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Relation Between the Gutman Index of a Tree and Matchings

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Abstract

Gutman (J Chem Inf Comput Sci, 34 (1994) 1087-1089) defined the Gutman index of a graph G with vertex set $V(G)$ as

$$Gut(G) = \sum_{\{u,v\}\subseteq V(G)} \deg_G(u) \deg_G(v) d_G(u,v)\,,$$

where $\deg_G(u)$ is the degree of vertex u and $d_G(u,v)$ is the distance between vertices u and v in G. In this paper, we show that if T is a tree with vertex set $\{v_1, v_2, \ldots, v_n\}$, then $Gut(T) = m(S(T)^\omega, n-2) \prod_{i=1}^{n} \deg_T(v_i)$, where $S(T)^\omega$ is an edge-weighted subdivision of T which is obtained from T by replacing each edge $e = (u,v)$ of T with a path $u - e^* - v$ of length two, and the edge-weighting function ω satisfies $\omega(ve^*) = \frac{1}{\deg_T(v_i)}$ for each edge ve^* of $S(T)^\omega$, and $m(S(T)^\omega, n-2)$ is the sum of weights of matchings with $n-2$ edges in $S(T)^\omega$.

1 Introduction

A graph invariant is a real number related to a graph G which is invariant under graph isomorphism, that is, it does not depend on the labeling or the pictorial representation of a graph. In chemistry, graph invariants are known as topological indices. Topological indices have many applications as tools for modeling chemical and other properties of molecules. The Wiener index is one of the most studied topological indices in mathematical chemistry,

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both from a theoretical point of view and applications. This index was the first topological index to be used in chemistry. Let G be a connected graph with vertex set $V(G)$. The Wiener index of G, denoted by $W(G)$, is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v), \tag{1}$$

where $d_G(u,v)$ is the distance between vertices u and v in G.

The name Wiener index or Wiener number for the quantity defined in Eq. (1) is usual in chemical literature, since Harold Wiener [20] in 1947 seems to be the first who considered it. Wiener himself conceived W only for acyclic molecules (i.e., trees) and defined it in a slightly different - yet equivalent - manner. It has found many applications in the modelling of physicochemical, pharmacological and biological properties of organic molecules [21–23]. The definition of the Wiener index in terms of distances between vertices of a graph, such as in Eq. (1), was first given by Hosoya [12]. The Wiener index has been studied extensively (see for example Refs [2, 5, 8–10, 14, 19]).

Based on the degrees and distances in a connected graph G, Gutman [7] defined a new index-Gutman index, denoted by $Gut(G)$, as

$$Gut(G) = \sum_{\{u,v\} \subseteq V(G)} \deg_G(u) \deg_G(v) d_G(u,v), \tag{2}$$

where $\deg_G(u)$ is the degree of vertex $u \in V(G)$. The Gutman index is also called the Schultz index of the second kind and has been studied by many combinatorists and theoretical chemists (see for example [1, 4, 6, 11, 25]).

Another two topological indices related to the Wiener and Gutman indices are the so-called Kirchhoff and degree Kirchhoff indices of a connected graph G, denoted by $K(G)$ and $K'(G)$, respectively, where the Kirchhoff index was defined by Klein and Randić [13] as

$$K(G) = \sum_{\{u,v\} \subseteq V(G)} \Omega_G(u,v), \tag{3}$$

and the degree Kirchhoff index was defined by Chen and Zhang [3] as

$$K'(G) = \sum_{\{u,v\} \subseteq V(G)} \deg_G(u) \deg_G(v) \Omega_G(u,v), \tag{4}$$

where $\Omega_G(u,v)$ is the resistance distance between the vertices u and v in G.

Obviously, if T is a tree, the Wiener and Kirchhoff indices of T coincide, and so do the Gutman and degree Kirchhoff indices of T. That is, for any tree T,

$$W(T) = K(T), \quad Gut(T) = K'(T). \tag{5}$$

The following peculiar result was communicated around 1990 independently in several papers [15–18]:

$$K(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i(G)}, \tag{6}$$

where G is a connected graph with n vertices, $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G) > \mu_n(G) = 0$ are the Laplacian eigenvalues of G.

The above result is an unexpected result, because it connects the Kirchhoff index (a quantity defined on the basis of graph distances) and matrix eigenvalues.

For the degree Kirchhoff index of a connected graph G with n vertices, there is a similar formula to Eq. (6) as follows [3].

$$K'(G) = 2m \sum_{i=1}^{n-1} \frac{1}{\lambda_i(G)}, \tag{7}$$

where $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) > \lambda_n(G) = 0$ are the normalized Laplacian eigenvalues of G, and m is the number of edges of G.

Hence, if T is a tree with n vertices, then

$$W(T) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i(T)}, \tag{8}$$

$$Gut(T) = 2(n-1) \sum_{i=1}^{n-1} \frac{1}{\lambda_i(T)}. \tag{9}$$

In order to state our result, we need to introduce some notations.

An edge-set $M \subseteq E(G)$ of a graph G is a *matching* if each vertex of G is incident with at most one edge in M. Let $m(G, j)$ denote the number of matchings with j edges in G. We set $m(G, 0) = 1$ and $m(G, j) = 0$ for $j > [|V(G)|/2]$. If G^ω is an edge-weighted graph, define the weight of a matching M of G as the product of weights of edges in M. We also use $m(G^\omega, j)$ to denote the sum of weights of matchings with j edges in G, i.e.,

$$m(G^\omega, j) = \sum_M \prod_{e \in M} \omega(e), \tag{10}$$

where the sum is over all matchings of G with j edges.

Let T be a tree with vertex set $V(T) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(T) = \{e_1, e_2, \ldots, e_{n-1}\}$. Denote the subdivision of T by $S(T)$, which is obtained from T by replacing each edge $e = (u, v)$ with a path $u - e^* - v$ of length two. That is, $S(T)$ is a tree with vertex set $V(S(T)) = V(T) \cup \{e^* | e \in E(T)\}$ and edge set $E(S(T)) = \{(u, e^*), (v, e^*) | e = (u, v) \in E(T)\}$. We need to weight each edge of $S(T)$ in two ways as follows. Weight each edge (u, e^*) of $S(T)$ with weight $1/\deg_T(u)$ (where $e = (u, v)$ is an edge of T) and we obtain an edge-weighted subdivision $S(T)^\omega$. Weight each edge (u, e^*) of $S(T)$ with weight $1/\sqrt{\deg_T(u)}$ and we obtain an edge-weighted subdivision $S(T)^{\omega'}$. For the tree T in Figure 1(a), $S(T)^\omega$ and $S(T)^{\omega'}$ are illustrated in Figure 1(b) and (c), respectively.

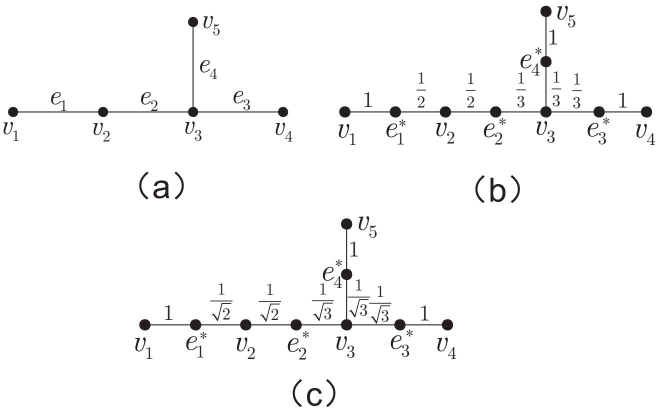

Figure 1. (a) A tree T. (b) The corresponding subdivision $S(T)^\omega$ of T. (c) The corresponding subdivision $S(T)^{\omega'}$ of T.

In [24], Yan and Yeh proved that if T is a tree with n vertices, then the Wiener index of T can be expressed by

$$W(T) = m(S(T), n-2). \tag{11}$$

A natural question is: does there exist a similar formula to Eq. (11) for the Gutman index of a tree T ?

In this work, we answer the question above and prove mainly that the Gutman index of a tree T can be calculated as $\prod_{i=1}^{n} \deg_T(v_i)$ times the sum of weights of matchings with $n-2$ edges in an edge-weighted subdivision tree $S(T)^\omega$. That is, we have the following theorem.

Theorem 1.1. Let T be a tree with n vertices $v_1, v_2, \ldots, v_n$. Keeping the notations above, then

$$Gut(T) = m(S(T)^{\omega}, n-2) \prod_{i=1}^{n} \deg_T(v_i). \tag{12}$$

2 Some lemmas

Let $M = (m_{ij})_{n\times(n-1)}$ be the vertex-edge weighted incidence matrix of a tree T with n vertices $v_1, v_2, \ldots, v_n$ and $n-1$ edges $e_1, e_2, \ldots, e_{n-1}$, defined as

$$m_{ij} = \begin{cases} \frac{1}{\sqrt{\deg_T(v_i)}} & \text{if } e_j = (v_i, \sim), \\ 0 & \text{otherwise.} \end{cases}$$

For the tree T showed in Figure 1(a),

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Lemma 2.1. Let T be a tree with the vertex set $V(T) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(T) = \{e_1, e_2, \ldots, e_{n-1}\}$, $M = (m_{ij})_{n\times(n-1)}$ be the vertex-edge weighted incidence matrix of T defined above. Then

$$MM^T = I_n + D^{-\frac{1}{2}} A D^{-\frac{1}{2}},$$

where M^T is the transpose of M, and A and D are the adjacency matrix and the diagonal matrix of vertex degrees of T, respectively.

Proof. For any $i, j \in \{1, 2, \ldots, n\}$, by the definition of M,

$$\left(MM^T\right)_{ii} = \sum_{k=1}^{n-1} m_{ik} m_{ik} = \sum_{v_k \in \Gamma(v_i)} \frac{1}{\deg_T(v_i)} = 1$$

and

$$\left(MM^T\right)_{ij} = \sum_{k=1}^{n-1} m_{ik} m_{jk},$$

where $\Gamma(v_i)$ is the set of vertices adjacent with v_i in T. Note that

$$m_{ik} m_{jk} = \frac{1}{\sqrt{\deg_T(v_i) \deg_T(v_j)}}$$

if and only if $e_k = (v_i, v_j) \in E(T)$, and $m_{ik}m_{jk} = 0$ otherwise. Hence

$$\left(MM^T\right)_{ij} = \sum_{k=1}^{n-1} m_{ik}m_{jk} = \frac{1}{\sqrt{\deg_T(v_i)\deg_T(v_j)}}$$

if $(v_i, v_j) \in E(T)$ and 0 otherwise.

Hence we have proved that $MM^T = I_n + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. ■

Let $L = D - A$ be the Laplacian matrix of a graph G with n vertices. The normalized Laplacian matrix of G is defined as $\mathcal{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = D^{-\frac{1}{2}}(D-A)D^{-\frac{1}{2}} = I_n - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. Two polynomials $\phi(G, x) = \det(xI_n - A)$ and $\chi(G, x) = \det(xI_n - \mathcal{L}(G))$ are called the characteristic polynomial and the normalized Laplacian characteristic polynomial of G, respectively.

Lemma 2.2. Let G be a connected bipartite graph with n vertices. Then the matrices $I_n - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ and $I_n + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ have the same spectrum.

Proof. Note that G is a bipartite graph. Then the matrices A and D have the following forms:

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}, D^{-\frac{1}{2}} = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}.$$

Hence

$$D^{-\frac{1}{2}}AD^{-\frac{1}{2}} = \begin{pmatrix} 0 & D_1BD_2 \\ D_2B^TD_1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & D_1BD_2 \\ (D_1BD_2)^T & 0 \end{pmatrix}.$$

Suppose α is an eigenvalue of $D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$, $x = \begin{pmatrix} x^{(1)} \\ x^{(2)} \end{pmatrix}$ is an eigenvector of $D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ corresponding to α. So

$$\begin{pmatrix} 0 & D_1BD_2 \\ (D_1BD_2)^T & 0 \end{pmatrix}\begin{pmatrix} x^{(1)} \\ x^{(2)} \end{pmatrix} = \alpha\begin{pmatrix} x^{(1)} \\ x^{(2)} \end{pmatrix}.$$

Then it may be verified that

$$\begin{pmatrix} 0 & D_1BD_2 \\ (D_1BD_2)^T & 0 \end{pmatrix}\begin{pmatrix} x^{(1)} \\ -x^{(2)} \end{pmatrix} = -\alpha\begin{pmatrix} x^{(1)} \\ -x^{(2)} \end{pmatrix}.$$

Thus, $-\alpha$ is also an eigenvalue of $D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$.

Hence the matrices $I_n - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ and $I_n + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ have the same spectrum. The lemma thus follows. ■

Let T_1 be an edge-weighted tree with vertex set $V(T_1) = \{v_1, v_2, \dots, v_n\}$ and edge-weighted function $\omega : E(T_1) \to \mathbb{R}^+$, that is weight each edge e in T_1 as $\omega_{T_1}(e)$. Let T_2 be an edge-weighted tree obtained from T_1 by changing the edge-weighted function into ω' :

$E(T_2) \to \mathbb{R}^+$, such that $\omega'_{T_2}(e) = \omega_{T_1}(e)^2$. Denote by $\mu(T_2, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(T_2, k) x^{n-2k}$ the matching polynomial of T_2, where $m(T_2, k)$ is the sum of weights of matchings of T_2 with k edges. With the notations above, we have the following lemma.

Lemma 2.3. The characteristic polynomial of the edge-weighted tree T_1 is equal to the matching polynomial of the edge-weighted tree T_2, i.e.

$$\phi(T_1, x) = \mu(T_2, x).$$

Proof. We may assume that T_1 has at least one edge, otherwise the assertion is trivial. Let u be an endpoint of T_1 and v its unique neighbor. Assume that the vertices are labelled so that u is the first and v is the second, and $\omega_{T_1}(uv) = a$. Let A_1, A'_1 and A''_1 be the adjacency matrices of T_1, $T_1 - u$ and $T_1 - u - v$, respectively, and let I_n, I_{n-1} and I_{n-2} denote the identity matrices of size n, $n-1$ and $n-2$, respectively. Then we have

$$\phi(T_1, x) = \det(xI - A_1) = \begin{vmatrix} x & -a & 0 & \cdots & 0 \\ -a & x & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & x \end{vmatrix}_{n \times n}.$$

If we expand this determinant by its first row, and then expand the second term by its first column, we obtain

$$\begin{aligned} \phi(T_1, x) &= \det(xI_n - A_1) \\ &= x \det(xI_{n-1} - A'_1) - a^2 \det(xI_{n-2} - A''_1) \\ &= x\phi(T_1 - u, x) - a^2 \phi(T_1 - u - v, x). \end{aligned}$$

For the tree T_2, we have $\omega'_{T_2}(uv) = a^2$. Note that, if $k \geq 1$, then $m(T_2, k) = m(T_2 - u, k) + \omega'_{T_2}(uv) m(T_2 - u - v, k-1)$. So we have

$$\begin{aligned} \mu(T_2, x) &= \sum_{k \geq 0} (-1)^k m(T_2, k) x^{n-2k} \\ &= \sum_{k \geq 0} (-1)^k m(T_2 - u, k) x^{n-2k} + \omega'_{T_2}(uv) \sum_{k \geq 1} (-1)^k m(T_2 - u - v, k-1) x^{n-2k} \\ &= x\mu(T_2 - u, x) + a^2 \sum_{i \geq 0} (-1)^{i+1} m(T_2 - u - v, i) x^{n-2(i+1)} \\ &= x\mu(T_2 - u, x) - a^2 \sum_{i \geq 0} (-1)^i m(T_2 - u - v, i) x^{n-2-2i} \\ &= x\mu(T_2 - u, x) - a^2 \mu(T_2 - u - v, x). \end{aligned}$$

Since $\phi(T_1, x)$ and $\mu(T_2, x)$ satisfies the same recurrence relation, the theorem follows by induction. ■

3 Proof of the main result

In this section, we give the proof of Theorem 1.1.

Proof of Theorem 1.1. Let M be the vertex-edge weighted incidence matrix defined in Section 2. By the definition of $S(T)^{\omega'}$, it is well known that the adjacency matrix of $S(T)^{\omega'}$, denoted by $A(S(T)^{\omega'})$, where (v_i, e_j^*)-entry of $A(S(T)^{\omega'})$ is $1/\sqrt{\deg_T(v_i)}$ for the vertices v_i and e_j^* adjacent, and 0 otherwise. So $A(S(T)^{\omega'})$ has the following form:

$$A(S(T)^{\omega'}) = \begin{pmatrix} 0 & M \\ M^T & 0 \end{pmatrix}.$$

Then the characteristic polynomial of $S(T)^{\omega'}$ can be expressed by:

$$\begin{aligned}
\phi(S(T)^{\omega'}, x) &= \det\left(xI_{2n-1} - A(S(T)^{\omega'})\right) \\
&= \det\begin{pmatrix} xI_n & -M \\ -M^T & xI_{n-1} \end{pmatrix} \\
&= x^{n-1} \det\begin{pmatrix} xI_n & -M \\ x^{-1}M^T & I_{n-1} \end{pmatrix} \\
&= x^{n-1} \det\begin{pmatrix} xI_n - x^{-1}MM^T & 0 \\ -x^{-1}M^T & I_{n-1} \end{pmatrix} \\
&= x^{n-1} \det\left(xI_n - x^{-1}MM^T\right) \\
&= x^{-1} \det\left(x^2 I_n - MM^T\right).
\end{aligned}$$

By Lemma 2.1, we have $MM^T = I_n + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. Hence we have

$$\phi(S(T)^{\omega'}, x) = x^{-1} \det\left(x^2 I_n - (I_n + D^{-\frac{1}{2}}AD^{-\frac{1}{2}})\right).$$

By Lemma 2.2, $I_n + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ and $\mathcal{L}(T) = I_n - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ have the same spectrum. Hence we have

$$\begin{aligned}
\phi(S(T)^{\omega'}, x) &= x^{-1} \det\left(x^2 I_n - (I_n + D^{-\frac{1}{2}}AD^{-\frac{1}{2}})\right) \\
&= x^{-1} \det\left(x^2 I_n - (I_n - D^{-\frac{1}{2}}AD^{-\frac{1}{2}})\right) \\
&= x^{-1} \det\left(x^2 I_n - \mathcal{L}(T)\right) \\
&= x^{-1}\chi(T, x^2),
\end{aligned} \tag{13}$$

where $\chi(T, x)$ denotes the normalized Laplacian characteristic polynomial of T.

By the definition of $S(T)^{\omega'}$, $S(T)^{\omega}$ and Lemma 2.3, we have

$$\phi(S(T)^{\omega'}, x) = \mu(S(T)^{\omega}, x). \tag{14}$$

By Eqs. (13) and (14),

$$\chi(T, x^2) = x\mu(S(T)^{\omega}, x). \tag{15}$$

By Eq. (9),

$$Gut(T) = 2(n-1)\sum_{k=1}^{n-1}\frac{1}{\lambda_k}, \tag{16}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} > \lambda_n = 0$ are the normalized Laplacian eigenvalues of T.

By Theorem 2.1 of [3],

$$\left(\prod_{i=1}^{n}\deg_T(v_i)\right)\left(\prod_{k=1}^{n-1}\lambda_k\right) = 2m\tau(T) = 2(n-1), \tag{17}$$

since the number $\tau(T)$ of spanning trees equals one.

By Eqs. (16) and (17), we have

$$Gut(T) = \left(\prod_{i=1}^{n}\deg_T(v_i)\right)\sum_{k=1}^{n-1}\frac{\lambda_1\lambda_2\cdots\lambda_{n-1}}{\lambda_k}. \tag{18}$$

Note that $\chi(T,x) = x(x-\lambda_1)(x-\lambda_2)\cdots(x-\lambda_{n-1})$. Then $(-1)^{n-2}\sum_{k=1}^{n-1}\frac{\lambda_1\lambda_2\cdots\lambda_{n-1}}{\lambda_k}$ is the coefficient of x^2 in $\chi(T,x)$.

By Eq. (15), the coefficient of x^4 in $\chi(T,x^2)$ equals the coefficient of x^3 in $\mu(S(T)^{\omega},x)$. Note that

$$\mu(S(T)^{\omega}, x) = \sum_{k=0}^{n-1}(-1)^k m(S(T)^{\omega}, k)x^{2n-1-2k}. \tag{19}$$

In Eq. (19), if $2n-1-2k = 3$, we obtain $k = n-2$. Then the coefficient of x^3 in $\mu(S(T)^{\omega}, x)$ is $(-1)^{n-2}m(S(T)^{\omega}, n-2)$.

So we have proved that

$$\sum_{k=1}^{n-1}\frac{\lambda_1\lambda_2\cdots\lambda_{n-1}}{\lambda_k} = m(S(T)^{\omega}, n-2). \tag{20}$$

By Eqs. (18) and (20),

$$Gut(T) = \left(\prod_{i=1}^{n}\deg_T(v_i)\right) m(S(T)^{\omega}, n-2).$$

The theorem thus follows. ∎

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