Linear Algebra and its Applications 451 (2014) 182–196

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

Walks and cycles on a digraph with application to population dynamics

J.W. Moon [a], Zhisheng Shuai [b,*], P. van den Driessche [c]

[a] Department of Mathematical and Statistical Sciences, University of Alberta, Edmonton, AB T6G 2G1, Canada
[b] Department of Mathematics, University of Central Florida, Orlando, FL 32816, United States
[c] Department of Mathematics and Statistics, University of Victoria, Victoria, BC V8W 2Y2, Canada

ARTICLE INFO

Article history:
Received 31 December 2013
Accepted 3 March 2014
Available online 2 April 2014
Submitted by R. Brualdi

MSC:
05C20
92D30

Keywords:
Spectral radius
Target reproduction number
Closed walk
Digraph
Infectious disease control

ABSTRACT

Several relations involving closed walks and closed cycles in a weighted digraph are established. These relations are used to derive new expressions for target reproduction numbers for controlling the spectral radius of nonnegative matrices. The results are illustrated by an application to infectious disease control.

* Corresponding author.
E-mail addresses: jwmoon@ualberta.ca (J.W. Moon), shuai@ucf.edu (Z. Shuai), pvdd@math.uvic.ca (P. van den Driessche).

http://dx.doi.org/10.1016/j.laa.2014.03.003

1. Introduction

Let $W = [w_{ij}]$ be a nonnegative $n \times n$ matrix. Its spectral radius, denoted by $\rho(W)$, gives the asymptotic growth rate of any matrix norm of W^k (see, for example, [5] and [7, Section 5.6]). This fact is of wide application in population dynamics. For example, in a Leslie matrix population model [3, Chapter 2], the spectral radius of the nonnegative projection matrix W determines whether the population grows or goes to extinction, depending on whether $\rho(W) > 1$ or $0 \leqslant \rho(W) < 1$. In an infectious disease model [1,4] with a nonnegative next-generation matrix W, the spectral radius $\rho(W)$, called the basic reproduction number in this content, often determines whether the disease persists or dies out, depending on whether $\rho(W) > 1$ or $\rho(W) < 1$. A natural question is how to reduce or enlarge one or more entries of W so that the controlled matrix W_c (that is obtained from W by reducing or enlarging those entries of W) has spectral radius 1. It turns out that the target reproduction number defined in [11] can be used to measure the magnitude of this reduction or enlargement.

Suppose that only one entry of W is targeted, say the entry w_{ij} for some i, j with $1 \leqslant i, j \leqslant n$. Let A denote the matrix obtained from W by replacing the entry w_{ij} by zero, i.e.,

$$A = W - P_i W P_j, \tag{1.1}$$

where P_i is the $n \times n$ projection matrix with the (i, i) entry equal to 1 and all other entries 0. If $\rho(A) < 1$, then the target reproduction number T_{ij} [11] is defined as

$$T_{ij} = w_{ij}(I - A)^{-1}_{ji}, \tag{1.2}$$

where I is the $n \times n$ identity matrix. To exclude trivial situations, we always assume that $\rho(W) > 0$ and that $T_{ij} > 0$ whenever it is well defined. The following special case of Theorem 4.4 in [11] gives a relation between $\rho(W)$ and T_{ij}.

Proposition 1.1. *Let W be an $n \times n$ nonnegative irreducible matrix such that $\rho(A) < 1$, where A is as defined in (1.1). Then either $1 < \rho(W) < T_{ij}$, $\rho(W) = T_{ij} = 1$, or $T_{ij} < \rho(W) < 1$.*

The next result, a special case of Theorem 2.2 in [11], shows how T_{ij} can be used to modify w_{ij} to find the controlled matrix W_c whose spectral radius equals 1.

Proposition 1.2. *Let W be an $n \times n$ nonnegative irreducible matrix such that $\rho(A) < 1$, where A is as defined in (1.1). If W_c is the controlled matrix obtained from W by replacing w_{ij} by w_{ij}/T_{ij}, then $\rho(W_c) = 1$.*

Example 1. Suppose $W = \left[\begin{smallmatrix} 0.5 & 0.7 \\ 0.7 & 0.5 \end{smallmatrix}\right]$; then $\det(\lambda I - W) = (\lambda + 0.2)(\lambda - 1.2)$, and thus $\rho(W) = 1.2$. In this case, it follows from (1.2) that $T_{11} = 0.5\left[\begin{smallmatrix} 1 & -0.7 \\ -0.7 & 1-0.5 \end{smallmatrix}\right]^{-1}_{11} =$

$50\left[\begin{smallmatrix}0.5 & 0.7\\ 0.7 & 1\end{smallmatrix}\right]_{11} = 25$. If we let $W_c = \left[\begin{smallmatrix}0.5/25 & 0.7\\ 0.7 & 0.5\end{smallmatrix}\right]$, we find that $\det(\lambda I - W_c) = (\lambda - 1) \times (\lambda + 0.48)$; so $\rho(W_C) = 1$, in accordance with Proposition 1.2.

Several applications of target reproduction numbers T_{ij} to infectious disease control problems have been considered in [11]. New results concerning such applications will be described in Section 5.

It turns out that the numbers T_{ij} also have a combinatorial interpretation. To describe this we need to introduce some definitions and notation from graph theory.

If $W = [w_{ij}]$ is any $n \times n$ nonnegative matrix, let $\mathcal{D} = \mathcal{D}(W) = (V(\mathcal{D}), \Gamma(\mathcal{D}))$ denote the associated weighted digraph with vertex set $V(\mathcal{D}) = \{1, 2, \dots, n\}$ and arc set $\Gamma(\mathcal{D}) = \{ij\colon w_{ji} > 0\}$. If $ij \in \Gamma$, then the arc ij (from vertex i to vertex j) has weight w_{ji}. Following [2, p. 65], we use w_{ji} for the weight of ij instead of w_{ij} for convenience in applications. If $w_{ii} > 0$, then the arc ii exists and is called the *loop* at vertex i. A digraph $\mathcal{H}$ is a *subdigraph* of $\mathcal{D}$ if $V(\mathcal{H}) \subseteq V(\mathcal{D})$, $\Gamma(\mathcal{H}) \subseteq \Gamma(\mathcal{D})$, and every arc ij in $\Gamma(\mathcal{H})$ has weight w_{ji}. If $V(\mathcal{H}) = V(\mathcal{D})$, then $\mathcal{H}$ is a *spanning* subdigraph of $\mathcal{D}$. The *weight* $w(\mathcal{H})$ of any subdigraph $\mathcal{H}$ is the product of the weights of the arcs in $\mathcal{H}$ with the understanding that an empty product equals 1 (when $\mathcal{H}$ has no arcs). A *walk* $\mathcal{F}_{az}$ in $\mathcal{D}$ from vertex a to vertex z is an alternating sequence of vertices and arcs of the form $a, ab, b, bc, \dots, yz, z$; if $a = z$ then the walk is *closed*. A *trivial* walk consists of a single vertex and no arcs. See [13] for additional graph-theoretic definitions.

We are now ready to describe the combinatorial interpretation of T_{ij}.

Theorem 1.3. *Let W be an $n \times n$ nonnegative irreducible matrix such that $\rho(A) < 1$, where A is as defined in (1.1). Then*

$$T_{ij} = \sum_{\mathcal{Q}} w(\mathcal{Q}), \tag{1.3}$$

where the sum is over all closed walks $\mathcal{Q}$ from i to i in $\mathcal{D} = \mathcal{D}(W)$ that contain the arc ji (of weight w_{ij}) exactly once and the unique occurrence of ji is as the last arc of the walk.

Proof. Since $\rho(A) < 1$, definition (1.2) can be rewritten as

$$T_{ij} = w_{ij}\left(I + A + A^2 + \cdots\right)_{ji}. \tag{1.4}$$

It is not difficult to see [11, Section 3.2] that the ji entry of $I + A + A^2 + \cdots$ enumerates the weighted walks $\tilde{\mathcal{F}}_{ij}$ in $\mathcal{D}$ from i to j that do not contain the arc ji (of weight w_{ij}). Thus,

$$T_{ij} = w_{ij}\tilde{f}_{ij}, \tag{1.5}$$

with

$$\tilde{f}_{ij} = \sum_{\tilde{\mathcal{F}}_{ij}} w(\tilde{\mathcal{F}}_{ij}), \tag{1.6}$$

where the sum is over all weighted walks $\tilde{\mathcal{F}}_{ij}$ just defined (i.e., all weighted walks in $\mathcal{D}$ from i to j that do not contain the arc ji). When the arc ji and the vertex i are added at the end of such walks and their weight is multiplied by the weight w_{ij}, expression (1.3) results. □

Notice that if $Z = I - A$, then the relation between its inverse and adjoint implies that (1.2) can be rewritten as

$$T_{ij} = (-1)^{i+j} w_{ij} \frac{\det Z(i|j)}{\det Z}, \tag{1.7}$$

where $Z(i|j)$ denotes the matrix obtained from Z by deleting the i-th row and the j-th column. Relations (1.3) and (1.7) imply the following result.

Corollary 1.4. *Let W be an $n \times n$ nonnegative irreducible matrix such that $\rho(A) < 1$, where A is as defined in (1.1), and let $Z = I - A$. Then*

$$\sum_{\mathcal{Q}} w(\mathcal{Q}) = (-1)^{i+j} w_{ij} \frac{\det Z(i|j)}{\det Z}, \tag{1.8}$$

where the sum is over all closed walks $\mathcal{Q}$ in $\mathcal{D} = \mathcal{D}(W)$ that contain the arc ji (of weight w_{ij}) exactly once and the unique occurrence of ji is as the last arc of the walk.

Our object is to extend relation (1.8) in certain ways. We begin in Section 2 by expressing some determinants as sums of the weights of subdigraphs of a weighted digraph $\mathcal{D}$ associated with a more general version of the matrix W. Our approach involves combinatorial interpretations and does not make any use of the result involving the inverse and adjoint of a matrix; nor does it require any considerations of convergence. In Section 3, we prove an identity involving the sum of the weighted walks between two vertices in a digraph. In Section 4, we give a new expression for T_{ij} in terms of cycles (cycle-unions as defined in Section 2). Finally, in Section 5, we use the relations established to give results applicable to disease control strategies in models of infectious disease dynamics.

2. Some determinant and cofactor expansions

In this and the next section, we consider the entries w_{ij} in the $n \times n$ matrix $W = [w_{ij}]$ as formal variables. So, in particular, a statement of equality between two generating functions involving sums of (finite) products of variables w_{ij} (plus, perhaps, a constant term) simply means that any particular product of m variables w_{ij} has the same (finite) coefficient in each of the generating functions, for $m = 0, 1, 2, \ldots$. See, e.g., Tutte [12] for an exposition of the calculus of operations on formal power series.

Brualdi and Cvetković [2, Chapter 4] give a non-traditional graph-theoretic approach to the elementary theory of determinants. In this section we formulate some basic determinant expansions in terms of sums of the weights of certain subdigraphs of a digraph. We use these expansions in the subsequent sections to derive our main results. First we give some additional definitions.

A *cycle-union* of the digraph $\mathcal{D}$ associated with the matrix $W = [w_{ij}]$, is a spanning subdigraph $\mathcal{U}$ such that each component of $\mathcal{U}$ is either a cycle or an isolated vertex. A *linear subdigraph* $\mathcal{L}$ of $\mathcal{D}$ is a cycle-union with no isolated vertices; that is, every vertex of $\mathcal{L}$ has indegree and outdegree 1. Let $c(\mathcal{U})$ and $c(\mathcal{L})$ denote the number of cycles in such digraphs. We now give the Harary–Coates formulation of the definition of the determinant $\det W$ of the matrix W (see [2, p. 65]).

Proposition 2.1.

$$\det W = (-1)^n \sum_{\mathcal{L}} (-1)^{c(\mathcal{L})} w(\mathcal{L}),$$

where the sum is over all linear subdigraphs $\mathcal{L}$ of $\mathcal{D}(W)$.

From this we can deduce an expression for the determinant of the matrix $Y = I - W$.

Proposition 2.2.

$$\det Y = \det(I - W) = \sum_{\mathcal{U}} (-1)^{c(\mathcal{U})} w(\mathcal{U}), \tag{2.1}$$

where the sum is over all cycle-unions $\mathcal{U}$ of $\mathcal{D}(W)$.

Proof. It follows from Proposition 2.1 that

$$\det(-W) = (-1)^n \det W = \sum_{\mathcal{L}} (-1)^{c(\mathcal{L})} w(\mathcal{L}).$$

To obtain the expansion of $\det Y$ from this, replace each factor $w_{ii} \neq 0$ that occurs in any term $w(\mathcal{L})$ by $1 - w_{ii}$ and then multiply out the resulting products. Choosing the $-w_{ii}$ term from each such factor gives the terms in the expansion of $\det(-W)$. But each time the 1 is chosen instead of the $-w_{ii}$, the loop at vertex i is removed, in effect, and $\mathcal{L}$ is converted into a cycle-union $\mathcal{U}$ with the weight function and exponent of -1 adjusted accordingly. (Notice that the cycle-union with no arcs contributes a term of 1 to $\det Y$.) □

Following [2, pp. 77, 103], we define a 1-*connection* of i to j in any weighted digraph to be a spanning subdigraph $\mathcal{E}_{ij}$ with the following properties: it contains a path from i

to j (of length 0 if $i = j$) and a (possibly empty) collection of $c(\mathcal{E}_{ij})$ cycles such that the path and cycles collectively are vertex disjoint.

Let $\mathcal{K}$ denote the n-vertex digraph in which there is an arc ij of weight $y_{ji} = \delta_{ji} - w_{ji}$ for $1 \leqslant i, j \leqslant n$; and if $\mathcal{H}$ is any subdigraph of $\mathcal{K}$, let $y(\mathcal{H})$ denote the product of the weights y_{ji} of the arcs ij in $\mathcal{H}$ (with the usual convention for empty products). Finally, if M is any $n \times n$ matrix, let $M(a, \ldots | b, \ldots)$ denote the matrix obtained from M by deleting rows $a, \ldots$ and columns $b, \ldots$ from M.

The following result [2, pp. 77, 105] contains an alternate formulation of the usual definition of cofactors in the expansion of a determinant. We adopt the convention that $Y(1|1) = 1$ when $n = 1$.

Proposition 2.3. *Let the cofactors C_{ij} of entries y_{ij} in the expansion of the determinant of the matrix $Y = I - W = [y_{ij}]$ be defined by the relations*

$$\det Y = \sum_{j=1}^{n} y_{ij} C_{ij} = \sum_{i=1}^{n} y_{ij} C_{ij}, \tag{2.2}$$

for $i = 1, 2, \ldots, n$ in the first sum and for $j = 1, 2, \ldots, n$ in the second. Then

$$C_{ij} = (-1)^{i+j} \det Y(i|j) = (-1)^n \sum_{\mathcal{E}_{ij}} (-1)^{1+c(\mathcal{E}_{ij})} y(\mathcal{E}_{ij}), \tag{2.3}$$

where the sum is over all 1-connections $\mathcal{E}_{ij}$ of i to j in $\mathcal{K}$.

Proposition 2.4. *Let $Y = I - W$.*

(*i*) *If $i \neq j$, then*

$$y_{ij} C_{ij} = \sum_{\mathcal{U}_{ij}} (-1)^{c(\mathcal{U}_{ij})} w(\mathcal{U}_{ij}) \tag{2.4}$$

where the sum is over all cycle-unions $\mathcal{U}_{ij}$ of $\mathcal{D}(W)$ that contain the arc ji.

(*ii*) *If $i = j$, then*

$$y_{ii} C_{ii} = (1 - w_{ii}) \sum_{\mathcal{U}'} (-1)^{c(\mathcal{U}')} w(\mathcal{U}'), \tag{2.5}$$

where the sum is over all cycle-unions $\mathcal{U}'$ of the digraph associated with $W(i|i)$.

Proof. Relation (2.4) follows readily upon comparing terms containing w_{ij} in Proposition 2.2 and in (2.2). Relation (2.5) follows from the definition of y_{ii} and the expansion obtained by replacing $\det Y$ by C_{ii} in Proposition 2.2. □

Expanding $\det Y$ along its n-th row and then expanding each factor $\det Y(n|j)$ that arises in this expansion along its last column gives the following result.

Lemma 2.5. *Let $Y = I - W$. If $n \geqslant 2$, then*

$$\det Y = y_{nn} \det Y(n|n) - \sum_{i,j=1}^{n-1} w_{in} w_{nj} (-1)^{i+j} \det Y(i,n|j,n). \tag{2.6}$$

Also expanding $\det Y(n|n-1)$ along its last column (which is now its $(n-1)$-st column) leads to another result.

Lemma 2.6. *Let $Y = I - W$. If $n \geqslant 2$, then*

$$\det Y(n|n-1) = \sum_{i=1}^{n-1} w_{in} (-1)^{n+i} \det Y(i,n|n-1,n). \tag{2.7}$$

There are, of course, more general versions of expansions (2.6) and (2.7); we have given only the expansions we use explicitly in the next section.

3. An identity involving the weights of walks in a digraph

For $1 \leqslant i, j \leqslant n$, let the generating function f_{ij} be defined as follows:

$$f_{ij} = \sum_{\mathcal{F}_{ij}} w(\mathcal{F}_{ij}),$$

where the sum is over all walks $\mathcal{F}_{ij}$ from i to j in the digraph $\mathcal{D} = \mathcal{D}(W)$ associated with the $n \times n$ matrix W. We now show, by induction on n, that f_{ij} satisfies the following relation.

Theorem 3.1. *If $1 \leqslant i, j \leqslant n$, then*

$$f_{ij} \det Y = C_{ij} = (-1)^{i+j} \det Y(i|j), \tag{3.1}$$

where $Y = I - W = [y_{ij}]$ and C_{ij} is the cofactor of y_{ij} in $\det Y$.

Proof. If $i = j = n = 1$, then

$$f_{11} \det Y = (1 - w_{11})\bigl(1 + w_{11} + w_{11}^2 + \cdots\bigr) = 1 = C_{11},$$

in view of our convention about C_{11} when $n = 1$; so (3.1) holds when $n = 1$.

We may suppose that $n \geqslant 2$ and that the analogue of relation (3.1) holds for all square matrices with $n - 1$ rows and columns. There are essentially two cases to consider for the proof of (3.1); namely, when $i = j$ and when $i \neq j$. For notational convenience we treat only the cases when $i = j = n$ and when $i = j + 1 = n$; the remaining cases follow by symmetry.

If $1 \leqslant i, j \leqslant n-1$, let f'_{ij} be defined as f_{ij} except that now the walks $\mathcal{F}'_{ij}$ are restricted to walks on the subdigraph $\mathcal{D}'$ associated with the matrix $W(n|n)$. Our induction hypothesis gives

$$f'_{ij} \det Y(n|n) = (-1)^{i+j} \det Y(i,n|j,n) \tag{3.2}$$

for $1 \leqslant i, j \leqslant n-1$.

Case 1: $i = j = n$. We assert that f_{nn} satisfies the recurrence relation

$$f_{nn} = 1 + w_{nn} f_{nn} + \sum_{i,j=1}^{n-1} w_{in} f'_{ij} w_{nj} f_{nn}. \tag{3.3}$$

The 1 records the weight of the trivial walk consisting of vertex n and no arcs. The term $w_{nn} f_{nn}$ records the weights of the walks that starts at n, proceed along the loop (of weight w_{nn}) back to n and may or may not proceed along another walk that eventually stops at n. The term $w_{in} f'_{ij} w_{nj} f_{nn}$ records the weights of the walks that immediately leave n by arc ni, of weight w_{in}, to some vertex i in $\mathcal{D}'$, continue along a walk in $\mathcal{D}'$ to some vertex j, from which they leave $\mathcal{D}'$ along the arc jn, of weight w_{nj}, and return to n for the first time; these walks may or may not continue until they return to n for the last time. Combining all these possibilities, the contribution of all walks starting and ending at n are included, as required.

Appealing successively to expansion (2.6), the induction hypothesis (3.2), and relation (3.3), we find that

$$\begin{aligned} f_{nn} \det Y &= f_{nn} \left((1 - w_{nn}) \det Y(n|n) - \sum_{i,j=1}^{n-1} w_{in} w_{nj} (-1)^{i+j} \det Y(i,n|j,n) \right) \\ &= \det Y(n|n) f_{nn} \left(1 - w_{nn} - \sum_{i,j=1}^{n-1} w_{in} f'_{ij} w_{nj} \right) = \det Y(n|n), \end{aligned} \tag{3.4}$$

as required.

Case 2: $i = j + 1 = n$. We assert that when $n \geqslant 2$, $f_{n,n-1}$ satisfies the recurrence relation

$$f_{n,n-1} = f_{nn} \sum_{i=1}^{n-1} w_{in} f'_{i,n-1}. \tag{3.5}$$

Any walk from n to $n-1$ starts with a (possibly trivial) walk starting at n and continuing until it returns to n for the last time; this accounts for the factor f_{nn} in (3.5). The walk then leaves n along some arc ni, of weight w_{in}, to a vertex i in $\mathcal{D}'$; it then proceeds along some walk in $\mathcal{D}'$ until it reaches $n-1$ for the last time; the sum records the contributions of this latter part of the walk.

Relation (3.5), conclusion (3.4), the induction hypothesis (3.2) for $f'_{i,n-1}$, and expression (2.7) imply that

$$\begin{aligned} f_{n,n-1} \det Y &= \det Y f_{nn} \sum_{i=1}^{n-1} w_{in} f'_{i,n-1} \\ &= \sum_{i=1}^{n-1} w_{in} \det Y(n|n) f'_{i,n-1} \\ &= \sum_{i=1}^{n-1} w_{in} (-1)^{i+n-1} \det Y(i,n|n-1,n) \\ &= (-1) \det Y(n|n-1) = (-1)^{2n-1} \det Y(n|n-1), \end{aligned}$$

as required. This suffices to prove relation (3.1) in view of the earlier remarks. □

Appealing to (2.3) and Proposition 2.2, we can rewrite relation (3.1) to give another expression for the sum of the weights of all walks from i to j in $\mathcal{D}(W)$.

Corollary 3.2. *If $1 \leqslant i, j \leqslant n$, then*

$$f_{ij} = \sum_{\mathcal{F}_{ij}} w(\mathcal{F}_{ij}) = \frac{(-1)^n \sum_{\mathcal{E}_{ij}} (-1)^{1+c(\mathcal{E}_{ij})} y(\mathcal{E}_{ij})}{\sum_{\mathcal{U}} (-1)^{c(\mathcal{U})} w(\mathcal{U})}, \tag{3.6}$$

where, as before, the sums are over all walks $\mathcal{F}_{ij}$ from i to j in $\mathcal{D}(W)$, all 1-connections $\mathcal{E}_{ij}$ of i to j in digraph $\mathcal{K}$ as defined in Section 2, and all cycle-unions in $\mathcal{D}(W)$, respectively.

We remark that the quotient of the two formal power series is well-defined since the series in the denominator has a non-zero constant term, namely, 1; see, e.g., [12, p. 118].

4. A new expression for T_{ij}

We now specialize the preceding results to obtain an expression for $\tilde{f}_{ij}$ defined in (1.6) as the sum of the weights of the walks from i to j in $\mathcal{D}$ that do not contain the arc ji. To accomplish this, let A denote, as before, the matrix obtained from W by replacing w_{ij} by zero as in (1.1), and let $Z = I - A$. Then it follows from (1.6) and Corollary 3.2 that

$$\tilde{f}_{ij} = (-1)^{i+j} \frac{\det Z(i|j)}{\det Z} = \frac{(-1)^n \sum_{\mathcal{E}_{ij}} (-1)^{1+c(\mathcal{E}_{ij})} z(\mathcal{E}_{ij})}{\sum_{\mathcal{V}_{ij}} (-1)^{c(\mathcal{V}_{ij})} w(\mathcal{V}_{ij})}, \tag{4.1}$$

where the sums are over all 1-connections $\mathcal{E}_{ij}$ of i to j in $\mathcal{K}$ and all cycle-unions $\mathcal{V}_{ij}$ of $\mathcal{D}(W)$ that do not contain the arc ji.

The following result provides a new expression for the target reproduction number T_{ij} in terms of cycle-unions.

Theorem 4.1. *Let W be an $n \times n$ nonnegative irreducible matrix. For $1 \leqslant i, j \leqslant n$,*

$$T_{ij} = w_{ij}\tilde{f}_{ij} = w_{ij}(-1)^{i+j}\frac{\det Z(i|j)}{\det Z} = \frac{\sum_{\mathcal{U}_{ij}}(-1)^{1+c(\mathcal{U}_{ij})}w(\mathcal{U}_{ij})}{\sum_{\mathcal{V}_{ij}}(-1)^{c(\mathcal{V}_{ij})}w(\mathcal{V}_{ij})}, \tag{4.2}$$

where the sums are over all cycle-unions $\mathcal{U}_{ij}$ and $\mathcal{V}_{ij}$ of $\mathcal{D}(W)$ that do and do not contain the arc ji, respectively.

Proof. The first two expressions for T_{ij} are (1.5) and (1.7). The last expression follows from (4.1), (2.1), (2.3), and expansions (2.4) and (2.5). Note that when $i = j$, the factor y_{ii} is replaced by w_{ii} in (2.5), and that if $\mathcal{U}'$ is a cycle-union of the digraph associated with $W(i|i)$, then

$$w_{ii}(-1)^{c(\mathcal{U}')}w(\mathcal{U}') = (-1)^{c(\mathcal{U}_{ii})-1}w(\mathcal{U}_{ii}) = (-1)^{1+c(\mathcal{U}_{ii})}w(\mathcal{U}_{ii}),$$

where $\mathcal{U}_{ii}$ is the cycle-union of $\mathcal{D}(W)$ obtained by adding the loop ii to $\mathcal{U}'$ and $c(\mathcal{U}_{ii}) = 1 + c(\mathcal{U}')$. □

Example 2. Let $W = \left[\begin{smallmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{smallmatrix}\right]$, and $\mathcal{D}(W)$ be the associated weighted digraph. There are five cycle-unions in $\mathcal{D}(W)$, and their weights are 1, w_{11}, w_{22}, $w_{12}w_{21}$, and $w_{11}w_{22}$, respectively. Theorem 4.1 determines whether the weight of a cycle-union appears in the denominator or numerator of the expression for T_{ij}, and the number of cycles in the cycle-union determines the sign. For instance, $T_{11} = \frac{w_{11}-w_{11}w_{22}}{1-w_{22}-w_{12}w_{21}}$, and $T_{12} = T_{21} = \frac{w_{12}w_{21}}{1-w_{11}-w_{22}+w_{11}w_{22}}$. If we apply the formula for T_{11} to the matrix $W = \left[\begin{smallmatrix} 0.5 & 0.7 \\ 0.7 & 0.5 \end{smallmatrix}\right]$ considered in Example 1 (Section 1), we find that $T_{11} = 0.25/0.01 = 25$. This agrees with the value we obtained in Example 1, but here we did not have to calculate the inverse of a matrix.

Although $T_{12} = T_{21}$ in Example 2, in general T_{ij} does not equal T_{ji}; see, e.g., [11, Section 5.3]. In the following we discuss the cases in which $T_{ij} = T_{ji}$.

It follows from Proposition 2.2 that

$$\det(I - W) = \sum_{\mathcal{U}_{ij}}(-1)^{c(\mathcal{U}_{ij})}w(\mathcal{U}_{ij}) + \sum_{\mathcal{V}_{ij}}(-1)^{c(\mathcal{V}_{ij})}w(\mathcal{V}_{ij}), \tag{4.3}$$

where the sums are over all cycle-unions $\mathcal{U}_{ij}$ and $\mathcal{V}_{ij}$ of $\mathcal{D}(W)$ that do and do not contain the arc ji. Thus, for the fraction in the last term of (4.2), the denominator minus the numerator always equals $\det(I - W)$, which is independent of the choices of i and j. Using this fact, we are able to establish the following criterion for the equality of the target reproduction numbers T_{ij} and T_{ji}.

Theorem 4.2. *Let W be an $n \times n$ nonnegative irreducible matrix such that* $\det(I - W) \neq 0$. *Then $T_{ij} = T_{ji}$ if and only if*

$$\sum_{\tilde{\mathcal{U}}_{ij}} (-1)^{c(\tilde{\mathcal{U}}_{ij})} w(\tilde{\mathcal{U}}_{ij}) = \sum_{\tilde{\mathcal{U}}_{ji}} (-1)^{c(\tilde{\mathcal{U}}_{ji})} w(\tilde{\mathcal{U}}_{ji}), \tag{4.4}$$

where the sums are over all cycle-unions $\tilde{\mathcal{U}}_{ij}$ and $\tilde{\mathcal{U}}_{ji}$ of $\mathcal{D}(W)$ that contain arc ji but not arc ij and that contain arc ij but not arc ji, respectively.

Proof. For convenience let $\lambda_{ij} = \sum_{\tilde{\mathcal{U}}_{ij}} (-1)^{c(\tilde{\mathcal{U}}_{ij})} w(\tilde{\mathcal{U}}_{ij})$ and $\lambda_{ji} = \sum_{\tilde{\mathcal{U}}_{ji}} (-1)^{c(\tilde{\mathcal{U}}_{ji})} w(\tilde{\mathcal{U}}_{ji})$, where the sums are over cycle-unions as given for (4.4). Also let $\lambda = \sum_{\tilde{\mathcal{U}}} (-1)^{c(\tilde{\mathcal{U}})} w(\tilde{\mathcal{U}})$ and $\hat{\lambda} = \sum_{\hat{\mathcal{U}}} (-1)^{c(\hat{\mathcal{U}})} w(\hat{\mathcal{U}})$, where the sums are over all cycle-unions $\tilde{\mathcal{U}}$ that contain both arcs ij and ji, and cycle-unions $\hat{\mathcal{U}}$ that contain neither arc ij nor ji. It follows from Theorem 4.1 that

$$T_{ij} = \frac{-\lambda - \lambda_{ij}}{\hat{\lambda} + \lambda_{ji}} \quad \text{and} \quad T_{ji} = \frac{-\lambda - \lambda_{ji}}{\hat{\lambda} + \lambda_{ij}}. \tag{4.5}$$

Hence $T_{ij} = T_{ji}$ if and only if $\frac{-\lambda-\lambda_{ij}}{\hat{\lambda}+\lambda_{ji}} = \frac{-\lambda-\lambda_{ji}}{\hat{\lambda}+\lambda_{ij}}$ if and only if $(\lambda_{ij} - \lambda_{ji})(\lambda + \hat{\lambda} + \lambda_{ij} + \lambda_{ji}) = (\lambda_{ij} - \lambda_{ji}) \det(I - W) = 0$, where (4.3) is used in the last equality. Since $\det(I - W) \neq 0$, it follows that $T_{ij} = T_{ji}$ if and only if $\lambda_{ij} = \lambda_{ji}$, as required. □

We remark that the assumption $\det(I - W) \neq 0$ is not required for the "if" statement in Theorem 4.2. That is, if (4.4) holds, then $T_{ij} = T_{ji}$ holds by (4.5).

Cycle $\mathcal{C}'$ in a digraph $\mathcal{D}$ is the *reverse* of cycle $\mathcal{C}$ if cycle $\mathcal{C}'$ passes through the same vertices as cycle $\mathcal{C}$ but in the reverse order. A weighted digraph $\mathcal{D}$ is *cycle-balanced* (e.g., see [9] or [11][1]) if for every cycle $\mathcal{C}$ of $\mathcal{D}$, the reverse cycle $\mathcal{C}'$ exists and $w(\mathcal{C}) = w(\mathcal{C}')$. The following result, which is a consequence of Theorem 4.2, first appeared in [11, Theorem 4.1] as a special case of Theorem 4.2 in [11].

Theorem 4.3. *Let W be an $n \times n$ nonnegative irreducible matrix. If $\mathcal{D}(W)$ is cycle-balanced, then $T_{ij} = T_{ji}$ for all $1 \leqslant i, j \leqslant n$.*

Proof. Since $\mathcal{D}(W)$ is cycle-balanced, for every cycle-union $\tilde{\mathcal{U}}_{ij}$ on the left-hand side of (4.4), its reverse $\tilde{\mathcal{U}}_{ji}$ appears on the right-hand side of (4.4) and has the same weight as $\tilde{\mathcal{U}}_{ij}$. Thus (4.4) holds for all i, j, which implies $T_{ij} = T_{ji}$, following the remark after Theorem 4.2. □

Notice that if a weighed digraph contains only cycles of lengths 1 or 2, then it is cycle-balanced. As a special case, any weighted digraph consisting of 2 vertices is cycle-balanced, and thus $T_{12} = T_{21}$ holds in Example 2.

[1] A cycle-balanced digraph is also called weight-balanced in [11].

It has been asked[2] whether the converse of Theorem 4.3 holds. It can be verified, using Theorem 4.2, that the converse of Theorem 4.3 holds for $n = 3$, but the general case for $n \geqslant 4$ remains open.

5. Application to infectious disease control

Consider a heterogeneous population model (formulated as a system of ordinary differential equations) where the individuals are subdivided into n epidemiologically different infected host types. The $n \times n$ nonnegative next-generation matrix $W = [w_{ij}]$ represents the transmission and spread of the infection from one generation to the next [4]. The entry w_{ij} of W is defined as the expected number of new cases that an infected individual of type j causes among the susceptible individuals of type i. As mentioned earlier, the spectral radius often determines whether the disease persists or dies out. The control strategy mentioned in Section 1 targets only a single entry w_{ij} in the matrix W and considers the effect of reducing the transmission of disease from infected individuals of type j to susceptible individuals of type i; and the target reproduction number T_{ij} defined in (1.2) gives a measure of the amount of reduction to ensure the disease would eventually die out (as a result of this particular reduction).

More general control strategies might simultaneously target several entries of W for reduction. For example, vaccinating susceptible individuals of host type i might reduce all the entries in the i-th row of W; or medical treatment to reduce the infectiousness of infected individuals of host type i could reduce all the entries of the i-th column of W. Target reproduction numbers T_{i*} and T_{*i} for such strategies may be defined as follows (see [6,10,11]). In particular, T_{i*} is also called the type reproduction number in [6,10].

If B denotes the matrix obtained from W by replacing all entries w_{ij} in the i-th row of W by zero, let

$$T_{i*} = \sum_{j=1}^{n} w_{ij}(I - B)^{-1}_{ji}. \tag{5.1}$$

And if D denotes the matrix obtained from W by replacing all entries w_{ji} in the i-th column of W by zero, let

$$T_{*i} = \sum_{j=1}^{n} w_{ji}(I - D)^{-1}_{ij}. \tag{5.2}$$

The usefulness of these quantities arises from the following result, a special case of Theorem 2.2 in [11].

Proposition 5.1. *Let W be an $n \times n$ nonnegative irreducible matrix. Assume that $\rho(B) < 1$ and $\rho(D) < 1$, where B and D are as defined above. If W_c denotes the matrix obtained*

[2] Yuan Lou, private communication.

from W *by (a) replacing* w_{ij} *by* w_{ij}/T_{i*} *for* $1 \leqslant j \leqslant n$ *or (b) replacing* w_{ji} *by* w_{ji}/T_{*i} *for* $1 \leqslant j \leqslant n$*, then* $\rho(W_c) = 1$*.*

Biologically, if (a) a proportion more than $1 - 1/T_{i*}$ of the population of type i can be effectively vaccinated or (b) the infectiousness of infected individuals of host type i can be reduced to a proportion less than $1/T_{*i}$, then the disease can be eradicated from all host populations.

It follows readily from definitions (5.1) and (5.2) that T_{i*} and T_{*i}, respectively, are the sums of the weights of the non-trivial closed walks in $\mathcal{D}(W)$ that start and end at vertex i and that contain (a) exactly one arc ending at vertex i or (b) exactly one arc starting at vertex i. Note that a non-trivial walk starting and ending at vertex i contains a unique arc ending at i if and only if it contains a unique arc starting at i. It follows that

$$T_{i*} = T_{*i} = \sum_{\mathcal{Q}_i} w(\mathcal{Q}_i), \tag{5.3}$$

where the sum is over all walks $\mathcal{Q}_i$ in $\mathcal{D}(W)$ that start at vertex i and terminate at vertex i the first time the walk returns to vertex i. Since there is equality in (5.3), we define $T_i = T_{i*} = T_{*i}$. Biologically, relation (5.3) indicates that in order to eradicate the disease from all host populations, the same proportion of transmission reduction is needed when vaccinating susceptible individuals of one type host population or when treating (using medicine, etc.) infectious individuals of the same type host population.

We now derive expressions for this sum based on its combinatorial interpretation.

Theorem 5.2. *Let* $Y = I - W = [y_{ij}]$*, where* $W = [w_{ij}]$ *is an* $n \times n$ *matrix of formal variables* w_{ij}*. Let*

$$T_i = \sum_{\mathcal{Q}_i} w(\mathcal{Q}_i),$$

where the sum is over all walks $\mathcal{Q}_i$ *in* $\mathcal{D}(W)$ *of the type defined above with respect to some given* i*,* $1 \leqslant i \leqslant n$*. Then*

$$T_i = \frac{C_{ii} - \det Y}{C_{ii}} = \frac{1}{C_{ii}} \sum_{j=1}^{n} C_{ij} w_{ij} = \frac{1}{C_{ii}} \sum_{j=1}^{n} w_{ji} C_{ji}, \tag{5.4}$$

where C_{ij} *denotes the cofactor of* y_{ij} *in* $\det Y$*.*

Proof. In Section 3, f_{ii} is defined to be the sum of all closed walks in $\mathcal{D}(W)$ starting and ending at vertex i, with no restriction on the number of times the walk visits vertex i. Recall that f_{ii} includes the contribution of the trivial walk of weight one that consists of vertex i itself and no arcs. Every non-trivial walk enumerated by f_{ii} contains an initial portion that starts at vertex i and continues until it returns to vertex i for the first time; there may be an additional portion that continues on from vertex i and may return to vertex i more times before returning to vertex i for the last time. It follows from this observation that

$$f_{ii} = 1 + T_i f_{ii}. \tag{5.5}$$

(See [8, p. 74] for another application of this relation to stochastic walks on a lattice.) From Theorem 3.1,

$$f_{ii} \det Y = C_{ii}. \tag{5.6}$$

The first part of relation (5.4) follows immediately from (5.5) and (5.6). The last two parts follow from the cofactor expansions of $\det Y$ along its i-th row or its i-th column, respectively, bearing in mind that $y_{ii} = 1 - w_{ii}$. □

We remark that $w_{ij}C_{ij}/C_{ii}$ and $w_{ji}C_{ji}/C_{ii}$ enumerate the contributions to T_{i*} and T_{*i} of those walks $\mathcal{Q}_i$ in which ji is the unique arc with i as its terminal vertex and those in which ij is the unique arc with i as its initial vertex.

Theorem 5.3. *Let W be an $n \times n$ nonnegative irreducible matrix. For $1 \leqslant i \leqslant n$,*

$$T_i = \frac{\sum_{\mathcal{U}_i} (-1)^{1+c(\mathcal{U}_i)} w(\mathcal{U}_i)}{\sum_{\mathcal{V}_i'} (-1)^{c(\mathcal{V}_i')} w(\mathcal{V}_i')}, \tag{5.7}$$

where the sums are over all cycle-unions $\mathcal{U}_i$ of $\mathcal{D}(W)$ in which vertex i is not an isolated vertex and all cycle-unions $\mathcal{V}_i'$ of the digraph associated with $W(i|i)$.

Proof. The expression in the denominator follows upon applying Proposition 2.2 to the cofactor C_{ii} in (5.4). The expression in the numerator follows upon applying Proposition 2.4 to the terms in the first sum in (5.4), bearing in mind that $y_{ij} = -w_{ij}$ when $i \neq j$. □

Note that the vertex i occurs in a cycle of each cycle-union in the numerator in (5.7) but does not occur in any of the cycle-unions in the denominator.

Acknowledgements

This research was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) through a Discovery Grant (PvdD) and by the University of Central Florida through a start-up fund (ZS).

References

[1] F. Brauer, P. van den Driessche, J. Wu (Eds.), Mathematical Epidemiology, Lecture Notes in Math., vol. 1945, Springer, Berlin, 2008.
[2] R.A. Brualdi, D. Cvetković, A Combinatorial Approach to Matrix Theory and Its Applications, CRC Press, Boca Raton, 2009.
[3] H. Caswell, Matrix Population Models: Construction, Analysis, and Interpretation, 2nd edition, Sinauer Associates, Sunderland, 2001.
[4] O. Diekmann, H. Heesterbeek, T. Britton, Mathematical Tools for Understanding Infectious Disease Dynamics, Princeton University Press, Princeton, NJ, 2013.
[5] I. Gelfand, Normierte ringe, Rec. Math. [Mat. Sbornik] N.S. 9 (1941) 3–24.
[6] J.A.P. Heesterbeek, M.G. Roberts, The type-reproduction number T in models for infectious disease control, Math. Biosci. 206 (2007) 3–10.
[7] R.A. Horn, C.R. Johnson, Matrix Analysis, 2nd edition, Cambridge University Press, Cambridge, UK, 2013.
[8] P.W. Kasteleyn, Graph theory and crystal physics, in: F. Harary (Ed.), Graph Theory and Theoretical Physics, Academic Press, New York, 1967, pp. 43–110.
[9] L. Yu Kolotilina, Lower bounds for the Perron root of a nonnegative matrix, Linear Algebra Appl. 180 (1993) 133–151.
[10] M.G. Roberts, J.A.P. Heesterbeek, A new method for estimating the effort required to control an infectious disease, Proc. R. Soc. Lond. Ser. B 270 (2003) 1359–1364.
[11] Z. Shuai, J.A.P. Heesterbeek, P. van den Driessche, Extending the type reproduction number to infectious disease control targeting contacts between types, J. Math. Biol. 67 (2013) 1067–1082.
[12] W.T. Tutte, On elementary calculus and the Good formula, J. Combin. Theory Ser. B 18 (1975) 97–137.
[13] D.B. West, Introduction to Graph Theory, Prentice Hall, Upper Saddle River, NJ, 1996.