A weighted graph zeta function involved in the Szegedy walk

Ayaka Ishikawa
Graduate School of Engineering Science
Yokohama National University
Hodogaya, Yokohama, 240-8501, JAPAN

Norio Konno
Department of Applied Mathematics, Faculty of Engineering
Yokohama National University
Hodogaya, Yokohama, 240-8501, JAPAN

Abstract

We define a new weighted zeta function for a finite graph and obtain its determinant expression. This result gives the characteristic polynomial of the transition matrix of the Szegedy walk on a graph.

1 Introduction

In this paper, we define a new graph zeta function which is not obtained as a specialization of the generalized weighted zeta function. Since it satisfies the adjacency condition, we can obtain the three expressions. The problem to consider in this paper is to give the Ihara expression. In the main theorem, we show that our graph zeta function has the Ihara expression for a finite graph and a finite digraph. The reason we deal with graphs is to consider the relationship between our graph zeta function and the “Szegedy walk” defined on a graph. On the other hand, we also treat digraphs. Since the Ihara expressions of generalized weighted zeta functions on graphs and digraphs are a slightly different (cf. [3, 4]), we can expect there are differences between our graph zeta functions for graphs and digraphs. In fact, the two Ihara expressions are found to be different. The reason lies in the difference in the definition of the inverse arc as expected. For a graph, we consider the symmetric digraph of the graph and define a pair of arcs assigned to each edge as inverse. Then the Ihara expression is the same form as in [3].
deal with this definition because the Szegedy walk adopts the definition. In other words, it is necessary to use the definition in order to consider the relationship between the Szegedy walk and our graph zeta function. In this paper, we deal with the other definition of the inverse motivated by [4]. For a digraph and an arc, we define the inverse as any arc with an opposite direction. Then the Ihara expression different from that derived by the previous definition.

The Szegedy walk is a quantum walk model, which is a generalization of the “Grover walk”. A quantum walk is the quantum version of a random walk, and it is studied in various fields: quantum algorithm, financial engineering, and laser isotope separation, for example (see e.g., [8, 10, 11]). The common interest in these fields is the behavior of quantum walks. Some important quantum walk properties, such as periodicity and localization, are determined by the eigenvalues of the transition matrix. For example, in the quantum search problem, the eigenvalues are crucial for deriving the quantum hitting time of the quantum walk on a graph [7]. In particular, the Grover transition matrix is an example of the “edge matrix” [9], which describes the Hashimoto expression for the Sato zeta function. By transforming the Hashimoto expression of the Sato zeta function into the Ihara expression, this process describes the eigenvalues of the Grover transition matrix [6]. Our graph zeta function has the edge matrix corresponding to the Szegedy transition matrix. Hence, our result shows that we can describe the eigenvalues of the Szegedy transition matrix by our graph zeta function.

The rest of the paper is organized as follows. In Section 2, we define a new graph zeta function as an exponential expression. We introduce the Szegedy walk and state the relation between our zeta function and the Szegedy walk. The Ihara expression of our zeta function is defined in Section 3 which is the main theorem of our paper. From the theorem, we can obtain the characteristic polynomial of the transition matrix of the Szegedy walk on a finite graph. In Section 4, we give two examples on a graph and a digraph.

Throughout this paper, graphs (resp. digraphs) are finite, and multiedge (resp. multi-arcs) and multi-loops are allowed. We use the following symbols. For positive integers $m$ and $n$, let $\text{Mat}(m, n; \mathbb{C})$ be the set of $m \times n$ matrices over $\mathbb{C}$. For a matrix $M \in \text{Mat}(n, n; \mathbb{C})$, let $\text{Spec}(M)$ be the spectrum of $M$. An $m \times n$ matrix with all one denotes by $\mathbb{1}_{m \times n}$. In particular, if $m = n$, we write $\mathbb{1}_{m \times n}$ as $\mathbb{1}_n$. For a proposition $P$, we define $\delta_P$ as follows: $\delta_P = 1$ if $P$ is true, $\delta_P = 0$ if $P$ is false. For the Kronecker delta $\delta_{uv}$, let $\overline{\delta}_{uv} = 1$ if $u \neq v$, $\overline{\delta}_{uv} = 0$ otherwise.
2 Preliminary

A graph $G = (V, E)$ is a pair of vertex set $V$ and edge set $E$, where $E$ consists of 2-subsets of $V$. If both $V$ and $E$ are finite, then $G$ is called finite. We call an edge $e = \{v, v\}$ a loop. The number $\deg(u) := |\{u \in V \mid v \in V\}$ is called the degree of $u$. If there is at most one edge between each two vertices and there are not loops, then the graph is called simple. Let $V$ be a vertex set and $A$ a set of ordered pairs of two vertices. We call the pair $\Delta = (V, A)$ a digraph and an element of $A$ an arc. For an arc $a = (u, v)$, $u$ and $v$ are called the tail and the head of $a$ denoted by $t(a)$ and $h(a)$, respectively. For two vertices $u, v \in V$ of a digraph $\Delta$, let $A_{uv} := \{a \in A \mid t(a) = u, h(a) = v\}$, $A_{vu} := \{a \in A \mid \text{h}(a) = u, \text{t}(a) = v\}$, and $A(u, v) := A_{uv} \cup A_{vu}$. For a graph $G = (V, E)$, let $A(G) := \{(u, v), (v, u) \mid e = \{v, u\} \in E\}$, and then the digraph $\Delta(G) = (V, A(G))$ is called the symmetric digraph of $G$. For an arc $a \in A(G)$, we denote by $\overline{a}$ the arc induced by the same edge as $a$.

A sequence of arcs $p = (a_i)_{i=1}^k$ is a path if it satisfies $h(a_i) = t(a_{i+1})$ for each $i = 1, 2, \ldots, k - 1$. The number $k$, called the length of $p$, is denote by $|p|$. If $h(a_k) = t(a_1)$, then the path $p$ is called closed. Let $X_k$ denote the set of closed paths of length $k$. For $C \subseteq X_k$, we denote by $C^n$ the closed path that connects $C$ $n$ times. It is called the $n$-th power of $C$. If $C$ cannot be expressed as a power of a closed path shorter than $C$, then it is called prime. For $C = (c_i)_{i=1}^k, C' = (c'_i)_{i=1}^k \subseteq X_k$, if there exists an integer $n$ such that $c_i = c'_i \in \theta^k$ for any $i$, where the indices are taken modulo $k$, then we denote the relation by $C \sim C'$. Clearly, the relation $\sim$ is an equivalence relation. An equivalence class is called a cycle, and we denote by $[C]$ the equivalence class of a closed path $C$. Since any closed path in $[C]$ have the same length, we define the length of $[C]$ to be the length of a closed path in $[C]$. We denote by $|C|$ the length of $[C]$. A cycle is prime if a closed path in the cycle is prime. We denote by $\mathcal{P}$ the set of prime cycles.

2.1 A new graph zeta function

Let $\Delta = (V, A)$ be a digraph. For a map $\theta : A \times A \rightarrow \mathbb{C}$ and a closed path $C = (c_i)_{i=1}^k \subseteq X_k$, let $\text{circ}_\theta(C)$ denote the circular product $\theta(c_1, c_2)\theta(c_2, c_3) \ldots \theta(c_k, c_1)$. Note that $\text{circ}_\theta(C) = \text{circ}_\theta(C')$ holds if $C \sim C'$. Let $N_k(\text{circ}_\theta) := \sum_{C \subseteq X_k} \text{circ}_\theta(C)$. We define a graph zeta function for $\Delta$.

Definition 1:
A graph zeta function for $\Delta$ is the following formal power series:

$$Z_\Delta(t; \theta) := \exp \left( \sum_{k \geq 1} \frac{N_k(\circ \theta)}{k} t^k \right).$$  \hspace{1cm} (1)

We call the map $\theta$ the weight of the graph zeta function, and the expression (1) the exponential expression \cite{9}. Let

$$E_\Delta(t; \theta) := \prod_{[C] \in \mathcal{P}} \frac{1}{1 - \circ \theta(C) t^{[C]}}, \quad H_\Delta(t; \theta) := \frac{1}{\det(I - t M_\theta)},$$

where $M_\theta = (\theta(a, a'))_{a, a' \in A}$. The expressions $E_\Delta(t; \theta)$ and $H_\Delta(t; \theta)$ are called the Euler expression and the Hashimoto expression, respectively (cf. \cite{9}).

**Proposition 1:**

If $\theta : A \times A \to \mathbb{C}$ satisfies the condition

$$\theta(a, a') \neq 0 \Rightarrow h(a) = t(a'),$$

then $Z_\Delta(t; \theta) = E_\Delta(t; \theta) = H_\Delta(t; \theta)$.

**Proof:** See \cite{9}. □

The above condition for $\theta$ is called the adjacency condition \cite{9}.

Before we introduce the “Ihara expression”, we will mention the definition of the inverse. For an arc $a$, let $a^{-1}$ denote the set of inverses of $a$. For a digraph $\Delta$, if $a \in A_{uv}$, then we define $a^{-1} := A_{vu}$. Note that for a loop $a \in A_{vv}$, $a \in a^{-1}$ holds. Unless otherwise specified, for a digraph, this definition is adopted. On the other hand, for the symmetric digraph $\Delta(G)$ of a graph $G$, we adopt the following definition. Let $a = (u, v)$ and $a' = (v, u)$ be induced by an edge $\{u, v\} \in E$, then we define $a^{-1} := \{a'\}$, and $a'$ denotes by $\pi$.

Let $\Delta = (V, A)$ be a digraph (not specified whether it is the symmetric digraph or not). For any maps $\tau_1, \tau_2 : A \to \mathbb{C}$, let $\tau$ be a map $A \times A \to \mathbb{C}$ defined by $\tau(a, a') := \tau_1(a) \tau_2(a')$. We define a new graph zeta function $Z_\Delta(t; \theta)$ with the weight

$$\theta(a, a') := \tau(a, a') \delta_{h(a)} t(a') - \delta_{a' \in a^{-1}},$$  \hspace{1cm} (2)
where $\delta_{h(a)t(a')} \equiv 1$ is the Kronecker delta, and $\delta_{a'\in a^{-1}} \equiv 1$ if $a'$ is an inverse of $a$, 0 otherwise. Note that if $\delta_{a'\in a^{-1}} = 1$, any arc $a' \in a^{-1}$ is in $A_{h(a)t(a)}$, and it satisfies $h(a) = t(a') = v$. If $\theta(a, a') \neq 0$ for $a, a' \in A$, then $\delta_{h(a)t(a')} = 1$ holds at least. Thus, the weight $\theta$ is satisfying the adjacency condition, and we can see $Z_\Delta(t; \theta) = E_\Delta(t; \theta) = H_\Delta(t; \theta)$.

We assume that $\theta_S := \theta|_{\tau_i \equiv 1}$. The graph zeta function with the weight $\theta_S$ is called the \textit{Sato zeta function} \cite{9, 12}. Since $\theta_S$ satisfies the adjacency condition, the Sato zeta function has the Euler expression and the Hashimoto expression. In addition, it also has the following determinant expression called the \textit{Ihara expression}.

**Proposition 2:** (Sato \cite{12}) Let $\Delta(G) = (V, A(G))$ be the symmetric digraph of a finite simple graph $G = (V, E)$, and $A_G^S = (a_{uv})_{u,v \in V}$ and $D_G^S = (d_{uv})_{u,v \in V}$ be defined as follows:

$$a_{uv} := \sum_{a \in A_{uv}} \tau(a), \quad d_{uv} := \sum_{a \in A_{uv}} \tau(a).$$

Then, $Z_{\Delta(G)}(t; \theta)$ equals

$$\frac{1}{(1-t^2)^{|E|-|V|} \det(I - tA_G^S + t^2(D_G^S - I))}.$$
2.2 Szegedy walk

First we give the definition of the Szegedy walk.

Definition 2: For the symmetric digraph \( \Delta = (V, \mathcal{A}(G)) \) of a simple graph \( G \), let \( p : \mathcal{A}(G) \to (0, 1] \) be a transition probability satisfying \( \sum_{a \in \mathcal{A}(G), t(a) = v} p(a) = 1 \) for each \( v \in V \). The Szegedy walk \[13\] is the quantum walk whose transition matrix \( U_{SZ} = (u_{SZ}(a, a'))_{a, a' \in \mathcal{A}(G)} \) is defined by

\[
u_{SZ}(a, a') := 2\sqrt{p(a)p(a')}\delta_{t(a)h(a')} - \delta_{a,a'}.
\]

For the weight \( [2] \), let \( \tau_1(a) = \sqrt{2p(a)} \) and \( \tau_2(a) = \sqrt{2p(a)} \) for each \( a \in \mathcal{A}(G) \). Then, we have \( \theta(a, a') = u_{SZ}(a', a) \).

Remark 1: The Grover walk \[2\] is a special case of the Szegedy walk, whose transition matrix is \( U_{GR} = \frac{2}{\text{deg} t(a)} \delta_{t(a)h(a')} - \delta_{a,a'} \) for each \( a \in \mathcal{A}(G) \). It is given by substituting \( p = \frac{2}{\text{deg} t(a)} \) for each \( u_{SZ}(a, a') \).

Konno and Sato \[6\] give the spectrum of the transition matrix of the Grover walk on \( G \) by the Ihara expression of \( Z_{\Delta(G)}(t; \theta) \).

Theorem 1: For a finite simple connected graph \( G \),

\[
\det(\lambda - U_{GR}) = (\lambda^2 - 1)^{|E| - |V|} \det((\lambda^2 + 1)I - 2\lambda T) = (\lambda^2 - 1)^{|E| - |V|} \prod_{\mu \in \text{Spec}(T)} ((\lambda^2 + 1) - 2\mu\lambda),
\]

where \( T = (T_{uv})_{u,v \in V} \) is defined as follows:

\[
T_{uv} = \begin{cases} \frac{1}{\text{deg}(u)} & \text{if } \{u, v\} \in E, \\ 0 & \text{otherwise}. \end{cases}
\]

Thus, we get

\[
\text{Spec}(U_{GR}) = \{ \pm 1 \}^{|E| - |V|} \sqcup \{ \lambda | \lambda^2 - 2\mu\lambda + 1 = 0, \text{ for each } \mu \in \text{Spec}(T) \}.
\]

Recall that \( \theta^S(a, a') = \theta(a, a')|_{\tau_1 = 1} = \tau_2(a')\delta_{h(a)h(a')} - \delta_{a,a'} \) for each two arcs \( a, a' \in \mathcal{A} \). For each \( a \in \mathcal{A}(G) \), substituting \( \frac{2}{\text{deg} t(a)} \) for \( \tau_2(a) \) of \( \theta^S \), we get the above theorem by the Ihara expression of \( Z_{\Delta(G)}(t; \theta^S) \). In order to consider a similar theorem for the Szegedy walk on a finite digraph \( \Delta \), it is necessary to show that \( Z_{\Delta}(t; \theta) \) has the Ihara expression.
3 Main theorem

Before stating the main theorem, we will show some lemmas.

**Lemma 1:** For a variable $t$ and a scalar $k$, the following hold
\[
(I + tk\mathbb{1}_n)^{-1} = I - (1 + t kn)^{-1}tk\mathbb{1}_n,
\]
\[
\det(I + tk\mathbb{1}_n) = 1 + t kn.
\]

**Proof:** It is easy to see from the following:
\[
(I + tk\mathbb{1}_n)(I - (1 + t kn)^{-1}tk\mathbb{1}_n) = I - (1 + t kn)^{-1}tk\mathbb{1}_n + tk\mathbb{1}_n - (1 + t kn)^{-1}t^2k^2n\mathbb{1}_n
\]
\[
= I + tk\mathbb{1}_n - (1 + t kn)^{-1}(1 + t kn)tk\mathbb{1}_n
\]
\[
= I.
\]
In the same way, we can see \(I - (1 + t kn)^{-1}tk\mathbb{1}_n)(I + tk\mathbb{1}_n) = I.\)

The determinant is given as follows:
\[
\begin{vmatrix}
1 + tk & tk & tk & \ldots \\
tk & 1 + tk & tk & \ldots \\
tk & tk & 1 + tk & \ldots \\
\vdots & \vdots & \vdots & \ddots
\end{vmatrix}
\]
\[
= \begin{vmatrix}
1 + tk & tk & tk & \ldots \\
-1 & 1 & 0 & \ldots \\
-1 & 0 & 1 & \ldots \\
\vdots & \vdots & \vdots & \ddots
\end{vmatrix}
\]
\[
= \begin{vmatrix}
1 + n(tk) & tk & tk & \ldots \\
0 & 1 & 0 & \ldots \\
0 & 0 & 1 & \ldots \\
\vdots & \vdots & \vdots & \ddots
\end{vmatrix}
\]
\[
= 1 + t kn.
\]
\]

\[
\square
\]

**Lemma 2:** Let $M_1 \in \text{Mat}(k, l; \mathbb{C})$ and $M_2 \in \text{Mat}(l, k; \mathbb{C})$ and $M := \begin{bmatrix} O & M_1 \\ M_2 & O \end{bmatrix}$. When the matrix $I_l - t^2 M_2 M_1$ is nonsingular, $(I + tM)^{-1}$ can be written by
\[
\begin{bmatrix}
(I_l - t^2 M_1 M_2)^{-1} & -tM_1(I_l - t^2 M_2 M_1)^{-1} \\
-t(I_l - t^2 M_2 M_1)^{-1}M_2 & (I_l - t^2 M_2 M_1)^{-1} \\
\end{bmatrix}.
\]
We also have \( \det(I + tM) = \det(I - t^2M_2M_1) = \det(I - t^2M_1M_2). \)

**Proof:** The matrix \( I + tM \) is decomposed as

\[
I + tM = \begin{bmatrix}
I & O \\
tM_2 & I
\end{bmatrix}
\begin{bmatrix}
I & O \\
O & I - t^2M_2M_1
\end{bmatrix}
\begin{bmatrix}
I & tM_1 \\
O & I
\end{bmatrix}.
\] (3)

Taking the inverse of both sides, we get

\[
(I + tM)^{-1} = \begin{bmatrix}
I & tM_1 \\
O & I
\end{bmatrix}^{-1}
\begin{bmatrix}
I & O \\
O & I - t^2M_2M_1
\end{bmatrix}^{-1}
\begin{bmatrix}
I & O \\
tM_2 & I
\end{bmatrix}^{-1}
\]

\[
= \begin{bmatrix}
I & -tM_1 \\
O & I
\end{bmatrix}
\begin{bmatrix}
I & O \\
O & (I - t^2M_2M_1)^{-1}
\end{bmatrix}
\begin{bmatrix}
I & O \\
-tM_2 & I
\end{bmatrix}
\]

\[
= \begin{bmatrix}
I + tM_1(I - t^2M_2M_1)^{-1}tM_2 & -tM_1(I - t^2M_2M_1)^{-1} \\
-(I - t^2M_2M_1)^{-1}tM_2 & (I - t^2M_2M_1)^{-1}
\end{bmatrix}.
\]

By the same way as in Lemma 1, it can be shown that \( I + tM_1(I - t^2M_2M_1)^{-1}tM_2 = (I_k - t^2M_1M_2)^{-1} \) holds.

The matrix \( I + tM \) is also decomposed as

\[
I + tM = \begin{bmatrix}
I & tM_1 \\
O & I
\end{bmatrix}
\begin{bmatrix}
I - t^2M_1M_2 & O \\
O & I
\end{bmatrix}
\begin{bmatrix}
I & O \\
O & I
\end{bmatrix}.
\] (4)

Taking the determinants of both sides of Equation (3) and (4), we get

\[
\det(I + tM) = \det(I - t^2M_1M_2) = \det(I - t^2M_2M_1).
\]

\(\square\)

**Remark 2:** For conformable matrices \( A, B, C, \) and \( D, \) the identity \( (A + BCD)^{-1} = A^{-1} - A^{-1}B(C^{-1} + DA^{-1}B)^{-1}DA^{-1} \) is called the **Woodbury matrix identity**.

### 3.1 The Ihara expression of the graph zeta function on a finite digraph

We fix a total order \( < \) on \( V, \) and if one writes \( A(u, v) \) then the condition \( u < v \) is always assumed. Let \( J = (j_{aa'})_{a,a' \in A}, \ K = (k_{av})_{a \in A, v \in V} \) and \( L = (l_{aa'})_{a \in V, a' \in A} \) be matrices defined by \( j_{aa'} = \delta_{a' \in a^{-1}}, \ k_{av} = \tau_i(a) \delta_{b(a)v} \) and \( l_{aa'} = \tau_2(a') \delta_{a_t(a')} \). For each \( (u, v) \in \Phi_\Delta, \) let \( J(u, v) := (j_{aa'})_{a,a' \in A(u,v)}, \ K(u, v) := (k_{aw})_{a \in A(u,v), w \in V} \) and \( L(u, v) := (l_{wa'})_{w \in V, a' \in A(u,v)}. \) Note that
one can choose a total order on $V$ which makes $J$ a diagonal matrix. We fix such a total order on $V$. Let $T$ denote the block diagonal matrix $I + tJ$, and the diagonal blocks are given by $T(u, v) := I + tJ(u, v)$. We denote $\det(T(u, v))$ by $f(u, v)$. Then, we can see that $\det(T) = \prod_{(u,v) \in \Phi} f(u, v)$ holds.

**Lemma 3:** For $(u, v) \in \Phi$, 
\[
f(u, v) = \begin{cases} 
1 - |A_{uv}||A_{vu}|t^2 & \text{if } u \neq v, \\
1 + |A_{uu}|t & \text{if } u = v.
\end{cases}
\]

**Proof:** For $(u, v) \in \Phi$ satisfying $u \neq v$, we assume that $|A_{uv}| = k$ and $|A_{vu}| = l$. The matrix $J(u, v)$ is given by $\begin{bmatrix} I_k & tI_{k \times l} \\
tI_{l \times k} & I_l \end{bmatrix}$. By Lemma 2, we have $\det(T(u, v)) = \det(I - t^2I_{k \times l}I_{l \times k})$. Since $I_{k \times l}I_{l \times k} = I_{k \times k}$ holds, and the identity $\det(I - t^2I_{k \times k}) = 1 - klt^2$ follows from Lemma 1.

For $(u, u) \in \Phi$, we assume that $|A_{uu}| = n$. Since the matrix $J(u, u)$ is equal to $1_n$, $T(u, u) = I + t1_n$ holds. From Lemma 1, we obtain $\det(I + t1_n) = 1 + nt$. □

We consider the following matrices
\[
A^\theta_{\Delta} = \sum_{(u,v) \in \Phi} L(u,v)K(u,v),
\]
\[
D^\theta_{\Delta} = \sum_{(u,v) \in \Phi} \frac{L(u,v)J(u,v)K(u,v)}{f(u,v)},
\]
\[
X^\theta_{\Delta} = \sum_{(u,v) \in \Phi} \delta_{uv} \frac{L(u,v)J(u,v)^2K(u,v)}{f(u,v)}.
\]

**Theorem 2:** The following identity holds:
\[
\det(I - tM_{\theta}) = \prod_{u,v \in V} f(u,v) \det(I - tA^\theta_{\Delta} + t^2D^\theta_{\Delta} - t^3X^\theta_{\Delta}).
\]

**Proof:** Let $H := (\tau(a, a')\delta_{b(a)\delta_0(a')})_{a, a' \in A}$. Then we have $M_{\theta} = H - J$. Since $\tau(a, a')\delta_{b(a)\delta_0(a')} = \sum_{v \in V} (\tau_1(a)\delta_{b(a)v})(\tau_2(a')\delta_{e_0(a')})$, we have $H = KL$. Thus
we obtain
\[ \det(I - tM_0) = \det(I - t(KL - J)) = \det(T - tKL). \]

For two conformable matrices \(X\) and \(Y\), it is known that \(\det(I - XY) = \det(I - YX)\) holds. Hence we have
\[ \det(T - tKL) = \det(T) \det(I - tT^{-1}KL) \]
\[ = \left( \prod_{(u,v) \in \Phi_\Delta} f(u, v) \right) \det(I - tLT^{-1}K). \]

For the direct sum decomposition \(T = \bigoplus_{(u,v) \in \Phi_\Delta} T(u, v)\), we arrange the submatrices \(J(u, v)\) and \(K(u, v)\) of \(J\) and \(K\) in order of submatrices \(T(u, v)\) of \(T\). Then, we can give the matrix \(LT^{-1}K\) by a sum
\[ \sum_{(u,v) \in \Phi_\Delta} L(u,v)T(u,v)^{-1}K(u,v). \]

The matrix \(T(u,v)\) is different for \(u = v\) and for \(u \neq v\). Thus we consider these two cases separately.

For \((u, u) \in \Phi_\Delta\), we assume \(|A(u, u)| = n\). Since any two arcs \(a, a' \in A(u, u)\) are inverses of each other, \(J(u, u) = \mathbf{1}_n\) and \(T(u, u) = I + t\mathbf{1}_n\) holds. By Lemma 1 and Lemma 3, we have
\[ L(u, u)T(u, u)^{-1}K(u, u) = L(u, u) \left( I - \frac{t}{1 + nt} \mathbf{1}_n \right) K(u, u) \]
\[ = L(u, u)K(u, u) - t \frac{L(u, u)J(u, u)K(u, u)}{f(u, u)}. \]

For \((u, v) \in \Phi_\Delta\) satisfying \(u \neq v\), we arrange the elements of \(A(u, v)\) by an order \(<\) such that \(a < a'\) for \(a \in A_{uv}\) and \(a' \in A_{vu}\). We assume that \(|A_{uv}| = k\) and \(|A_{vu}| = l\). Then, \(T(u, v) = \begin{bmatrix} I & t\mathbf{1}_{k \times l} \\ t\mathbf{1}_{l \times k} & I \end{bmatrix}\). From Lemma 2, \((1, 1)\)-block and \((2, 2)\)-block of \(T(u, v)^{-1}\) are \((I_k - t^2\mathbf{1}_{k \times k})^{-1} = (I_k - t^2\mathbf{1}_{k \times k})^{-1}\) and \((I_l - t^2\mathbf{1}_{l \times l})^{-1} = (I_l - t^2\mathbf{1}_{l \times l})^{-1}\). Thus, \(T(u, v)^{-1}\) is given by
\[ \begin{bmatrix} (I_k - t^2\mathbf{1}_{k \times k})^{-1} & -t\mathbf{1}_{k \times l}(I_l - t^2\mathbf{1}_{l \times l})^{-1} \\ -t(I_l - t^2\mathbf{1}_{l \times l})^{-1}\mathbf{1}_{l \times k} & (I_l - t^2\mathbf{1}_{l \times l})^{-1} \end{bmatrix}. \]
By Lemma 1 and Lemma 3, we have

\[ T(u,v)^{-1} = \begin{bmatrix} I_k + \frac{t^2}{1 - klt^2} I_k & -t I_k \times I_k & 1 - \frac{klt^3}{1 - klt^2} I_k \times I_k \\ -t I_k \times I_k & I_k + \frac{t^3}{1 - klt^2} I_k \times I_k & 1 - \frac{klt^3}{1 - klt^2} I_k \times I_k \\ 1 - \frac{klt^3}{1 - klt^2} I_k \times I_k & 1 - \frac{klt^3}{1 - klt^2} I_k \times I_k & \frac{1}{1 - klt^2} I_k \times I_k \\ \end{bmatrix} \]

Hence \( L(u,v)T(u,v)^{-1}K(u,v) \) equals

\[ L(u,v)K(u,v) - t \frac{L(u,v)J(u,v)K(u,v)}{f(u,v)} + t^2 \frac{L(u,v)J(u,v)^2K(u,v)}{f(u,v)}. \]

Therefore, \( LT^{-1}K \) is given by

\[ \sum_{(u,v) \in \Phi} \left\{ L(u,v)K(u,v) - t \frac{L(u,v)J(u,v)K(u,v)}{f(u,v)} + t^2 \frac{L(u,v)J(u,v)^2K(u,v)}{f(u,v)} \right\}. \]

It follows from the definition that \( LT^{-1}K = A_\Delta^6 - t D_\Delta^6 + t^2 X_\Delta^6 \), which completes the proof. \( \square \)

**Remark 3:** The entries of \( A_\Delta^6 = (a_{uv})_{u,v \in V} \), \( D_\Delta^6 = (d_{uv})_{u,v \in V} \) and \( X_\Delta^6 = (x_{uv})_{u,v \in V} \) are given by

\[ a_{uv} = \sum_{a \in A_{uv}} \tau(a, a), \]

\[ d_{uv} = \delta_{uv} \sum_{w \in V} \left( \sum_{a \in A_{uw}, a' \in A_{wu}} \frac{\tau(a', a)}{f(u, w)} \right), \]

\[ x_{uv} = \delta_{uv} \frac{|A_{uv}|}{f(u, v)} \left( \sum_{a, a' \in A_{uv}} \tau(a, a') \right). \]

### 3.2 The Ihara expression of the graph zeta function on a finite graph

In order to give the characteristic polynomial of the Szegedy transition matrix by our graph zeta function, we derive the Ihara expression of
Remark 4: The entries of $A_G^\theta = (a_{uv})_{u,v \in V}$ and $D_G^\theta = (d_{uv})_{u,v \in V}$ are given by
\[ a_{uv} = \sum_{a \in \mathcal{A}_{uv}} \tau(a, a), \quad d_{uv} = \delta_{uv} \sum_{a \in \mathcal{A}_u} \tau(\overline{a}, a). \]

$Z_{\Delta(G)}(t; \theta)$ for a graph $G$. Accordingly, we adopt the “usual” definition of inverse for symmetric digraphs.

Let $G$ be a graph, and $\Delta(G) = (V, \mathcal{A}(G))$ the symmetric digraph for $G$. Let $\mathcal{A}(e)$ denote the set of two arcs induced by $e \in E$. The two arcs in each $\mathcal{A}(e)$ are inverses of each other. Let $J(e) := (\delta_{a' \in \mathcal{A}(e)}a, a' \in \mathcal{A}(e)), K(e) := (\tau_1(a) \delta_{(a)\in \mathcal{A}(e)}, v \in V)$ and $L(e) := (\tau_2(a') \delta_{(a')\in \mathcal{A}(e)})v \in V, a' \in \mathcal{A}(e)$. Note that $J(e)$ is the square matrix $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ for any $e \in E$, and $J = \bigoplus_{e \in E} J(e)$ holds. Let $T(e) := I + tJ(e)$ and $T = \bigoplus_{e \in E} T(e)$, then we can see that $\det(T(e)) = 1 - t^2$ and $\det(T) = (1 - t^2)^{|E|}$. We consider the following matrices:

$$A_G^\theta := \sum_{e \in E} L(e)K(e), \quad D_G^\theta := \sum_{e \in E} L(e)J(e)K(e).$$

**Theorem 3:** The following identity holds:

$$Z_{\Delta(G)}(t; \theta)^{-1} = (1 - t^2)^{|E| - |V|} \det(I - tA_G^\theta + t^2(D_G^\theta - I)). \quad (5)$$

**Proof:**

As in Theorem 2, $\det(I - tM_\theta)$ is given by

$$\det(T - tKL) = \det(T)\det(I - tLT^{-1}K) = (1 - t^2)^{|E|} \det(I - tLT^{-1}K).$$

Since $T = \bigoplus_{e \in E} T(e)$, we have $LT^{-1}K = \sum_{e \in E} L(e)T(e)^{-1}K(e)$. For each $e \in E$, $T(e)^{-1} = (1 - t^2)^{-1} \begin{bmatrix} 1 & \frac{-t}{1} \\ -t & 1 \end{bmatrix} = (1 - t^2)^{-1}(I - tJ(e))$, and we get

$$L(e)T(e)^{-1}K(e) = (1 - t^2)^{-1}\{L(e)K(e) - L(e)J(e)K(e)\}.$$

Since $LT^{-1}K = \sum_{e \in E}(1 - t^2)^{-1}\{L(e)K(e) - L(e)J(e)K(e)\}$ holds, we see

$$\begin{align*}
(1 - t^2)^{|E|} & \det(I - tLT^{-1}K) \\
&= (1 - t^2)^{|E| - |V|} \det((1 - t^2)I - t\sum_{e \in E}(L(e)K(e) - L(e)J(e)K(e))) \\
&= (1 - t^2)^{|E| - |V|} \det(I - tA_G^\theta + t^2(D_G^\theta - I)).
\end{align*}$$

$\square$

**Remark 4:** The entries of $A_G^\theta = (a_{uv})_{u,v \in V}$ and $D_G^\theta = (d_{uv})_{u,v \in V}$ are given by

$$a_{uv} = \sum_{a \in \mathcal{A}_{uv}} \tau(a, a), \quad d_{uv} = \delta_{uv} \sum_{a \in \mathcal{A}_u} \tau(\overline{a}, a).$$
As was mentioned in the introduction, we obtain a generalization of the Konno-Sato’s theorem [6].

**Corollary 1:** For a graph $G = (V, E)$ without loops, the characteristic polynomial of the transition matrix of the Szegedy walk on $G$ is given as follows:

$$
\det(\lambda I - U_{SZ}) = (\lambda^2 - 1)^{|E| - |V|} ((\lambda^2 + 1)I - 2\lambda T)
$$

$$
= (\lambda^2 - 1)^{|E| - |V|} \prod_{\mu \in \text{Spec}(T)} ((\lambda^2 + 1) - 2\mu \lambda),
$$

where $T = \left( \sum_{a \in A_{uv}} \sqrt{p(a)p(\overline{a})} \right)_{u,v \in V}$.

**Proof:** Let $\tau_1(a) = \sqrt{2p(a)}$ and $\tau_2(a) = \sqrt{2p(\overline{a})}$ for $a \in \mathcal{A}(G)$. Then $\theta(a, a') = u_{SZ}(a', a)$ and $M_{\theta} = ^t U_{SZ}$ hold. The matrices $A^\theta_G$ and $D^\theta_G$ of Equation (5) are given by

$$
A^\theta_G = \left( \sum_{a \in A_{uv}} 2\sqrt{p(a)p(\overline{a})} \right)_{u,v \in V} = 2T, \quad D^\theta_G = \left( \delta_{uv} \sum_{a \in A_{uv}} 2p(a) \right)_{u,v \in V} = 2I_{|V|}.
$$

Thus, we obtain

$$
\det(\lambda I - U_{SZ}) = \det(\lambda I - ^t U_{SZ})
$$

$$
= \det(\lambda I - M_\theta)
$$

$$
= (\lambda^2 - 1)^{|E| - |V|} \det(\lambda^2 I - \lambda A^\theta_G + (D^\theta_G - I))
$$

$$
= (\lambda^2 - 1)^{|E| - |V|} \det(\lambda^2 I - 2\lambda T + I).
$$

□

4 Example

Let $\Delta = (V, \mathcal{A})$ be a digraph with $V = \{v_1, v_2, v_3\}$ and $\mathcal{A} = \{a_1 = (v_1, v_1) < a_2 = (v_1, v_1) < a_3 = (v_1, v_2) < a_4 = (v_1, v_2) < a_5 = (v_2, v_1) < a_6 = (v_2, v_1) < a_7 = (v_2, v_3) < a_8 = (v_3, v_2) < a_9 = (v_1, v_3) < a_{10} = \ldots\}$. 

---
Figure 1: digraph $\Delta = (V, A)$

$(v_3, v_1)$ (see Figure 1). The matrices $J, K,$ and $L$ are as follows:

$$J = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} \tau_1(a_1) \\ \tau_1(a_2) \\ \tau_1(a_3) \\ \tau_1(a_4) \\ \tau_1(a_5) \\ \tau_1(a_6) \end{bmatrix}, \quad L = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ \tau_2(a_1) & \tau_2(a_2) & \tau_2(a_3) & \tau_2(a_4) & \tau_2(a_5) & \tau_2(a_6) & \tau_2(a_7) & \tau_2(a_8) & \tau_2(a_9) & \tau_2(a_{10}) \end{bmatrix}.
Then, $A_\Delta^\theta$, $D_\Delta^\theta$ and $X_\Delta^\theta$ are

\[
A_\Delta^\theta = \begin{bmatrix}
\tau(a_1, a_1) + \tau(a_2, a_2) & \tau(a_3, a_3) + \tau(a_4, a_4) & \tau(a_9, a_9) \\
\tau(a_5, a_5) + \tau(a_6, a_6) & 0 & \tau(a_7, a_7) \\
\tau(a_{10}, a_{10}) & \tau(a_8, a_8) & 0
\end{bmatrix},
\]

\[
D_\Delta^\theta = \begin{bmatrix}
d_{v_1,v_1} + d_{v_1,v_2} + d_{v_1,v_3} & 0 & 0 \\
0 & d_{v_2,v_1} + d_{v_2,v_3} & 0 \\
0 & 0 & d_{v_3,v_1} + d_{v_3,v_2}
\end{bmatrix},
\]

\[
X_\Delta^\theta = \begin{bmatrix}
0 & x_{v_1,v_2} & x_{v_1,v_3} \\
x_{v_2,v_1} & 0 & x_{v_2,v_3} \\
x_{v_3,v_1} & x_{v_3,v_2} & 0
\end{bmatrix},
\]

where

\[
d_{v_1,v_1} = \frac{\tau(a_1, a_1) + \tau(a_2, a_2) + \tau(a_3, a_1) + \tau(a_2, a_2)}{1 + 2t},
\]

\[
d_{v_1,v_2} = \frac{\tau(a_5, a_3) + \tau(a_6, a_3) + \tau(a_5, a_4) + \tau(a_6, a_4)}{1 - 4t^2},
\]

\[
d_{v_2,v_1} = \frac{\tau(a_3, a_5) + \tau(a_4, a_5) + \tau(a_3, a_6) + \tau(a_4, a_6)}{1 - 4t^2},
\]

\[
d_{v_3,v_1} = \frac{\tau(a_9, a_{10})}{1 - t^2},
\]

\[
d_{v_3,v_2} = \frac{\tau(a_7, a_8)}{1 - t^2},
\]

\[
x_{v_1,v_2} = \frac{2(\tau(a_3, a_3) + \tau(a_3, a_4) + \tau(a_4, a_3) + \tau(a_4, a_4))}{1 - 4t^2},
\]

\[
x_{v_2,v_1} = \frac{2(\tau(a_5, a_5) + \tau(a_5, a_6) + \tau(a_6, a_5) + \tau(a_6, a_6))}{1 - 4t^2},
\]

\[
x_{v_1,v_3} = \frac{\tau(a_{10}, a_{10})}{1 - t^2},
\]

\[
x_{v_2,v_3} = \frac{\tau(a_8, a_8)}{1 - t^2}.
\]

Let $G = (V, E)$ be a graph with $V = \{v_1, v_2, v_3\}$ and $E = \{e_1 = \{v_1, v_1\}, e_2 = \{v_1, v_2\}, e_3 = \{v_1, v_3\}, e_4 = \{v_2, v_3\}, e_5 = \{v_1, v_3\}\}$. Assign $e_1$ to $\{a_1, a_2\}$, $e_2$ to $\{a_3, a_5\}$, $e_3$ to $\{a_4, a_6\}$, $e_4$ to $\{a_7, a_8\}$ and $e_5$ to $\{a_9, a_{10}\}$, where the directions of $a_1, \ldots, a_{10}$ are the same as in $\Delta$. Thus, the symmetric digraph $\Delta(G)$ is the same as $\Delta$. Note that the two arcs corresponding to the same edge are inverses of each other, and they do not have any other inverses. Let $\Delta(G) = (V, \mathcal{A}(G))$ be the symmetric digraph of $G$ with $\mathcal{A}(G) = \{a_1 < a_2 < a_3 < a_5 < a_4 < a_6 < a_7 < a_8 < a_9 < a_{10}\}$. The
matrices $J, K,$ and $L$ are as follows:

$$J = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix},$$

$$K = \begin{bmatrix} \tau_1(a_1) \\ \tau_1(a_2) \\ \tau_1(a_3) \\ \tau_1(a_4) \\ \tau_1(a_5) \\ \tau_1(a_6) \\ \tau_1(a_7) \\ \tau_1(a_8) \\ \tau_1(a_9) \\ \tau_1(a_{10}) \end{bmatrix},$$

$$L = \begin{bmatrix} \tau_2(a_1) & \tau_2(a_2) & \tau_2(a_3) & \tau_2(a_4) \\ \tau_2(a_5) & \tau_2(a_6) & \tau_2(a_7) & \tau_2(a_9) \\ \tau_2(a_8) & \tau_2(a_{10}) \end{bmatrix}.$$
where

\[ d_{v_1,v_1} = \tau(a_1,a_2) + \tau(a_2,a_1), \quad d_{v_1,v_2} = \tau(a_5,a_3) + \tau(a_6,a_4), \quad d_{v_1,v_3} = \tau(a_{10},a_9), \]
\[ d_{v_2,v_1} = \tau(a_3,a_5) + \tau(a_4,a_6), \quad d_{v_2,v_3} = \tau(a_8,a_7), \]
\[ d_{v_3,v_1} = \tau(a_9,a_{10}), \quad d_{v_3,v_2} = \tau(a_7,a_8). \]

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