A basis for the ensemble of walks on digraphs with non-commuting edge weights

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Abstract

We demonstrate that any walk on a directed graph $G$ can be decomposed into an underlying simple path and a nested collection of bare cycles, where simple paths and bare cycles are open and closed walks that are forbidden from visiting any vertex more than once. We define a convention for the nesting structure of the bare cycles that makes this path decomposition unique. In contrast to existing decompositions based on the cycle space of a graph, our walk decomposition natively respects the ordering of the edges in a walk, allowing a natural extension to walks on weighted directed graphs with non-commutative edge weights. We thus show that the sum of all walks on $G$ can be recast as a finite sum over simple paths only. We provide two applications of this result: firstly, we derive a continued-fraction expression for the walk-generating matrix of an arbitrary directed graph, and secondly, we obtain an expression relating the communicability and subgraph centrality of any vertex of $G$ to the communicability and subgraph centrality of vertices in arbitrarily chosen subgraphs of $G$.

Keywords: directed graph, quiver, path algebra, non-commutative algebra, walk-generating function, subgraph centrality, communicability

2010 MSC: 05C38, 05C20, 05C22

1. Introduction

Many problems and solutions from the fields of computer science, engineering, mathematics, and physics are naturally formulated in terms of walks on directed graphs. In this article, we present a result on the fundamental structure of such walks. In particular, we show that every walk on a directed graph can be decomposed into a simple path and a collection of nested bare cycles, and that this decomposition can be done uniquely. Further, this decomposition can be performed in a manner that natively respects the ordering of edges in the original walk. We show that the sum of all walks on a weighted directed graph can consequently be written as a finite sum over appropriately-weighted simple paths, and that this result is valid whether the edge weights commute with one another or not.

This article is organized as follows. In Section 2, we present a brief summary of the notation and terminology used throughout the article. In Section 3, we present and prove the path decomposition of a walk, which is the main result of this work. In Section 4, we show that the infinite sum of all walks on a directed graph can be rewritten as a finite sum over simple paths; this is a natural consequence of the path decomposition result of Section 3. In Sections 5 and 6, we present examples of the application of our results by obtaining a continued-fraction representation of the walk-generating function of a directed graph, and an expression linking the communicabilities and subgraph centralities of vertices in different parts of a graph.

2. Notation and terminology

Basic notation. In order to establish our notation and terminology, we begin by summarizing some concepts in graph theory. A directed graph $G$ is a pair $(\mathcal{V}, \mathcal{E})$ comprising a set $\mathcal{V}$ of vertices and a set $\mathcal{E}$ of directed edges among these...
vertices. In this article we consider only finite graphs; i.e. the sets \( G \) and \( E \) are finite. We consider the case where \( G \)
may contain self-loops, but not multiple edges. However, the latter restriction is solely for the purpose of notational
clarity, and all of our results can be straightforwardly extended to cases where \( G \) does contain multiple edges. We
will denote the vertices of \( G \) by Greek letters \( \alpha, \beta, \ldots \), and the graph obtained by deleting vertices \( \alpha, \beta, \ldots \) from \( G \) by
\( G \setminus \{ \alpha, \beta, \ldots \} \). We define maps \( h : E \to V \) and \( t : E \to V \) such that for a given edge \( e \in E \) that starts on \( \mu \) and ends on \( \nu \), \( h(e) \) is its head \( \mu \) and \( t(e) \) is its tail \( \nu \). This allows an edge \( e \) to be uniquely denoted by \( (h(e)t(e)) \).

Walks. A walk \( w \) of length \( n \geq 1 \) from \( \alpha \) to \( \omega \) on \( G \) is a sequence \((\alpha_1 \mu_2) (\mu_2 \mu_3) \cdots (\mu_n \omega)\) of \( n \) contiguous edges. We will
equivalently denote \( w \) by its vertex string \((\alpha \mu_2 \mu_3 \cdots \mu_\omega)\). We define the head and tail vertices of \( w \) to be \( h(w) = \alpha \)
and \( t(w) = \omega \), respectively; the remaining vertices \( \mu_2, \ldots, \mu_n \) are the internal vertices of \( w \). In addition to walks of
positive length, we define for every vertex \( \mu \in V \) a trivial walk of length zero off \( \mu \), which we will denote by \((\mu)\). When convenient, these trivial walks may be inserted into the edge sequence of a longer walk: thus \((\alpha \mu_2)(\mu_2 \omega)(\omega)\) represent the same walk of length 2 from \( \alpha \) to \( \omega \). A walk \( w \) that satisfies \( h(w) = t(w) \) will be
referred to as a closed walk. The set of all walks from \( \alpha \) to \( \omega \) on \( G \) will be denoted by \( W_{G, \alpha \omega} \).

Paths. The terms path and simple path will be used interchangeably to refer to a walk whose vertices are all distinct.
The set of all paths from \( \alpha \) to \( \omega \) on \( G \) will be denoted by \( P_{G, \alpha \omega} \). Since \( G \) has a finite number of vertices, the set \( P_{G, \alpha \omega} \)
is finite.

Cycles. A cycle off \( \alpha \) is a walk \( w \) that starts and ends on \( \alpha \), but does not revisit \( \alpha \) in between. Every cycle is therefore
a closed walk, but not every closed walk is a cycle. A cycle will be called a bare cycle if it visits each of its internal
vertices only once, or a compound cycle otherwise. A bare cycle is necessarily a self-loop if it is of length 1, a
backtrack if it is of length 2, and a triangle, square, etc. if it is of length 3, 4, … The set of all cycles off \( \alpha \) on \( G \)
will be denoted by \( C_{G, \alpha} \). The set of bare cycles off \( \alpha \) on \( G \) will be denoted by \( C_{G, \alpha}^b \); this set is finite.

Concatenating walks. For any two walks \( W_1 \) and \( W_2 \) such that \( h(W_2) = t(W_1) \), their concatenation \( W_1 W_2 \) is the walk
obtained by concatenating their edge sequences. It is convenient to extend this concept to sets of walks: given two
sets \( W_1 \) and \( W_2 \) such that \( h(W_2) = t(W_1) \) for every \( w_1 \in W_1 \) and \( w_2 \in W_2 \), the set \( W_1 \circ W_2 \) is defined as

\[
W_1 \circ W_2 = \{ w_1 w_2 : w_1 \in W_1, w_2 \in W_2 \}.
\]

Note that a set of closed walks may be concatenated with itself. Given a set \( W \) of closed walks off \( \mu \), we define
\( W^0 = \{ (\mu) \} \) and \( W^i = W^{i-1} \circ W \) for \( i \geq 1 \). Finally, we define the Kleene star \( W^* \) of a set \( W \) of closed walks to be the
set of walks formed by concatenating any number of elements of \( W \):

\[
W^* = \bigcup_{i=0}^{\infty} W^i.
\]

Nesting walks. Let \( w_1 = (\beta_1 \mu_2 \cdots \mu_n \beta) \) be a closed walk of length \( m \) off \( \beta \), and let \( w_2 = (\alpha \mu_2 \cdots \beta \cdots \omega) \) be a
walk of length \( n \) that has \( \beta \) as exactly one internal vertex. Then the walk of length \( m + n \) with vertex sequence
\( (\alpha \mu_2 \cdots \beta \mu_2 \cdots \mu_n \beta \cdots \omega) \) will be said to consist of \( w_1 \) nested into \( w_2 \). This walk is formed by making the replacement
\( \beta \to w_1 \) in the vertex string of \( w_2 \).

The walk algebra \( KG \). Let \( K \) be a field. Then the walk algebra (also called the path algebra) \( KG \) is the vector space
over \( K \) with basis \( B_{KG} \) given by the set of all walks on \( G \). Note that \( KG \) is a finite-dimensional vector space if and
only if \( G \) contains no cycles. Multiplication in \( KG \) is given by the associative operation

\[
w_1 \cdot w_2 = \begin{cases} w_1 w_2 & \text{if } h(w_2) = t(w_1), \\ 0 & \text{otherwise.} \end{cases}
\]
3. Decomposing the set of walks on $G$

In this section we present a universal result on the structure of walks on graphs. Specifically, we show that any walk on a graph can be decomposed into a simple path plus a collection of nested bare cycles, and that this decomposition can be done uniquely. The simple path and nested bare cycles then form a unique fundamental representation of the original walk, analogous to the way in which a prime factorization forms a unique fundamental representation of an integer. This result holds for both directed and undirected graphs, either with or without self-loops, and may be extended to treat the case where $G$ contains multiple edges.

**Theorem 3.1.** Every walk on an arbitrary directed graph $G$ can be decomposed into a simple path $p$ on $G$ and a collection of nested bare cycles off the vertices of $p$. This decomposition is unique if a consistent convention for the nesting structure of the bare cycles is chosen. The basis for the walk algebra $K_G$ can therefore be written as

$$B_{K_G} = \bigcup_{\alpha, \omega} \bigcup_{(\alpha \gamma_2 - \omega \gamma_2) \in P_{G, \omega \gamma_2}} \tilde{C}_{G, \alpha} \circ \{(\alpha \gamma_2)\} \circ \tilde{C}_{G, (\alpha \gamma_2 \gamma_2 \omega)\gamma_2} \circ \cdots \circ \{(\nu \gamma_2 \omega)\} \circ \tilde{C}_{G, (\alpha \nu \omega)\gamma_2}$$

(4a)

where

$$\tilde{C}_{G, \alpha} = \bigcup_{(\alpha \eta_2 - \alpha \eta_2) \in C_{G, \alpha}} \{(\alpha \eta_2)\} \circ \tilde{C}_{G, (\alpha \eta_2 \eta_2 \omega)\eta_2} \circ \cdots \circ \{(\nu \eta_2 \omega)\} \circ \tilde{C}_{G, (\alpha \nu \omega)\eta_2}$$

(4b)

**Proof.** This result follows directly from Lemmas 3.2–3.4.

**Lemma 3.2.** An arbitrary walk of length $n$ from $a$ to $\omega$ on $G$ can be decomposed into a path $p$ of length $\ell \leq n$ on $G$ and a collection of closed walks off the vertices of $p$. This decomposition is unique if a consistent convention for the structure of the closed walks is chosen. The set of all walks from $a$ to $\omega$ on $G$ can therefore be written as

$$W_{G, \omega \gamma_2} = \bigcup_{(\alpha \gamma_2 - \omega \gamma_2) \in P_{G, \omega \gamma_2}} \{(\alpha \gamma_2)\} \circ W_{G, (\alpha \gamma_2 \gamma_2 \omega)\gamma_2} \circ \cdots \circ \{(\nu \gamma_2 \omega)\} \circ W_{G, (\alpha \nu \omega)\gamma_2}.$$  

(5)

**Proof.** We first describe how an arbitrary walk $w$ can be decomposed into a path plus a collection of closed walks. We then show that although this decomposition is not unique in every case, it can be made unique by choosing a consistent convention for the structure of the closed walks.

Let $(\alpha \eta_2 \cdots \eta_n \omega)$ be the string of vertices visited by $w$, and let $S$ be a set of substrings of this string such that (i) each substring in $S$ has the form $(\eta_1, \cdots, \eta_l)$; (ii) the substrings in $S$ do not overlap; (iii) no further substrings satisfying (i) can be added to $S$ without violating (ii). Then the set $S$ contains all of the closed walks present in $w$. Further, the vertex string obtained from $w$ by making the replacement $\eta_1 \cdots \eta_l \rightarrow \eta_l$ for each element of $S$ contains no repeated vertices, and so defines a path $p$. The pair $(p, S)$ will be referred to as a path decomposition of $w$.

It is always possible to identify a (possibly empty) set $S$ that satisfies conditions (i)-(iii) above, and so it is always possible to find a path decomposition of $w$. However, the path decomposition of $w$ is not always unique: specifically, multiple possibilities for $(p, S)$ exist whenever $w$ contains a substring of the form $(\eta_1, \cdots, \eta_l)$. In this case either $(\eta_1, \cdots, \eta_l)$ or $(\eta_1, \cdots, \eta_l)$ (but not both, by condition (ii)) may be included in $S$. As a simple example, consider the walk $w = (13212)$, which may be decomposed either as $p = (12)$, $S = \{1321\}$, or $p' = (132), S' = \{212\}$. In order to choose between the different decompositions in such cases we adopt the convention that whenever $w$ contains overlapping substrings, the leftmost one should be included in $S$. Equivalently, we choose the canonical decomposition to be the one that places the closed walks as early in the path as possible, so that $w = (13212)$ is decomposed as $p = (12), S = \{1321\}$.

This convention assigns to every walk a unique path decomposition consisting of a path $p = (\alpha \nu_2 \cdots \nu_\omega)$ and a collection $S = \{w_i\}$ of closed walks off the vertices of $p$, with the restriction that $w_i$ does not visit any of the vertices $\alpha, \cdots, \nu_{i-1}$. This restriction follows from the observation that any decomposition that contains a closed walk $w_i$ that visits an earlier vertex $\nu_j$ is necessarily non-canonical, since it can be restructured by lengthening $w_j$ and shortening $w_i$.

Since every walk from $a$ to $\omega$ admits a unique path decomposition, the walk set $W_{G, \omega \gamma_2}$ consists of the union of all possible path decompositions: i.e. the set of all possible combinations of a path from $a$ to $\omega$ and a collection of restricted closed walks. This proves Lemma 3.2.
Lemma 3.3. An arbitrary closed walk \( w \) off \( \alpha \) on \( \mathcal{G} \) can be decomposed into a sequence of \( n = 0, 1, 2, \ldots \) cycles off \( \alpha \). The set of all closed walks off \( \alpha \) on \( \mathcal{G} \) can therefore be written as \( \mathcal{W}_{G,\alpha} = \mathcal{C}_{G,\alpha}^* \).

**Proof.** We define the trivial walk \((\alpha)\) to consist of zero cycles. Otherwise, let \((\alpha_{n-1} \cdots \alpha_0 \alpha)\) be the string of vertices visited by \( w \). In addition to the endpoints, let \( \alpha \) appear \( n \geq 0 \) times in the interior of the string. Then \( w \) consists of \( n + 1 \) cycles, which are identified by splitting the vertex string at each internal appearance of \( \alpha \). This proves Lemma 3.3.

Lemma 3.4. An arbitrary cycle of length \( n \) off \( \alpha \) on \( \mathcal{G} \) can be decomposed into a bare cycle \( c \) of length \( m \leq n \) off \( \alpha \), plus a collection of closed walks off the internal vertices of \( c \). This decomposition is unique if a consistent convention for the structure of the closed walks is chosen. The set of all cycles off \( \alpha \) on \( \mathcal{G} \) can therefore be written as

\[
\mathcal{C}_{G,\alpha}^* = \bigcup_{(\alpha_0 \alpha_1 \cdots \alpha_{n-1} \alpha_0) \in \mathcal{C}_{G,\alpha}} \left( (\alpha_n \eta_1) \circ \mathcal{C}_{G[\alpha_0, \eta_2]}^* \circ \cdots \circ \mathcal{C}_{G[\alpha_{n-2}, \eta_{n-1}, \eta_2]}^* \circ \{(\eta_n \alpha)\}. \right)
\]

where the result of Lemma 3.3 has been used to write \( \mathcal{C}_{G,\alpha}^* \) for the walk set \( \mathcal{W}_{G,\alpha} \).

**Proof.** A cycle \( \tilde{c} \) off \( \alpha \) can be decomposed into a bare cycle \( c \) off \( \alpha \) and a collection of closed walks \( S = \{w_i\} \) by an essentially identical procedure to that described in the proof of Lemma 3.2. The only differences are that the vertex string obtained from \( \tilde{c} \) by making the replacement \( \eta_i \cdots \eta_j \rightarrow \eta_i \) for each element of \( S \) defines not a path, but rather a bare cycle \( c \), and that the closed walks contained in \( S \) do not originate off the head or tail vertices of \( c \), but only off the internal vertices. The pair \((c, S)\) will be referred to as a cycle decomposition of \( \tilde{c} \).

In order to make the cycle decomposition unique, we adopt the convention that closed walks should be placed as early as possible in the bare cycle. Then \((c, S)\) consists of a bare cycle \( c = (\alpha \eta_1 \cdots \eta_{n-1} \alpha) \) and a collection of closed walks \( S = \{w_i\} \) off the internal vertices of \( c \), restricted such that \( w_i \) does not visit any of the vertices \( \alpha, \ldots, \eta_{i-1} \).

Since every closed walk admits a unique cycle decomposition, the walk set \( \mathcal{W}_{G,\alpha} \) consists of the union of all possible cycle decompositions: i.e. the set of all possible combinations of a bare cycle off \( \alpha \) and a collection of restricted closed walks. This proves Lemma 3.4.

It is important to note that although the decomposition we present here is similar in spirit to the prime factorization theorem for integers, the base objects of our decomposition — i.e. simple paths and bare cycles — are not the same as the prime cycles that are previously known in graph theory [1]. We note two important properties of the bare cycles: firstly, any finite graph contains only a finite number of bare cycles; and secondly, a bare cycle cannot be built from shorter cycles by concatenation or nesting. Prime cycles fulfill neither of these properties. In particular, Lemma 3.4 implies:

**Proposition 3.5.** Let \( p \) be a prime cycle on \( \mathcal{G} \). Then \( p \) may be decomposed into a collection of bare cycles through concatenation and nesting. This decomposition is unique if a consistent convention for the nesting structure of the bare cycles is chosen.

In this sense, bare cycles are more fundamental than prime cycles.

4. Converting the sum of all walks on a graph to a sum of simple paths

The results of Section 3 give a detailed understanding of the structure of the set of walks on \( \mathcal{G} \). In this section we use this result to recast the sum of all walks linking a given pair of vertices on \( \mathcal{G} \) into a compact form consisting of a finite number of terms. Specifically, we separate the sum over the elements of the walk set \( \mathcal{W}_{G,\alpha} \) into a sum over the elements of the path set \( \mathcal{P}_{G,\alpha} \) and a collection of sums over closed walks, and formally resum each of the sums of closed walks into a recursive closed form. This procedure allows the sum of all walks on \( \mathcal{G} \) to be rewritten as a sum over simple paths only, so long as each path is appropriately modified to include all possible closed walks off each vertex it visits.

**Theorem 4.1.** Let \( \Sigma_{G,\alpha} \) denote the sum of all walks from \( \alpha \) to \( \omega \) on \( \mathcal{G} \). Then

\[
\Sigma_{G,\alpha} = \sum_{\mathcal{P}_{G,\alpha}} \sum_{\mathcal{C}_{G,\alpha}} (\alpha)'_G (\alpha \omega) (\alpha \omega)'_G (\alpha \omega)'_G \cdots (\alpha \omega)'_G (\alpha \omega)'_G (\alpha \omega)'_G (\alpha \omega)'_G \cdots (\alpha \omega)'_G (\alpha \omega)'_G (\alpha \omega)'_G (\alpha \omega)'_G ,
\]

(7)
where \( (\alpha)'_G \) denotes the dressed vertex \( \alpha \) on \( G \), defined by

\[
(\alpha)'_G \equiv \sum_{\omega \in \mathcal{G}} (\alpha)(\alpha_1\eta_2)(\eta_2\eta_3)\cdots(\eta_m\alpha)(\alpha), \tag{8a}
\]

\[
= \left[(\alpha) - \sum_{\ell \in \mathcal{G}} (\alpha)(\alpha_\ell_2)(\mu_2)(\mu_2\mu_3)\cdots(\mu_m)G_{[\alpha_\ell_\cdots \mu_{m-1}]}(\mu_m\alpha)(\alpha)\right]^{-1}, \tag{8b}
\]

where \( [(\alpha) - \sum_{\mathcal{G}} (\alpha)(\alpha_\mu_2)\cdots(\alpha)]^{-1} \) represents the formal power series \( \sum_{p=0}^{\infty} \left[ \sum_{\mathcal{G}} (\alpha)(\alpha_\mu_2)\cdots(\alpha) \right]^p \).

**Proof.** We rewrite the first equality of Theorem 4.4 as

\[
\sum_{\omega \in \mathcal{G}} (\alpha)(\alpha_1\eta_2)(\eta_2\eta_3)\cdots(\eta_m\alpha)(\alpha) \equiv \sum_{\omega \in \mathcal{G}} (\alpha)(\alpha_\eta_2)(\eta_2\eta_3)\cdots(\eta_m\alpha)(\alpha) \tag{9}
\]

In this form the result follows from the result of Lemma 3.2 by starting from the decomposition of \( W_{G,\text{iso}} \) presented in Eq. (5), summing over set elements and using Eq. (8a) to define a dressed vertex, Eq. (9) is obtained immediately.

Secondly, we show that the dressed vertex \( (\alpha)' G \) has the recursive closed-form expression of Eq. (8b). Starting from the result of Lemma 3.3 and summing over set elements yields

\[
(\alpha)'_G = \sum_{n=0}^{\infty} \sum_{\ell \in \mathcal{G}} (\alpha)(\alpha_\ell_1\eta_2)(\eta_2\eta_3)\cdots(\eta_m\alpha)(\alpha), \tag{10a}
\]

\[
= \sum_{n=0}^{\infty} \left[ \sum_{\ell \in \mathcal{G}} (\alpha)(\alpha_\ell_1\eta_2) \left( \sum_{w \in \mathcal{G}_{[\alpha_\ell_1\eta_2]}} w \right) (\eta_3\eta_3)\cdots(\eta_m\alpha)(\alpha) \right]^{n}, \tag{10b}
\]

where the second equality follows from the result of Lemma 3.3. By using Eq. (8a) to define a dressed vertex and converting the infinite sum into a formal closed form, Equation (8b) is obtained.

**Definition 4.2.** A weighted graph \( (G, f) \) is a graph \( G \) paired with a weight function \( f \) that assigns a weight \( f(e) \) to each edge \( e \) of \( G \). In this article we consider the case where the edge weights assigned by \( f \) are matrices over \( \mathbb{C} \), the field of complex numbers. Specifically, we associate with each vertex \( \mu \) in \( G \) a complex vector space \( V_\mu = \mathbb{C}^{d_\mu} \) of dimension \( d_\mu \). Then \( f(\mu
u) \) is a \( d_\nu \times d_\mu \) matrix that represents a linear map from \( V_\mu \) to \( V_\nu \). We extend the domain of \( f \) to the walk algebra \( KG \) by setting \( f(\mu) = 1 \) for every trivial walk \( (\mu) \), where \( I \) is the identity matrix of dimension \( d_\mu \).

\[
f[1,e] = f[e], \tag{11a}
\]

\[
f[w_1 + w_2] = f[w_1] + f[w_2] \tag{11b}
\]

for edges \( e \) and \( e \), satisfying \( h(e) = t(e) \), and

for walks \( w_1, w_2 \) satisfying \( h(w) = h(w) \) and \( t(w) = t(w) \). Note that the ordering of the weights when two edges are concatenated is suitable for the matrix multiplications to be carried out.

**Corollary 4.3.** Provided the required inverses exist, the weight of the sum of all walks from \( \alpha \) to \( \omega \) on a weighted graph \( (G, f) \) is given by

\[
f[\Sigma_{G,\text{iso}}] = \sum_{\omega \in \mathcal{G}} F_{G_\alpha}[\alpha \cdots \omega_\alpha] w_{\omega_2} \cdots F_{G_\alpha}[\alpha_\alpha] w_{\alpha_1} F_{G_\alpha}, \tag{12}
\]

where \( w_{\omega_1} \in \mathbb{C}^{d_\omega \times d_\mu} \) is the weight of the edge \( (\mu, \nu) \), and

\[
F_{G_\alpha} \equiv f(\alpha)'_G = \left[1 - \sum_{\ell \in \mathcal{G}} w_{\ell_\mu} F_{G_\alpha}[\alpha_\ell_\cdots \mu_{m-1}] w_{\mu_{m-1}} \cdots F_{G_\alpha}[\alpha_{m-1}] w_{\mu_{m-1}} \right]^{-1}, \tag{13}
\]

where \( w^{-1} \) represents the matrix inverse of \( w \).
**Proof.** This Corollary follows from applying the weight function to the right hand side of Eq. (7) and to Eq. (8b), together with the properties of the weight function Eq. (11).

The result of Corollary 4.3 has been used to develop a new approach to matrix functions [7]. Here we give two alternative examples of how the result of Corollary 4.3 can be applied. Firstly, we compute the walk-generating functions of arbitrarily chosen subgraphs of \( \tilde{G} \).

Let \( G \) be a graph on \( n \) vertices with adjacency matrix \( A \). Then the walk-generating matrix \( G \) of \( G \) is a formal power series in \( z \) defined by \([3]\)

\[
G_G(z) = \sum_{\ell=0}^{\infty} z^\ell A^\ell = (1 - zA)^{-1},
\]

(14)

where \( I \) is the identity matrix of dimension \( n \). The individual entries \( g_{G,i,j}(z) = (G(z))_{ij} \) of the walk-generating matrix are called the walk-generating functions of \( G \).

Let \( \{\mathcal{V}^{(i)}\} \) be a partition of the vertex set of \( G \), and let \( G^{(i)} \) be the graph obtained from \( G \) by deleting all vertices not in \( \mathcal{V}^{(i)} \), and let \( A_i \) be the corresponding adjacency matrix. Note that \( A_i \) is a submatrix of \( A \), and can therefore be written as \( A_i = R_i A R_i^T \), where \( R_i \) and \( R_i^T \) are zero-one gather and scatter matrices respectively. The graph \( G^{(i)} \) may be disconnected, since there is no restriction on how the sets \( \mathcal{V}^{(i)} \) are chosen. Let \( \tilde{G} \) be the \( k \)-vertex graph obtained from \( G \) by merging together all vertices belonging to \( \mathcal{V}^{(i)} \), for each \( i \). We will denote the vertices of \( \tilde{G} \) by Roman letters: i.e. the vertex of \( \tilde{G} \) produced by merging all the vertices in \( \mathcal{V}^{(i)} \) is denoted \( i \).

Finally, let \( G^{(j)} \) for \( j \neq i \) be the graph obtained from \( G \) by deleting all vertices of \( G \) that do not belong to either \( \mathcal{V}^{(i)} \) or \( \mathcal{V}^{(j)} \), and deleting all edges of the resultant graph except for those that lead from a vertex of \( \mathcal{V}^{(i)} \) to a vertex of \( \mathcal{V}^{(j)} \). We define the adjacency matrix \( A_{ij} \) of \( G^{(i)} \) to be \( A_{ij} = R_i A R_j^T \). The ensembles of graphs \( \{G^{(i)}\} \) and \( \{G^{(j)}\} \) respectively encode the intra- and inter-vertex-set structure of \( G \).

**Proposition 5.1.** Let \( G_{\tilde{G},i,j}(z) \) be the walk-generating matrix for all the walks with heads in \( \mathcal{V}^{(i)} \) and tails in \( \mathcal{V}^{(j)} \). Then

\[
G_{\tilde{G},i,j}(z) = \sum_{P_{\tilde{G},i,j}} z^\ell G_{\tilde{G},(i \ldots p_1;i)j}(z) A_{j p_1} \cdots G_{\tilde{G},(i \ldots p_{\ell};2)q_2}(z) A_{q_2} \cdots A_{q_m} G_{\tilde{G},(i \ldots q_m;i)q_m}(z),
\]

(15a)

where \( \ell \) is the length of the path \( (i p_2 \ldots p_1; j) \in P_{\tilde{G},i,j} \) and

\[
G_{\tilde{G},i,j}(z) = \left[ 1 - \sum_{C_{\tilde{G}}} z^m A_{q_m} G_{\tilde{G},(i \ldots q_{m-1};q_m)q_m}(z) \cdots A_{q_2} G_{\tilde{G},(i \ldots 2;q_2)q_2}(z) A_{q_2} \cdots A_{q_m} G_{\tilde{G},(i \ldots q_m;i)q_m}(z) \right]^{-1},
\]

(15b)

where \( m \) is the length of the bare cycle \( (i q_1 \ldots q_m i) \in C_{\tilde{G},i,j} \).

**Proof.** Let \( f \) be a weight function on \( \tilde{G} \) that assigns the matrix \( zA_i \) to the loop \( (ii) \) and the matrix \( zA_{ij} \) to the edge \( (ij) \). Then \( G_{\tilde{G},i,j}(z) \) is equal to the sum of the weights of all walks from \( i \) to \( j \) on \( \tilde{G} \). By using Corollary 4.3 to recast the sum of walk weights to a sum of paths, Eq. (15) are obtained directly.

Note that if each of the vertex sets \( \mathcal{V}^{(i)} \) contains only a single vertex, then \( \tilde{G} \equiv G \) and Proposition 5.1 yields the walk-generating functions.
Proposition 5.2. The walk-generating function $g_{\mathcal{G}\cdot_{a,w}}(z) = (G_{\mathcal{G}}(z))_{a,w}$ is given by
\[
g_{\mathcal{G}\cdot_{a,w}}(z) = \sum_{P_{\mathcal{G}\cdot_{a,w}}} z^\ell g_{\mathcal{G}\cdot_{1,\ldots,\ell},a_{\omega}}(z) \cdots g_{\mathcal{G}\cdot_{1,\ldots,\ell},w}(z) g_{\mathcal{G}\cdot_{a,\omega}}(z),
\]
where $\ell$ is the length of the path $(a_{\nu}, \ldots, w_{\omega}) \in P_{\mathcal{G}\cdot_{a,w}}$, and
\[
g_{\mathcal{G}\cdot_{a,\omega}}(z) = \left[1 - \sum_{c_{\mathcal{G}\cdot_{a,\omega}}} z^m g_{\mathcal{G}\cdot_{1,\ldots,\mu},a_{\omega}}(z) \cdots g_{\mathcal{G}\cdot_{1,\ldots,\mu},w}(z) \right]^{-1},
\]
where $m$ is the length of the bare cycle $(a_{\mu}, \ldots, a_{\mu}) \in C_{\mathcal{G}\cdot_{a,\omega}}$.

Example 5.3. Let $\mathcal{G}$ be the directed graph defined by the adjacency matrix
\[
A = \begin{pmatrix}
1 & 1 & 1 & 0 \\
1 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}.
\]

Firstly we illustrate Proposition 5.1. Choosing $\mathcal{V}^{(1)} = \{1, 2\}$ and $\mathcal{V}^{(2)} = \{3, 4\}$, we find
\[
A_1 = \begin{pmatrix}
1 & 1 \\
1 & 1
\end{pmatrix}, \quad A_2 = \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}, \quad A_{12} = \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}, \quad A_{21} = \begin{pmatrix}
0 & 1 \\
0 & 0
\end{pmatrix}.
\]

Then the graph $\tilde{\mathcal{G}}$ is the complete graph on two vertices with a self-loop on each vertex. As an example of Proposition 5.2, we find that $G_{\tilde{\mathcal{G}}\cdot_{1,1}}$ is given by
\[
G_{\tilde{\mathcal{G}}\cdot_{1,1}} = \left[1 - zA_1 - z^2A_{12}[1 - zA_{12}^{-1}A_{21}] \right]^{-1} = \frac{1}{z^3 - z^2 - 2z + 1} \begin{pmatrix}
(z-1)^2(z+1) & z^2 - z^3 & (z-1)^2(z+1)
\end{pmatrix} = \begin{pmatrix}
G_{\tilde{\mathcal{G}}\cdot_{1,1}}(z) & G_{\tilde{\mathcal{G}}\cdot_{1,2}}(z) & G_{\tilde{\mathcal{G}}\cdot_{1,3}}(z)
\end{pmatrix}.
\]

Secondly we compute the walk-generating function $g_{\tilde{\mathcal{G}}\cdot_{1,2}}(z)$ using Proposition 5.2. The set of paths from vertex 1 to vertex 2 on $\mathcal{G}$ is $P_{\mathcal{G}\cdot_{1,2}} = \{(12), (132)\}$, so that
\[
g_{\mathcal{G}\cdot_{1,2}}(z) = z g_{\mathcal{G}\cdot_{1,1}}(z) g_{\mathcal{G}\cdot_{1,2,2}}(z) + z^2 g_{\mathcal{G}\cdot_{1,1}}(z) g_{\mathcal{G}\cdot_{1,3,3}}(z) g_{\mathcal{G}\cdot_{1,3,2,2}}(z).
\]

Using the fact that $C_{\tilde{\mathcal{G}}\cdot_{1,1}} = \{(11), (121), (1321)\}$, we find
\[
g_{\mathcal{G}\cdot_{1,1}}(z) = (1 - z - z^2) g_{\mathcal{G}\cdot_{1,1,2,2}}(z) + z^3 g_{\mathcal{G}\cdot_{1,1,3,3}}(z) g_{\mathcal{G}\cdot_{1,3,2}}(z) g_{\mathcal{G}\cdot_{1,3,3}}(z) g_{\mathcal{G}\cdot_{1,3,2,2}}(z),
\]

and
\[
g_{\mathcal{G}\cdot_{1,2,2}} = (1 - z)^{-1}, \quad g_{\mathcal{G}\cdot_{1,3,3}} = (1 - z^2) g_{\mathcal{G}\cdot_{1,3,4,4}}^{-1}, \quad g_{\mathcal{G}\cdot_{1,3,2,2}} = (1 - z)^{-1} \quad \text{and} \quad g_{\mathcal{G}\cdot_{1,3,4,4}} = 1.
\]

Assembling these expressions we find that
\[
g_{\mathcal{G}\cdot_{1,2}}(z) = z \left(1 - z - z^2(1 - z)^{-1} - z^3(1 - z^2)^{-1}(1 - z)^{-1}\right) (1 - z)^{-1}
\]
\[
+ z^2 \left(1 - z - z^2(1 - z)^{-1} - z^3(1 - z^2)^{-1}(1 - z)^{-1}\right)^{-1} (1 - z)^{-1} \left(1 - z^2\right)^{-1} (1 - z)^{-1},
\]
\[
= z + 3z^2 + 6z^3 + 14z^4 + 31z^5 + \cdots.
\]

which agrees with the result obtained in Eq. (19).

6. Communicability and Subgraph Centrality

Two quantities commonly used to describe the pattern of connectivity within a graph are the communicability and the subgraph centrality [3, 4]. Given a graph $\mathcal{G}$, the communicability of a pair of vertices $\alpha$, $\omega$ of $\mathcal{G}$ is defined as
\[
Co_{\mathcal{G}\cdot_{a,\omega}} = (\exp(A))_{a,\omega},
\]
while the subgraph centrality of a vertex \( \alpha \) is

\[
C_{S_{G,\alpha}} = (\exp A)_{\alpha\alpha},
\]

(23b)

These quantities provide important insights into the connectivity of complex networks. Here we provide an expression relating the communicability and subgraph centrality of any vertex of \( G \) to the communicability and subgraph centrality of vertices in arbitrarily chosen subgraphs of \( G \).

Let \( \mathcal{L}[x(t)] = \tilde{x}(s) \) be the Laplace transform of the function \( x(t) \), where \( s \) is the Laplace-domain variable conjugate to \( t \). Let \( \text{Co}_{G,\alpha\omega}(s) = \mathcal{L}[\exp(tA)_{\alpha\omega}] \) and \( \text{CS}_{G,\alpha}(s) = \mathcal{L}[\exp(tA)_{\alpha\alpha}] \), so that \( \text{Co}_{G,\alpha\omega} = \mathcal{L}^{-1}[\text{Co}_{G,\alpha\omega}(s)] \) and \( \text{CS}_{G,\alpha} = \mathcal{L}^{-1}[\text{CS}_{G,\alpha}(s)] \). Then:

**Proposition 6.1.** The communicability of a pair of vertices \( \alpha, \omega \) on a graph \( G \) and the subgraph centrality of a vertex \( \alpha \) on \( G \) fulfill the Laplace-domain relations

\[
\tilde{\text{Co}}_{G,\alpha\omega} = \sum_{P_{G,\alpha\omega}} \tilde{\text{CS}}_{G \setminus \{\alpha, \ldots, \omega\}; \omega} \cdots \tilde{\text{CS}}_{G \setminus \{\alpha\}; \omega} \tilde{C}_{G,\alpha},
\]

(24a)

where \( \ell \) is the length of the path (\( \alpha \omega_2 \ldots \omega_\ell \omega \)) \( \in P_{G,\alpha\omega} \), and

\[
\tilde{\text{CS}}_{G,\alpha} = \left[s - \sum_{C_{G,\alpha}} \tilde{\text{CS}}_{G \setminus \{\alpha, \ldots, \mu_\alpha\}; \mu_\alpha} \cdots \tilde{\text{CS}}_{G \setminus \{\alpha\}; \mu_\alpha}\right]^{-1},
\]

(24b)

where \( m \) is the length of the bare cycle (\( \alpha \mu_2 \ldots \mu_m \alpha \)) \( \in C_{G,\alpha} \).

**Proof.** Note that \( \exp A = \exp(tA)_{\alpha\alpha} = \mathcal{L}^{-1}\left[(1s - A)^{-1}\right]_{\alpha\alpha} \). Then Proposition 6.1 follows from Proposition 5.1. Note that one can also define the communicability and matrix subgraph centrality of any ensemble of vertices of a graph as being the matrix of communicabilities and subgraph centralities of all the vertices of that ensemble. Then this matrix communicability and subgraph centrality fulfills relations similar to those of Proposition 6.1 as follows from Proposition 5.1

**Example 6.2.** To illustrate Proposition 6.1, consider again the directed graph \( G \) defined by the adjacency matrix of Eq. (17). Suppose that we are interested in the relation between the subgraph centrality of vertex 3 on \( G \) and the subgraph centrality \( \text{CS}_{G \setminus \{3,4\};2} \) of vertex 2 on the subgraph \( G \setminus \{3,4\} \) of \( G \). Since \( G_{3,3} = \{(343), (3213)\} \), Proposition 6.1 indicates that

\[
\tilde{\text{CS}}_{G,\alpha} = \left[s - \tilde{\text{CS}}_{G \setminus \{\alpha, 4\};4} - \tilde{\text{CS}}_{G \setminus \{\alpha, 3\};4} \right]^{-1}
\]

(25)

Now note that \( \tilde{\text{CS}}_{G_{3,3};4} = s^{-1} \) since there is no loop on vertex 4, \( \tilde{\text{CS}}_{G_{3,3};3} = (s - 1)^{-1} \) since there is a loop on vertex 1, and \( \tilde{\text{CS}}_{G_{3,3};2} = \tilde{\text{CS}}_{G_{3,4};2} \). Thus the required relation between the subgraph centralities is

\[
\tilde{\text{CS}}_{G,3} = \left[s - s^{-1} - (s - 1)^{-1} \tilde{\text{CS}}_{G_{3,4};2}\right]^{-1}.
\]

(26)

7. Conclusion

In this article we demonstrated that every walk on an arbitrary directed graph \( G \) with self-loops can be decomposed into a simple path and a collection of nested bare cycles on \( G \), and that this can be done uniquely. This decomposition is reminiscent of the well-known result that an arbitrary positive integer can be uniquely decomposed into a product of prime factors. We presented an explicit expression for the basis of the walk algebra \( KG \) in terms of the sets of simple paths and bare cycles of \( G \). Further, we showed that the sum of all walks between a given pair of vertices on \( G \) can be rewritten as a sum over simple paths and a collection of sums over closed walks. We subsequently formally resummed each of the sums over closed walks into a recursive closed form, thereby reducing the (typically infinite) sum over walks to a (finite) sum over paths.

Note that our bare cycles, which play the role of the prime numbers in an integer factorization, differ from the ‘prime cycles’ that appear in the definition of the Ihara zeta function. In particular, the latter include compound cycles, which are not fundamental insofar as they may be decomposed into bare cycles. It would therefore be interesting to investigate the significance of Theorems 3.1 and 4.1 to the zeta functions of graphs.

Finally, we note that the results presented in this article have already found applications in linear algebra, where matrix functions can be expressed as infinite sums over walks on directed graphs with matrix-valued edge weights.
References

[1] A. Terras, Zeta Functions of Graphs, Cambridge University Press, 2011.
[2] N. Biggs, Algebraic Graph Theory, Cambridge University Press, Cambridge, 2nd edition, 1993.
[3] E. Estrada, J. A. Rodríguez-Velázquez, Phys. Rev. E 71 (2005) 056103.
[4] E. Estrada, N. Hatano, Phys. Rev. E 77 (2008) 036111.
[5] L. Da F. Costa, F. A. Rodrigues, G. Travieso, P. R. Villas Boas, Adv. Phys. 56 (2007) 167.
[6] O. Mason, M. Verwoerd, IET Syst. Biol. 1 (2007) 89.
[7] P.-L. Giscard, S. J. Thwaite, D. Jaksch, arXiv:1112.1588v2 (2011). Submitted to SIAM J. Mat. Anal. Appl.