10 most central nodes. This can be seen in Figure 6.2 which depicts the 536 537 nonbacktracking and classical Katz normalized centrality values for the union of the 10 most central nodes in the static network. The left bar chart in Figure 6.2 indicates 538 that both classical and nonbacktracking Katz agree on the 10 most central nodes of 539 which 'Anthony Fauci' is most central when $t = 0.5/\rho$. However the rightmost figure 540depicts a complete divergence in the ten most highly-ranked nodes produced by classic 541and nonbacktracking Katz centralities respectively. In particular we see that while 542the 'Anthony Fauci' node remains fairly central according to both measures, nodes 543 belonging to the clique shown in Figure 6.1 have overtaken it in the ranking induced by 544nonbacktracking Katz centrality. The clique identified in this case consists exclusively 545of participants (i.e., either directly sent or received an email within the thread, or were 546 547 CC'd in an email within the thread) in the so-called 'Red Dawn' email thread that was used throughout the pandemic "to provide thoughts, concerns, raise issues, share 548 information across various colleagues responding to Covid-19" [8]. 549

The effect of weighted edges on the rankings produced by nonbacktracking and classical Katz centralities for the static network is demonstrated in Figure 6.3. The figure contains two scatter graphs of the normalized nonbacktracking Katz centrality vector ($t = 0.95/\rho(B^{\circ 1/2})$) plotted against the Katz centrality vector ($t = 0.95/\rho(A)$) for both the original network (right) and a binarized modified network (left), which is formed from the original network by setting all edge weights to 1.

In particular we see that the presence of non-uniformly weighted edges in the network produces greater variation in the nonbacktracking and classical Katz centrality vectors.



Fig. 6.3: Scatter plots of normalized NBT Katz centrality against normalized classical Katz centrality corresponding to binarized and non-binarized static networks with attenuation factor $t = 0.95/\rho$.

6.2. Analysis on Temporal Networks. We now move on to the case of a time-dependent network, and we note that the special case of an unweighted network with backtracking permitted corresponds to the work in [15] wherein the *dynamic communicability matrix* Q(t) associated to such a network is defined as the product of the successive resolvents

564 (6.1)
$$Q(t) = (I - tA^{[1]})^{-1} (I - tA^{[2]})^{-1} \cdots (I - tA^{[N]})^{-1}$$

Here $A^{[i]}$ is the adjacency matrix associated to the *i*-th time-stamp of the temporal network \mathcal{G} . Katz centrality can then be computed via the formula

567 (6.2)
$$\boldsymbol{x}(t) = \boldsymbol{\mathcal{Q}}(t)\mathbf{1}$$

This formula accounts for all walks across the temporal network \mathcal{G} including those that backtrack in space and between time-stamps.

The temporal network \mathcal{G} analyzed in this section is the largest temporal strong component [9] of the provided email data, i.e., the largest component that is connected in the sense that there exists a time-respecting path between any two nodes contained within. This network consists of a collection of 100 directed networks associated with the date 2018-09-04 and the 99 consecutive days between 2020-01-26 and 2020-05-05. In this network we have a directed weighted edge $(i, j) \in E(G^{[\tau_t]})$, if node j is a recipient of, or is CC'd in, an email sent by node i. The weight of such an edge is equal to the number of such emails sent during the t-th timestamp.

We reiterate here that when treating temporal networks there is a range of possible nonbacktracking regimes, as outlined in Definition 5.4. The choice of appropriate backtracking regime is highly context-dependent. For the data set analyzed here, it is reasonable to forbid backtracking entirely, since the time-stamps associated with the temporal network have an almost uniform spacing of one day, and the time taken to reply to an email is on a similar scale to the spacing between time-stamps. It is



Table 6.2: Temporal network convergence information.



Fig. 6.4: The time-evolving network centrality vector values for both NBT and classical Katz with attenuation factor $t = 0.5/\rho$ and $t = 0.95/\rho$ respectively. In each plot we display the union of the ten most central nodes according to each centrality measure.

worth mentioning that this choice to fully forbid backtracking is subjective and other regimes may also be reasonable.

Our analysis of the spectrum of the global temporal transition matrix M associated to the graph \mathcal{G} with backtracking fully-forbidden yields the permitted ranges of attenuation factor t shown in Table 6.2. We contrast this with the permitted range of t in the case of classical Katz centrality via the dynamic communicability matrix \mathcal{Q} as defined in (6.1).

Figure 6.4 depicts two bar charts which display the normalized centrality values for both classical and nonbacktracking Katz centralities for $t = 0.5/\rho$ and $t = 0.95/\rho$ 592respectively, where $1/\rho$ is the upper-limit of the respective regime as given in Table 6.2. 593In particular $1/\rho$ is equal to $1/\rho(M)$ (see the proof of [25, Theorem 5.2]) in the case 594of nonbacktracking Katz centrality, where M is the matrix described in Definition 5.4 (iv) that is, the form of M in which all forms of backtracking are forbidden. In the 596 case of classical Katz centrality $1/\rho$ is given by $1/\max_i(\rho(A^{[i]}))$, the reciprocal of the 597largest principal eigenvalue of the adjacency matrices. In Figure 6.4 we report results 598for 12 nodes, which are selected by taking the union of the 10 most highly ranked 599nodes for classical Katz and the 10 most highly ranked nodes for NBT Katz, when 600 $t = 0.95/\rho$. 601

In Figure 6.5 we plot for the weighted temporal network both the classical and nonbacktracking Katz centrality values of 10 selected nodes against the attenuation factor t which ranges from 0% to 99% of its permitted range (as given in Table 6.2). The 10 nodes were selected such that they are the most central for large values of t.

Figure 6.6 presents results for the same experiment, this time carried out with the binarized version of the temporal network, i.e., the temporal network with all non-zero weights set to 1. It is interesting to note that nonbacktracking Katz identifies a node distinct from "Anthony Fauci" as the most central node for large values of t, favouring instead the node "Jeremy Farrar" which is considerably lower ranked in the static networks produced from the same data set. Furthermore by comparing Figures 6.5 and 6.6, we observe the large effect that weighting has on the two centrality measures.



Fig. 6.5: Plots of the normalized Katz (upper) and nonbacktracking Katz (lower) centralities vector values for 10 most prominent nodes (i.e., those with the largest centrality value as of the upper limit of the attenuation factor t) within the weighted temporal network

614 **7. Discussion.** Our aim in this work was to develop a useful theory for the 615 enumeration of nonbacktracking walks as well as for associated centrality measures, 616 in the case of edge weights that are combined multiplicatively. We showed in The-617 orem 3.1 that in contrast to the unweighted case where a four-term recurrence is 618 sufficient to count nonbacktracking walks of different lengths, the weighted case gives 619 rise to a recurrence where the walk count at length k depends on walk counts for all



Fig. 6.6: Plots of the normalized Katz (upper) and nonbacktracking Katz (lower) centralities vector values for 10 most prominent nodes (i.e., those with the largest centrality value as of the upper limit of the attenuation factor t) within the binarized temporal network.

shorter lengths. Despite this added complexity, the resulting formulas for the standard generating function in Theorem 3.3 and corresponding node centrality measure

622 in Corollary 3.4 are straightforward to evaluate.

We also showed in Theorem 4.5 that when working at the line graph level, the introduction of appropriate componentwise square roots allows us to develop a theory that extends to the unweighted case, with Theorem 4.6 summarizing the results, and Theorem 5.7 dealing with more general time-evolving graph sequences.

A practical take-home message is that a theory of nonbacktracking walk counts for static or dynamic weighted graphs is available, with corresponding computational algorithms that have the same complexity as in the unweighted case. Acknowledgements. We thank the Editor and the Referees for their usefulcomments.

632 **References.**

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