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Non-backtracking PageRank: From the classic model to hashimoto matrices

David Aleja[a,c], Regino Criado[a,b,c], Alejandro J. García del Amo[a,b,c,*], Ángel Pérez[a], Miguel Romance[a,b,c]

[a] Departamento de Matemática Aplicada, Ciencia e Ingeniería de los Materiales y Tecnología Electrónica, ESCET Universidad Rey Juan Carlos, C/Tulipán s/n, Móstoles Madrid 28933, Spain
[b] Center for Computational Simulation, Universidad Politécnica de Madrid, Pozuelo de Alarcón Madrid 28223, Spain
[c] Data, Complex Networks and Cybersecurity Research Institute, University Rey Juan Carlos, Madrid 28028, Spain

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ABSTRACT

Non-backtracking centrality was introduced as a way to correct what may be understood as a deficiency in the eigenvector centrality, since the eigenvector centrality in a network can be artificially increased in high-degree nodes (hubs) because a hub is central because its neighbors are central, but these, in turn, are central just because they are hub neighbors. We define the non-backtracking PageRank as a new measure modifying the well-known classic PageRank in order to avoid the possibility of the random walker returning to the node immediately visited (non-backtracking walk). But, as we show, this measure presents a gap and a remarkable difference between the limit of "no penalty for return trips" and the direct calculation of the non-backtracking PageRank. Also, as it is shown in the applications presented, in certain cases this new measure produces notable variations with respect to the classifications obtained by the classic PageRank.

1. Introduction

A fundamental problem facing the so-called Science of Complexity is to determine which are the most relevant elements of a complex system [3,5,12,20–22,39,54]. This problem is directly related to understanding the relevance of each element within the structure of a system, which is a first step to understand its behavior. Analyzing and determining the relevance of the elements of a network or system is a problem that arises in multiple social, technological and biological contexts [2,6,11,20,24,29,54]. A way to determine the relevance of the elements of a network or a system consists in associating a numerical value to each one of these elements. Centrality measures can be very different in nature but they allow us to sort the nodes according to a ranking of relevance within the network. Among them, PageRank centrality [41] is a culminating point since it is the basic ingredient in web information in general and in Google's web search engine in particular. Since its appearance in 1998 to classify web pages to the present day, a large number new applications and refinements of PageRank algorithm have emerged in the scientific literature [1,8,15,19,20,23,27,43,44,52,53,56,59]. These refinements are very varied in nature, and new methodologies and tools are being developed in the literature to detect both the most relevant nodes and the competing nodes [15,23,44,52,53,56,59]. The use of a personalization vector to modify the ranking obtained (personalized PageRank) [15,43,45] and a new vision of this algorithm that allows to extend PageRank to multiplex networks [20,27,40,45,48,57] are other advances that have appeared in recent years. On the other hand, it is known that the centrality of the eigenvector [9] takes into account the importance of the neighbors of a node, in the sense that a node is more important (or influential) if the nodes with which it is connected are, in turn, important or influential nodes. However, although this measure of centrality has been analyzed in different applications and contexts [5,14,36–38,42,46,54] and leads to several extensions in different environments, it is known to be artificially high for high-grade nodes (hubs) as evidenced in [36]. This is because a hub transmits part of its high centrality to its neighbors, who in turn increase its centrality and artificially inflate the hub's centrality. Therefore, if we can avoid these "round-trip centrality assignments", centrality will

* Corresponding author at: Center for Computational Simulation, Universidad Politécnica de Madrid, Pozuelo de Alarcón Madrid 28223, Spain.

E-mail addresses: david.aleja@urjc.es (D. Aleja), regino.criado@urjc.es (R. Criado), alejandro.garciadelamo@urjc.es (A.J. García del Amo), angel.perez@urjc.es (Á. Pérez), miguel.romance@urjc.es (M. Romance).

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behave much more realistically. Thus, in [36] an attempt is proposed to correct this weakness by using the so-called non-backtracking centrality. The idea is to calculate the eigenvector centrality as usual but with an important change: to calculate the eigenvector centrality of a particular node, one considers the centrality of its neighbors but in this case calculated in the absence of that particular node. But this measure of centrality, non-backtracking centrality, as shown in [16], has a built-in problem because in certain contexts, by eliminating round trips, the adjacency matrix on which calculations have to be made may be not irreducible, so the Perron–Frobenius theorem cannot be used [37], compromising the existence and uniqueness of the centrality vector that collects the centralities of the network nodes.

However, in [16] a new centrality measure is defined, the α-non-backtracking centrality, that makes possible to solve the problems related to the uniqueness of non-backtracking principal eigenvector and, by the way, directly calculate the centrality of edges. The idea consists in not eliminating completely the round trips, but to associate to these round trips a weight α, diminishing its contribution making tend this parameter to zero. The convergence of the α-non-backtracking centrality is proved in [16] when $\alpha \to 0^+$ and the techniques used makes it possible to demonstrate the convergence of the α-centrality principal eigenvector when $\alpha \to 0^+$ and also the convergence of PageRank vectors when the damping factor $q \to 1^-$. As it is pointed out in [16], to calculate the α-non-backtracking centrality it is needed to use the Hashimoto or non-backtracking matrix [28,33]. This matrix is closely related to the adjacency matrix of the line graph corresponding to the network under consideration which is extremely useful because, in some cases (v.g., cybersecurity, intentional cyber-risk, urban traffic networks [10,17,18]) it is much more useful for us to calculate the centrality of the edges than that of the nodes and, in any case, to be able to recover the centrality of the edges from the centrality of the nodes and reciprocally [15]. The main goal of this work is defining and analyzing a new centrality measure, the non-backtracking PageRank, that incorporates the ideas related to the non-backtracking centrality introduced in [36] and analyzed and developed in [16].

The structure of the paper is as follows. After this introduction, Section 2 is devoted to recall some preliminary results and definitions. In Section 3 a non-backtracking version of PageRank for the nodes of weighted and directed network is introduced and some interesting results related to this new centrality measure are obtained. Finally, in Section 4 we present some numerical experiments on some real-world problems in order to illustrate the results of the previous sections.

2. Notation and related concepts

In the sequel, for a vector $v \in \mathbb{R}^n$, we will denote by v^T its transpose vector and its 1-norm is defined as $||v||_1 = \sum_{i=1}^{n} |v_i|$. The vector v is said to be *positive* if $v_i > 0$ for every i and this fact is denoted with $v > 0$. Let $\mathbf{1} \in \mathbb{R}^n$ denote the vector $(1, 1, \dots, 1)^T$.

Throughout this paper we consider a *weighted directed network* $G = (X, E, w)$, where $X = \{1, \dots, n\}$ is the set of *vertices* or *nodes*, $E \subseteq X \times X$ is the set of *edges* and w is a function $w : E \longrightarrow [0, +\infty)$ such that for each edge $(i, j) \in E$, the coefficient $w(i, j)$ is called *weight* of (i, j). We will also use the notation $i \to j$ for an edge (i, j) when convenient. If we have a directed network $G = (X, E)$ and this network does not have an associated weight-function, then we will say that G is a *unweighted* network. We will consider networks without loops, that is, for every $i \in X$ we have that $(i, i) \notin E$, and also without multiple edges.

Given a directed and weighted network $G = (X, E, w)$, the *(weighted) adjacency matrix* of G is the matrix $A(G) = A = (a_{ij}) \in M_{n\times n}$ given by

$$a_{ij} = \begin{cases} w(i, j), & \text{if there exists an edge } (i, j) \in E, \\ 0, & \text{otherwise.} \end{cases} \quad (2.1)$$

If $G = (X, E)$ is a unweighted directed graph, its *adjacency matrix* is the matrix $A(G) = A = (a_{ij}) \in M_{n\times n}$ given by

$$a_{ij} = \begin{cases} 1, & \text{if there exists an edge } (i, j) \in E, \\ 0, & \text{otherwise,} \end{cases} \quad (2.2)$$

i.e., we interpret each directed unweighted network as a directed weighted network, by considering, for each $(i, j) \in E$, $w(i, j) = 1$.

Finally, whenever we deal with a non-directed network (X', E'), we will transform it into a directed network in the standard way, that is, by constructing a directed network (X, E) with the same set of nodes $X = X'$ and two directed edges $i \to j$ and $j \to i$ in E for each non-directed edge $\{i, j\}$ in E'. A more detailed explanation about this notation for directed and non-directed networks (weighted or not) may be found in [5].

2.1. Non-backtracking centrality

Non-backtracking centrality was introduced in [36] as an attempt to correct some deficiencies of eigenvector centrality. The heuristics to remove the feedback produced by back and forth edges is revealed in the Hashimoto matrix ([28]) and goes as follows: the centrality of edge $k \to l$ is proportional to the sum of the centralities of all edges **incident** on $k \to l$ **except** edge $l \to k$. Here $i \to j$ is incident on $k \to l$ if $j = k$. Then, if (X, E) is a unweighted directed network, after fixing an order in E (for instance the lexicographic order), the Hashimoto matrix is defined as:

$$B(0)_{i\to j, k\to l} = \begin{cases} 1 & \text{if } j = k \text{ and } i \neq l, \\ 0 & \text{otherwise,} \end{cases}$$

that is,

$$B(0)_{i\to j, k\to l} = \delta_{jk}(1 - \delta_{il}),$$

where δ_{ij} is the Kronecker's delta, i.e.,

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Notice that the Hashimoto matrix is closely related to the adjacency matrix of $L(G)$ (see [16]), the line graph of G, defined as

$$(M_{L(G)})_{i\to j, k\to l} = \delta_{jk} = \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{otherwise,} \end{cases}$$

(here $i \to j$ is incident on $k \to l$ if $j = k$).

As an illustrative example, if $X = \{1, 2, 3\}$ and $E = \{(1, 2); (2, 3); (3, 1); (3, 2)\}$, we can get the adjacency matrix of $L(G)$ and the Hashimoto matrix $B(0)$ associated to G (note the relationship between both matrices):

$$B(0) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad M_{L(G)} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

The relation between $B(0)$, the adjacency matrix of $L(G)$ and their respective associated graphs is illustrated in Fig. 1.

At this point it is important to highlight the existence of strong relationships between the eigenvector centrality of a given graph G, the eigenvector centrality of its line graph $L(G)$ and the eigenvector centrality of the bipartite graph $B(G)$ associated to G, both in the case of G being an undirected network [12] and in the case of G being a directed network [13].

So, in this context, the non-backtracking centrality for edges is defined [36], when possible, as a function η: $E \to [0, 1]$ that satisfies:

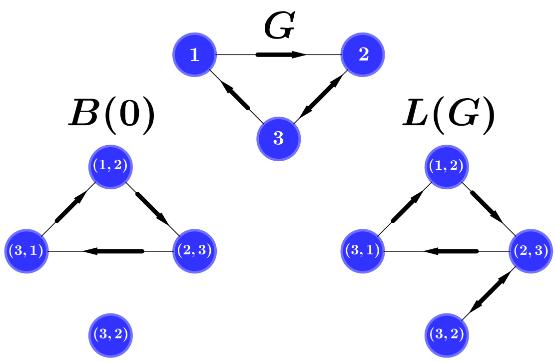

Fig. 1. An example of a directed graph G with 3 nodes to obtain $L(G)$ and the graph associated to the Hashimoto matrix $B(0)$.

- $\sum_{k\to l\in E} \eta(k\to l) = 1$ (normalization).
- $\eta(i\to j)$ is proportional to the sum of $\eta(k\to i)$ where $k=j$ is disregarded.

In terms of $B(0)$,

$$\eta(i\to j) \equiv \eta_{i\to j} = \frac{1}{\lambda}\sum_{k\to l\in E} B(0)_{k\to l, i\to j}\eta_{k\to l}.$$

Thus, if $\eta = (\eta_{i\to j})_{i\to j\in E}$, then $\lambda\eta^T = \eta^T B(0)$.

We remark that the non-backtracking centrality of each edge in E is ranked by means of the normalized non-negative eigenvector of $B(0)$.

So, at this point it is possible to define [36] the non-backtracking centrality of nodes as the sum of non-bactracking centralities of all edges incident on i, in other words, the sum of centralities of all edges $i\to k$. But, in order to avoid the irreducibility problem that results in lack of unicity for the non-backtracking eigenvector as it is shown in [16], it is possible to consider a parametrized centrality measure introduced in that work. This measure is called α-non-backtracking centrality in [16]. In the sequel, we choose to parametrize it by $\mu\in[0, 1]$ instead of α to avoid confusions with the damping factor of PageRank, which is also usually denoted by α. The measure is associated with a matrix which satisfies that, for $\mu=0$ we get the Hashimoto matrix $B(0)$, while for $\mu=1$ the matrix of $L(G)$ is recovered. In other words, the edge μ-non-backtracking centrality η_μ: $E\to[0, 1]$ is defined from the following edge adjacency matrix:

$$B(\mu)_{i\to j,k\to l} = \begin{cases} 1 & \text{if } j=k \text{ and } i\neq l,\\ \mu & \text{if } j=k \text{ and } i=l,\\ 0 & \text{if otherwise,}\end{cases}$$

that is,

$$B(\mu)_{i\to j,k\to l} = \delta_{jk}(1+(\mu-1)\delta_{il}),$$

and satisfies (see [16]):

- $\sum_{k\to l\in E} (\eta_\mu)_{k\to l} = 1$ (normalization),
- $(\eta_\mu)_{k\to l}$ is proportional to the sum of $(\eta_\mu)_{j\to k}$, where $j\to k$ is incident on $k\to l$ and the case $j=l$ is admissible although dampened by μ.

2.2. PageRank

Now, it is important to recall how PageRank works. One suggestive way to describe the idea behind PageRank is the following [8] (random walker hypothesis): If we move on the network in a *random* way, we will pass *more often* through the more *accessible* nodes. In order to mathematically model this idea, we must consider a specific type of Markov chains: *the random paths in a network*. Thus, PageRank may be defined formally as the stationary distribution of a stochastic process whose states are the nodes of the network. The associated matrix to PageRank is a stochastic matrix, bearing in mind that we can solve the problem of nodes with no outlinks (dangling nodes) by substituting every null row with a positive vector $y>0$ such that $||y||_1 = 1$. Thus, in contrast to what happens with non-backtracking centrality, we will not have the problem of existence and uniqueness of the eigenvector that will allow us to obtain the centrality of each edge and each node. So, if $G=(X, E)$ is a directed network with n nodes and adjacency matrix A, $q\in(0, 1)$ and $v=(v_1,\dots,v_n)\in\mathbb{R}^n$ is such that $v>0$ and $\|v\|_1 = 1$, then the *PageRank vector* of G with *damping factor* q and *personalization vector* v is the unique vector $PR(G, q, v) = PR\in\mathbb{R}^n$ such that

1. $PR\geq 0$ and $\|PR\|_1 = 1$.
2. PR is an eigenvector corresponding to the eigenvalue 1 of the matrix $\Psi=(\psi_{ij})$ given by

$$\psi_{ij} = q\,\theta_{ij} + (1-q)v_j, \quad \theta_{ij} = a_{ij}/\sum_k a_{ik}, \tag{2.3}$$

i.e., $PR\cdot\Psi = PR$.

Because of this, for each node $i\in X=\{1,\dots n\}$ the *PageRank* of the node i is the value $PR(G, q, v, i) = PR(i)$, the ith coordinate of the vector PR.

In the above definition, note that each coordinate $PR(i)$ of the PageRank vector is interpreted as the frequency with which a random walker passes through the i node as he moves randomly through the network, taking q (at each step) as the probability of following the network structure through the edges connected to the current node, and taking the distribution given by the v vector if he jumps unexpectedly to another node in the network.

2.3. Weighted line graph and edges' PageRank

In [15] the weighted line graph associated to a weighted network is defined in the following way: if $G=(X, E, w)$ is a directed and weighted network with adjacency matrix A, then the weighted line graph associated to G is defined as another weighted network $L(G) = (E, \tilde{E}, \tilde{w})$, where

$$\tilde{E} = \{(i\to j, j\to k);\ \ i\to j, j\to k\in E\} \tag{2.4}$$

and $\tilde{w}:\tilde{E}\longrightarrow[0, +\infty)$ whose expression is $\tilde{w}(i\to j, j\to k) = a_{ij}a_{jk}$.

The authors of [15] provide two different definitions for the PageRank of an edge of G. In the first definition, the PageRank of nodes of G is computed and then it is "propagated" to the edges, namely the PageRank $PR(i\to j)$ of edge $i\to j$ is defined as an appropriate fraction of $PR(i)$, where $PR(i)$ is the PageRank of node i. On the other hand, for the second definition, the PageRank of edge $i\to j$ is computed directly in the line graph $L(G)$ and denoted with $LPR(i\to j)$. Subsequently it is shown that, if $PR(i\to j)$ is computed by using a personalization vector v and $LPR(i\to j)$ is computed with respect to a personalization vector w chosen as an appropriate function of v, then both centrality measures for edges coincide (see [15] for details).

3. Non-backtracking PageRank

The aim of this section is to define a non-backtracking version of PageRank for the nodes of weighted and directed network $G=(X, E, w)$. In the spirit of [16], and in order to get a richer spectrum of centrality measures, we consider a family of PageRank vectors parametrized by $\mu\in[0, 1]$. The parameter μ can be interpreted as how much the importance of back and forth edges is mitigated when computing PageRank. For $\mu = 1$ the usual PageRank is recovered while the influence of these edges decreases as μ tends to zero. In addition we define another PageRank vector based on a Hashimoto like matrix. As an interesting fact, the latter does not always equal the one obtained when $\mu \to 0^+$. Therefore, we also study under which conditions both measures coincide.

Let $G = (X, E, w)$ be a weighted directed network with adjacency matrix A and $L(G) = (E, \tilde{E}, \tilde{w})$ its associated weighted line graph, both as defined in Section 2. Let $B \equiv B(1)$ be the adjacency matrix of $L(G)$ and recall that $b_{i\to j,k\to l} = a_{ij}a_{kl}$ if $j = k$ and equals 0 otherwise. In the sequel, we will always assume that G has no dangling nodes, which are defined as nodes with no outlinks (this corresponds to A having no null rows). It immediately follows that $L(G)$ neither has dangling nodes. Note that this is always the case when G is constructed from a non-directed network as explained in Section 2.

Now, we define a family of row stochastic matrices $\{C_\mu\}$ parametrized by $\mu \in (0, 1]$. The idea is taking as a starting point the adjacency matrix B of the line graph and, whenever both $i \to j,\ j \to i \in E$, multiply both corresponding coefficients $b_{i\to j,j\to i}$ and $b_{j\to i,i\to j}$ by μ. Subsequently, the resulting matrix is normalized by rows (this can be done as there are no null rows). More precisely, each coefficient of C_μ is defined as:

$$(c_\mu)_{i\to j,k\to l} = \begin{cases} 0 & \text{if } j \neq k, \\ \dfrac{b_{i\to j,k\to l}}{\sum\limits_{\beta\to\gamma} b_{i\to j,\beta\to\gamma}} & \text{if } j = k \text{ and } j \to i \notin E, \\ \dfrac{b_{i\to j,k\to l}}{\sum\limits_{(\beta\to\gamma)\neq(j\to i)} b_{i\to j,\beta\to\gamma} + \mu b_{i\to j,j\to i}} & \text{if } j = k,\ j \to i \in E \text{ and } l \neq i, \\ \dfrac{\mu b_{i\to j,j\to i}}{\sum\limits_{(\beta\to\gamma)\neq(j\to i)} b_{i\to j,\beta\to\gamma} + \mu b_{i\to j,j\to i}} & \text{if } j = k,\ j \to i \in E \text{ and } l = i. \end{cases}$$

For $\mu = 0$ we define the matrix C_0 as the limit, coefficient-wise, of C_μ when $\mu \to 0^+$, that is, $(c_0)_{i\to j,k\to l} = lim_{\mu\to 0^+}(c_\mu)_{i\to j,k\to l}$.

Finally we define from B a matrix C in the spirit of the Hashimoto matrix (taking into account that B is a weighted matrix). Essentially we repeat previous construction taking $\mu = 0$ and then normalize by rows, obtaining:

$$c_{i\to j,k\to l} = \begin{cases} 0 & \text{if } j \neq k, \\ \dfrac{b_{i\to j,k\to l}}{\sum\limits_{\beta\to\gamma} b_{i\to j,\beta\to\gamma}} & \text{if } j = k \text{ and } j \to i \notin E, \\ \dfrac{b_{i\to j,k\to l}}{\sum\limits_{(\beta\to\gamma)\neq(j\to i)} b_{i\to j,\beta\to\gamma}} & \text{if } j = k,\ j \to i \in E \text{ and } l \neq i, \\ 0 & \text{if } j = k,\ j \to i \in E \text{ and } l = i. \end{cases}$$

Note that the coefficients of C_0 and C are usually equal, but may differ in the forth line of the respective definitions. In order to determine when this happens, we introduce the following definition:

Definition 3.1. Let $G = (X, E, w)$ a weighted directed network and $j \in X$. We say that j is *an almost terminal node* if there exists another node $i \in X$ with $i \neq j$ such that $i \to j,\ j \to i \in E$ and every other node $k \in X$ with $k \neq i$ satisfies that $j \to k \notin E$.

Intuitively, an almost terminal node is a node j with indegree and outdegree one such that both the outlink and the inlink are connected to the same node i.

Lemma 3.2. *Let $G = (X, E, w)$ a weighted directed network and C and C_0 the matrices previously defined. Then $c_{i\to j,k\to l} \neq (c_0)_{i\to j,k\to l}$ if and only if $(k \to l) = (j \to i)$ and j is an almost terminal node. Moreover, if this is the case, $c_{i\to j,j\to i} = 0$ and $(c_0)_{i\to j,j\to i} = 1$.*

Proof. First note that the first and second lines in the definition of $(c_\mu)_{i\to j,j\to i}$ do not depend on μ and coincide with those in the definition of $c_{i\to j,j\to i}$, therefore equality holds between $c_{i\to j,k\to l}$ and $(c_0)_{i\to j,k\to l}$. With respect to the third line, it is straightforward that $(c_0)_{i\to j,k\to l} = lim_{\mu\to 0^+}(c_\mu)_{i\to j,j\to i} = c_{i\to j,j\to i}$. The same happens with the forth line if j is not an almost terminal node, because, if this is the case, the summation has at least one term. On the other hand, if j is an almost terminal node, then

$$(c_\mu)_{i\to j,j\to i} = \frac{\mu b_{i\to j,j\to i}}{\mu b_{i\to j,j\to i}} = 1$$

for every $\mu > 0$, which imply that $(c_0)_{i\to j,j\to i} = 1$. □

Note that, because B has no dangling nodes, the matrices C_μ for $\mu > 0$ have no null rows. As a consequence of previous theorem, the same is true for C_0. But nevertheless the matrix C may have null rows: this happens if it corresponds to an almost terminal node. More precisely:

Remark 3.3. The row of C labeled with $i \to j$ is a null row if and only if j is an almost terminal node.

Now, since matrices C_μ are row stochastic, we are ready to define corresponding PageRank vectors for edges, but first we need to choose a personalization vector. As pointed out in Section 2, it was shown in [15] that if A is the adjacency matrix of G and $v \in \mathbb{R}^n$ is a personalization vector for the computation of the PageRank of G, then choosing u such that

$$u_{i\to j} = \frac{a_{ij}}{\sum_k a_{ik}} v_i \tag{3.4}$$

guarantees that the two PageRank measures defined for edges in [15] coincide. Motivated by this fact we choose u in this way in our following definition:

Definition 3.5. Let A and $\{C_\mu\}_{\mu\in[0,1]}$ be matrices defined before, $q \in (0, 1)$, $v \in \mathbb{R}^n$ such that $v > 0$ and $||v||_1 = 1$, and u defined as in (3.4). Let H_μ be the following matrix:

$$H_\mu = qC_\mu + (1 - q)\mathbf{1}u^T.$$

Then the *μ-non-backtracking PageRank vector* of $L(G)$ with *damping factor* q and *personalization vector* v is the unique postive vector $\mu NBLPR(G, q, v) = \pi_\mu$ such that $||\pi_\mu||_1 = 1$ and $\pi_\mu^T H_\mu = \pi_\mu^T$.

Note that the existence and uniqueness of π_μ is guaranteed, in the same way as usual PageRank, by PerronFrobenius theory (see, for instance, [37]).

When we want to define an analogous PageRank vector for the matrix C, we need to take into account that there may be null rows in this matrix. In this case we choose the usual approach (see, for example Section 4 of [34]) and substitute these null rows with the personalization vector u. In order to construct the matrix H associated to C in this way, we first define a vector ξ indexed by the edge set E such that $\xi_{i\to j} = 1$ if j is an almost terminal node and $\xi_{i\to j} = 0$ otherwise. As we have previously stated, $\xi_{i\to j} = 1$ if and only if the row of C indexed with $i \to j$ is a null row.

Definition 3.6. Let A and C be matrices defined before, $q \in (0, 1)$ and $v \in \mathbb{R}^n$ such that $v > 0$ and $||v||_1 = 1$ and u defined as in (3.4). Let H be the following matrix:

$$H = q(C + \xi u^T) + (1 - q)\mathbf{1}u^T.$$

Then the *non-backtracking PageRank vector* of $L(G)$ with *damping factor* q and *personalization vector* v is the unique positive vector $NBLPR(G, q, v) = \pi$ such that $||\pi||_1 = 1$ and $\pi^T H = \pi^T$.

Again the existence and uniqueness of π is guaranteed by Perron Theorem, since H is a positive matrix.

Finally we are able to provide non-backtracking PageRank definitions for nodes induced by the measures we have defined for edges:

Definition 3.7. Let $G=(X,E,w)$ be a weighted directed network with adjacency matrix A, $q\in(0,1)$ and $v\in\mathbb{R}^n$ such that $v>0$ and $||v||_1=1$. Let $\{\pi_\mu\}_{\mu\in[0,1]}$ and π the non-backtracking PageRanks from Definitions 3.5 and 3.6. For every node $j\in E$ and every $\mu\in[0,1]$ define:

- the *μ-non-bactraking PageRank* of node j as
$$NBPR_\mu(j)=\sum_{j\to k}(\pi_\mu)_{j\to k},$$
- the *non-bactraking PageRank* of node j as
$$NBPR(j)=\sum_{j\to k}(\pi)_{j\to k},$$

both with respect to damping factor q and personalization vector v.

Once the measures are defined, it is a natural question to ask if the limit when $\mu\to 0^+$ of the μ-non-bactraking PageRank equals the 0-non-bactraking PageRank. The answer is positive and proven below. As a tool to show this result we will use the following result from [60]:

Theorem 3.8 (page 514 in [60]). *Let M be a Google matrix and $\hat{x}$ be the PageRank vector. Suppose that $\tilde{M}=M+F$ is the perturbed Google matrix and $\tilde{x}$ is the associated PageRank vector, then*
$$||\tilde{x}-\hat{x}||_1\le\frac{1}{1-q}||F||_\infty,$$
where $||\cdot||_1$ and $||\cdot||_\infty$ denote the 1-norm and ∞-norm of a vector or a matrix, respectively.

Next we use previous result to prove the convergence of the μ-non-bactraking PageRank:

Theorem 3.9. *Let $G=(X,E,w)$ be a weighted directed network with adjacency matrix A, $q\in(0,1)$ and $v\in\mathbb{R}^n$ such that $v>0$ and $||v||_1=1$. For every $j\in E$ and $\mu\in[0,1]$ let $NBPR_\mu(j)$ be the μ-non-bactraking PageRank of j as defined in Definition 3.7. Then*
$$\lim_{\mu\to 0^+}NBPR_\mu(j)=NBPR_0(j).$$

Proof. Consider $\mu>0$. Using the notation of Theorem 3.8, take $M=H_0$ and $\tilde{M}=H_\mu$. Then $\hat{x}=\pi_0$ and $\tilde{x}=\pi_\mu$ are PageRank vectors of H_0 and H_μ, respectively, and we can apply Theorem 3.8 to obtain
$$||\pi_\mu-\pi_0||_1\le\frac{1}{1-q}||H_\mu-H_0||_\infty.$$
Let us analyze the difference
$$H_\mu-H_0=qC_\mu+(1-q)\mathbf{1}u^T-qC_0-(1-q)\mathbf{1}u^T=q(C_\mu-C_0)$$
from which we conclude that
$$||\pi_\mu-\pi_0||_1\le\frac{q}{1-q}||C_\mu-C_0||_\infty.$$
Taking into consideration that C_0 is the coefficient-wise limit of C_μ when $\mu\to 0^+$ and that ∞-norm is a continuous function of the coefficients of a matrix, it follows that $lim_{\mu\to 0^+}||C_\mu-C_0||_\infty=0$ and therefore the same holds for $||\pi_\mu-\pi_0||_1$, which in turn implies that $lim_{\mu\to 0^+}\pi_\mu=\pi_0$.

The result follows easily from the definitions of $NBPR_\mu(j)$ and $NBPR_0(j)$. □

At this point it is worth analyzing the relationship between π_0 and π. As our experiments will show in Section 4, there are networks where these two vectors are different, therefore leading to different non-backtracking PageRank rankings for the nodes. However, in the next result, we provide an analytical sufficient condition for these two vectors to coincide:

Proposition 3.10. *Let $G=(X,E,w)$ be a weighted directed network and π_0,π be the vectors from Definitions 3.5 and 3.6 respectively. Then, if G has no almost terminal nodes, then $\pi_0=\pi$.*

Proof. This result follows directly from Lemma 3.2. □

Corollary 3.11. *Let $G=(X,E,w)$ be a weighted directed network with no almost terminal nodes. For every $j\in X$ and $\mu\in[0,1]$, let $NBPR_\mu(j)$ and NBPR(j) be the PageRank measures defined in Definition 3.7. Then*
$$\lim_{\mu\to 0^+}NBPR_\mu(j)=NBPR(j).$$

Proof. This follows from Theorem 3.9 and Proposition 3.10. □

It is worth pointing out that we can formulate an almost reciprocal statement for Proposition 3.10 as follows:

Proposition 3.12. *Let $G=(X,E,w)$ be a weighted directed network and π_0,π be the vectors from Definitions 3.5 and 3.6 respectively. Then, if $\pi_0=\pi$, it follows that either G has no almost terminal nodes or every node in G is almost terminal.*

Proof. Assume that $\pi_0=\pi$ and let us reasoning by *Reductio ad absurdum*. Let us suppose that there are two nodes such that one of them is almost terminal while the other is not.

Since $\pi_0=\pi$, we have that $\pi^TH=\pi^TH_0$. It follows that
$$\pi^Tq(C+\xi u^T)=\pi^TqC_0,$$
which implies that
$$\pi^T(C_0-C)=\pi^T\xi u^T. \tag{3.13}$$
Recall that, from Lemma 3.2, most coefficients in the matrix C_0-C equal 0 except for those which equal 1. And there are precisely as many coefficients equal to 1 as almost terminal nodes. As not every node is almost terminal, by Lemma 3.2 the matrix C_0-C must have at least one null column, namely any column indexed by $k\to l$ where k is not almost terminal. Then it follows that $(\pi^T(C_0-C))_{k\to l}=0$.

On the other hand, the vector ξ has at least one coordinate equal to 1, as there is at least one almost terminal node. Let $i\to j$ be an edge such that j is almost terminal. Then we have that $(\pi^T\xi u^T)_{k\to l}\ge\pi_{i\to j}u_{k\to l}>0$, where the last inequality is a consequence of both π and u being positive vectors.

By combining these two facts with Eq. (3.13) we obtain an absurd, which proves the stated result. □

Finally, it is interesting to point out that the directed networks such that every node is an almost terminal node are easy to characterize: they are disjoint unions of directed complete networks with 2 nodes.

4. Some experimental results

In this section, we report some numerical experiments, in which μ-non-bactracking PageRank of $L(G)$ for different real-world networks are calculated. Note that, by using [34], this computation is equivalent to finding the solution of the linear system
$$x^T(I-qC_\mu)=u^T, \tag{4.1}$$
and obtaining
$$\pi_\mu=(1-q)x.$$

Indeed, by using [4], we deduce that $(I-qC_\mu)^{-1}$ exists and has all nonnegative entries because

$$(I-qC_\mu)\mathbf{1} = (1-q)\mathbf{1} > 0$$

and $I-qC_\mu$ has nonpositive off-diagonal entries. Then, it follows from (4.1) that

$$x > 0 \quad \text{and} \quad \|x\|_1 = x^T\mathbf{1} = u^T(I-qC_\mu)^{-1}\mathbf{1} = 1/(1-q). \tag{4.2}$$

Therefore, $\|\pi_\mu\|_1 = 1$. Moreover, according to Definition 3.5, we deduce that

$$\pi_\mu^T H_\mu = q\pi_\mu^T C_\mu + (1-q)u^T = \pi_\mu^T.$$

Now, the numerical approximation of x is given by the Jacobi method (see, for example [47]). The iterations are defined by

$$\begin{cases} x_0^T = (0,0,\dots,0), \\ x_k^T = qx_{k-1}^T C_\mu + u^T, \quad k \in \mathbb{N}. \end{cases} \tag{4.3}$$

Note that [26] shows that these iterations may converge faster that the power method and are less sensitive to changes in the personalization vector. Also, due to C_μ is a row stochastic matrix and by (4.2), we can consider the following bound between the μ-non-bactracking PageRank of $L(G)$ and its approximation,

$$\|(1-q)x_k - \pi_\mu\|_1 \le q^k\|x^T C_\mu^k\|_1 \le q^k. \tag{4.4}$$

Similarly, we obtain the non-bactracking PageRank of $L(G)$. Due to C can have some null rows, i.e., in the case that the line graph has dangling nodes, we proceed as in [34] and we take

$$\tilde{C} = QCQ^T = \begin{pmatrix} \tilde{C}_1 & \tilde{C}_2 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \tilde{u} = Qu = \begin{pmatrix} \tilde{u}_N \\ \tilde{u}_D \end{pmatrix}, \tag{4.5}$$

where Q is a permutation matrix such that all null rows are at the bottom of the matrix $\tilde{C}$. Then, the solution of

$$\tilde{x}_N^T(I-q\tilde{C}_1) = \tilde{u}_N^T \quad \text{and} \quad \tilde{x}_D^T = q\tilde{x}_N^T\tilde{C}_2 + \tilde{u}_D^T \tag{4.6}$$

determines that

$$\pi = \frac{Q^T\tilde{x}}{\|\tilde{x}\|_1}, \quad \text{with } \tilde{x}^T = (\tilde{x}_N^T, \tilde{x}_D^T).$$

Indeed, by (4.5) and (4.6), we have that

$$\tilde{x}^T(I-q\tilde{C}) = \tilde{u}^T. \tag{4.7}$$

Moreover, $(I-q\tilde{C})^{-1}$ exists and has all nonnegative entries because

$$(I-q\tilde{C})\mathbf{1} = \mathbf{1}^* > 0 \quad \text{with } \mathbf{1}^* = \begin{pmatrix} (1-q)\mathbf{1}_N \\ \mathbf{1}_D \end{pmatrix}.$$

Then, since

$$\tilde{x}^T Q(q\xi + (1-q)\mathbf{1}) = \tilde{x}^T\mathbf{1}^* = \tilde{u}^T(I-q\tilde{C})^{-1}\mathbf{1}^* = 1,$$

it follows of (4.5) and (4.7) that

$$\pi^T(I-qC) = \pi^T(q\xi + (1-q)\mathbf{1})u^T,$$

and, consequently, π satisfies Definition 3.6. Therefore, the approximation of $\tilde{x}$,

$$\tilde{x}_k^T = (\tilde{x}_{N,k}^T, \tilde{x}_{D,k}^T),$$

is calculated as follows

$$\begin{cases} \tilde{x}_{N,0}^T = (0,0,\dots,0), \\ \tilde{x}_{N,k}^T = q\tilde{x}_{N,k-1}^T\tilde{C}_1 + \tilde{u}_N^T, \end{cases} \quad \text{and} \quad \tilde{x}_{D,k}^T = q\tilde{x}_{N,k}^T\tilde{C}_2 + \tilde{u}_D^T. \tag{4.8}$$

Since $\tilde{x}_N$ is approximated by Jacobi method and the sum of the elements of each row of $\tilde{C}$ is less or equal than 1, we deduce that

$$\|\tilde{x} - \tilde{x}_k\|_1 = \|\tilde{x}_N - \tilde{x}_{N,k}\|_1 + \|\tilde{x}_D - \tilde{x}_{D,k}\|_1 \le (1+q)q^k\|\tilde{x}\|_1,$$

and the bound of error is given by

$$\left\| \pi - Q^T\frac{\tilde{x}_k}{\|\tilde{x}_k\|_1} \right\|_1 \le 2\frac{\|\tilde{x}_k - \tilde{x}\|_1}{\|\tilde{x}\|_1} \le 2(1+q)q^k. \tag{4.9}$$

Also, it is possible to apply the method of Jacobi directly to (4.7) as in Gleich [25], but we have chosen the below algorithm because the dimension of $\tilde{C}_1$ is less than $\tilde{C}$.

Finally, we compute the standard PageRank in a similar way as in (4.3), but by using θ_{ij} and v (see (2.3)), with an error bound as in (4.4), and compare it with the ranking provides by μ-non-bactracking PageRank. For this purpose, we use the Kendall's Tau coefficient [30], which is denoted by

$$\tau_1(\mu) = \text{Kendall's Tau coefficient } PR \text{ vs } NBPR_\mu. \tag{4.10}$$

However, in the case that G has some almost terminal nodes, it is possible that $NBPR_0 \neq NBPR$ and thus, the rankings can be different. Therefore, we introduce also

$$\tau(\mu) = \text{Kendall's Tau coefficient } \begin{cases} NBPR \text{ vs } NBPR_\mu & \text{if } \mu \neq 1, \\ NBPR \text{ vs } PR & \text{if } \mu = 1. \end{cases} \tag{4.11}$$

The numerical experiments were run on a iMac18,3 with 4,2 GHz Intel Core i7 and RAM 16 GB, under the macOS High Sierra operating system. All the experimental results were obtained by using a Python 3.7 implementation with machine precision $\varepsilon \approx 2.22 \times 10^{-16}$.

4.1. Madrid underground system

In this subsection, we study the Madrid Underground System [61]. Following a similar interpretation as in [15], we choose a damping factor $q = 0.91$. Therefore, we stop in $k = 405$ to get an error less that 10^{-16} in (4.4) and (4.9). Also, note that this network possesses exactly eleven almost terminal nodes which produce big differences between the rankings provided by $NBPR_0$ and $NBPR$ as we will see next.

Firstly, we choose a uniform personalization vector, $v = \mathbf{1}/n$, and calculate the PageRank and the μ-non-bactracking PageRank for

$$\mu_i = 1 - \frac{i}{10}, \quad i = 1, 2, \dots 10.$$

Fig. 2 shows the changes introduced by the parameter μ, reflecting some variations in the ranking of the first fifteen stations. For example, it can be observed that the μ-non-backtracking does not affect to the first, second and fifteenth positions, which occupy the stations *Avenida de América, Vodafone Sol* and *Sainz de Baranda*, respectively, but, however, the rest of stations exchange their places, being significant the decrease of *Oporto* or the increase of *Diego de León* when μ goes to 0. Also, Fig. 3 provides Kendall's Tau coefficients, defined in (4.10) and (4.11), when the first fifteen stations are considered. It shows that the rankings are not the same and reflects the result proved in Proposition 3.12, because $\tau(0) \approx 0.71$. Now, we are going to consider two personalization vectors chosen in [15]. They take into account two situations: the morning traffic and the after-work traffic. For them, the 80% of passengers is assumed to enter the system in stations located in urban areas with many residents, surrounding suburbs, dormitory districts or nearby peripheral cities to define the personalization vector of the morning traffic, while the 80% is given to stations located in the vicinity of the main work centers in the case of after-work traffic.

The differences between the rankings are bigger with morning traffic than with after-work traffic. It can be seen in Fig. 4.

Moreover, some of the first fifteen stations, according with the PageRank, change their positions drastically. In the Table 1,

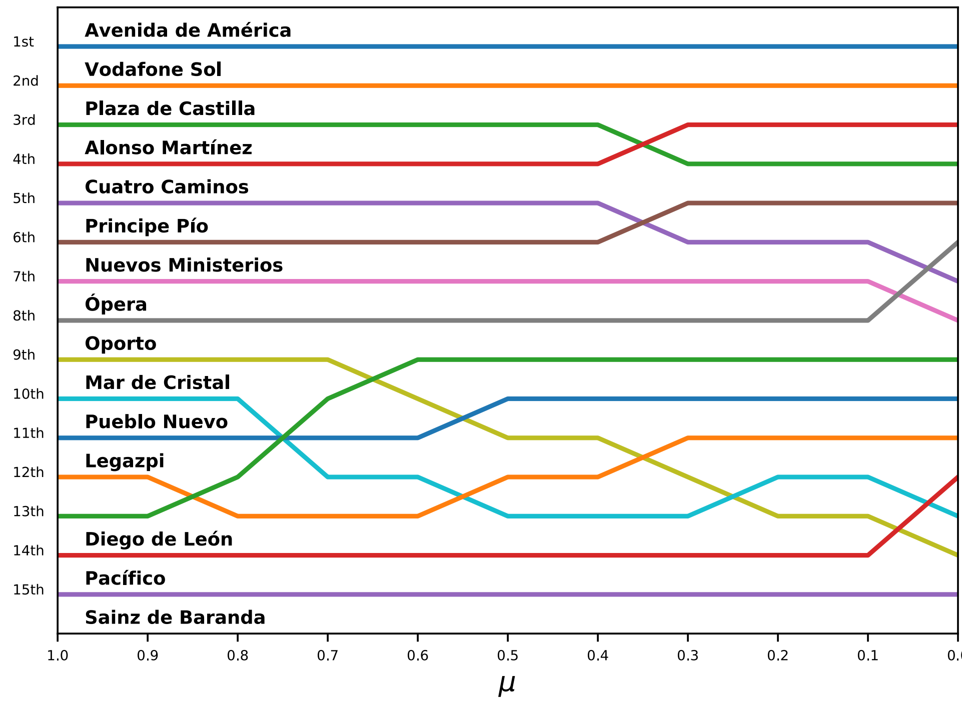

Fig. 2. Ranking of Madrid Underground with $v = \mathbf{1}/n$.

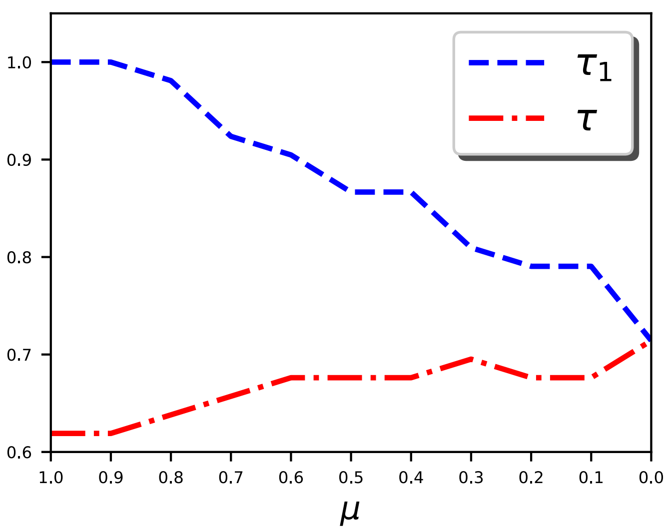

Fig. 3. Kendall's Tau coefficients of the 15-top stations with $v = \mathbf{1}/n$.

Table 1
Ranking of Madrid Underground with morning traffic.

Station	*PR*	$NBPR_{0.5}$	$NBPR_0$	*NBPR*
Puerta del Sur	1st	1st	1st	1st
Las Suertes	2nd	22nd	57th	94th
La Poveda	3rd	23rd	64th	99th
Reyes Católicos	4th	30th	56th	95th
La Peseta	5th	36th	59th	97th
Las Musas	6th	35th	52nd	108th
Arroyo Culebro	7th	3rd	4th	2nd
Parque de los Estados	8th	5th	5th	4nd
Conservatorio	9th	4th	6th	3rd
Fuenlabrada Central	10th	6th	8th	5th
Alonso de Mendoza	11th	7th	7th	6th
Parque Europa	12th	9th	9th	7th
Getafe Central	13th	8th	10th	8th
Juan de la Cierva	14th	10th	11th	10th
Hospital de Fuenlabrada	15th	11th	12th	9th

it can be observe that *Las Suertes, La Poveda, Reyes Católicos, La Peseta* and *Las Musas*, which are in the 6-top, are located above the fifty position if the 0-non-bactracking PageRank is considered, and higher of the ninety position in the case of non-backtracking PageRank.

4.2. Other real networks

Finally, Kendall's Tau coefficients, (4.10) and (4.11), are calculated for a variety of real networks. The first four networks of Table 2 can be found in [32] and the remainder in [49]. Also, they are studied in: *Pretty Good Privacy* [7], *Contiguous USA* [31], *Euroroad* [55], *US power grid* [58], *rt-retweet* [50,51] and *rec-amazon* [35].

For these simulations, we choose a uniform personalization vector and damping factor, $q = 0.85$. Then, we stop in $k = 235$ to obtain a error less that 10^{-16} in (4.4) and (4.9). Finally, for the results of Table 2, the 15-top positions, according to PageRank, are considered when is a small network as *Contiguous USA* and *rt-retweet*, and the 30-top positions for a medium network as *Pretty Good Privacy, Euroroad, US power grid* and *road-minnesota*. The Kendall's tau coefficients for the network, *rec-amazon*, are calculated with the 50-top positions.

Table 2
Kendall's Tau coefficients for different networks.

Network	$\tau_1(0.5)$	$\tau_1(0)$	$\tau(0)$	$\tau(1)$
Pretty good privacy	0.96	0.91	0.54	0.47
Contiguous USA	0.94	0.92	0.69	0.65
Euroroad	0.90	0.77	0.43	0.34
US power grid	0.94	0.88	0.30	0.23
road-minnesota	0.72	0.45	−0.14	−0.33
rt-retweet	1	0.98	0.69	0.71
rec-amazon	0.80	0.57	−0.21	−0.27

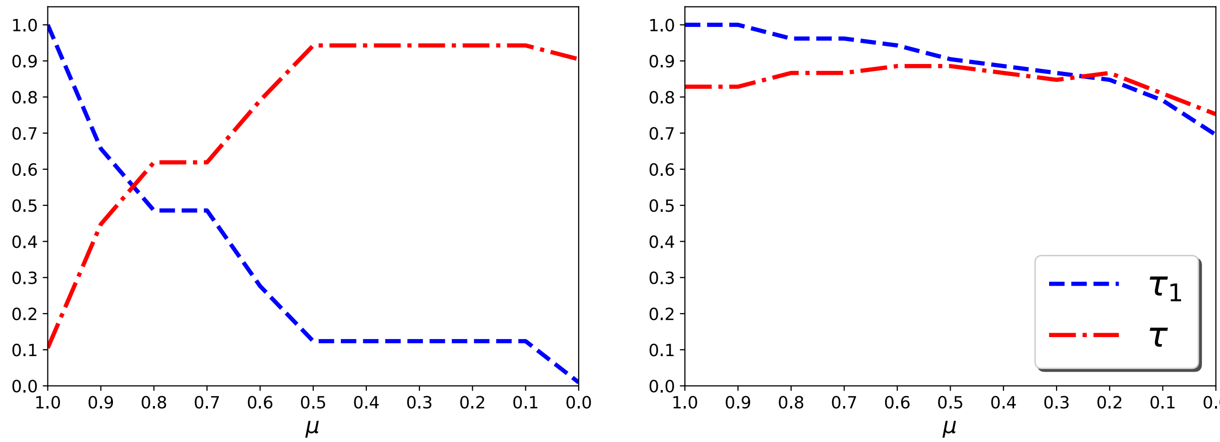

Fig. 4. Kendall's Tau coefficients of the 15-top stations with morning traffic (left) and after-work traffic (right).

5. Conclusions

We introduced and studied Non-backtracking PageRank (NBPR) as a new measure of centrality modifying the classic PageRank in order to avoid the possibility of the random walker returning to the node immediately visited by using the line graph associated to a directed network and the Hashimoto matrix. Indeed, we studied the convergence when $\mu \to 0^+$ of the tuned version of Non-backtracking PageRank and some analytical relationships are established between the μ-Non-backtracking PageRank and its non-tuned version. Furthermore, our numerical experiments showed that the differences between the rankings provided for the classical PageRank and the different NBPR approaches may differ widely under certain circumstances.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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