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Combinatorial Green's function of a graph and applications to networks

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ABSTRACT

Given a finite weighted graph G and its Laplacian matrix L, the *combinatorial Green's function* $\mathcal{G}$ of G is defined to be the inverse of $L + J$, where J is the matrix each of whose entries is 1. We prove the following intriguing identities involving the entries in $\mathcal{G} = (g_{ij})$ whose rows and columns are indexed by the vertices of G: $g_{aa} + g_{bb} - g_{ab} - g_{ba} = \kappa(G_{a*b})/\kappa(G)$, where $\kappa(G)$ is the complexity or tree-number of G, and G_{a*b} is obtained from G by identifying two vertices a and b. As an application, we derive a simple combinatorial formula for the resistance between two *arbitrary* nodes in a finite resistor network. Applications to other similar networks are also discussed.

1. Introduction

Given a finite graph G with n vertices and its Laplacian matrix $L = L(G)$, we define the *augmented Laplacian matrix* of G to be $\mathcal{L} = \mathcal{L}(G) = L + J$, where J denotes the $n \times n$ matrix each of whose entries is 1. The *tree-number* or *complexity* of G, denoted by $\kappa(G)$, is the number of spanning trees in G. Temperley [7] showed

$$n^2 \cdot \kappa(G) = \det \mathcal{L}(G), \tag{1.1}$$

which is an analog of the Matrix-Tree theorem [3] that states every cofactor of L equals $\kappa(G)$.

An important reason for our interest in the augmented Laplacian matrix $\mathcal{L}$ is that it is invertible when $\kappa(G)$ is nonzero, unlike the Laplacian matrix L. Moreover, $\mathcal{L}^{-1}$ acts as an "inverse" of L for solving the Laplace equations $L\mathbf{x} = \mathbf{y}$ in the sense that $\mathbf{x} = \mathcal{L}^{-1}\mathbf{y}$ is a desired solution if $\mathbf{y}$ is in the column space of L (see Section 4). An interesting application of these observations can be found in

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Stephenson and Zelen's work on the information centrality for networks (see Appendix in [6]). Similar methods using Green's functions were applied to compute the resistances in a finite resistor network in terms of the eigenvalues and eigenvectors of the associated Kirchhoff matrix (see e.g. [2,10]).

We define the *combinatorial Green's function* $\mathcal{G} = \mathcal{G}(G)$ of a connected finite graph G to be the inverse of its augmented Laplacian matrix $\mathcal{L}(G)$:

$$\mathcal{G}(G) = \mathcal{L}(G)^{-1}.$$

The main result of this paper is the following intriguing identities involving the entries in $\mathcal{G}(G) = (g_{ij})$ whose rows and columns are indexed by the vertices of G. Let G_{a*b} denote the *contraction* of G obtained by identifying two *arbitrary* vertices a and b (see Section 2). We will show

$$g_{aa} + g_{bb} - g_{ab} - g_{ba} = \frac{\kappa(G_{a*b})}{\kappa(G)}. \tag{1.2}$$

The proof of (1.2) will be based on a generalization of (1.1) and combinatorial analysis of the Laplacian matrix of G_{a*b}. In subsequent sections, we will see that all of our definitions and results are also valid for a finite weighted graph G where the weights are non-negative.

As an application of our main result, we will derive a combinatorial formula for the network resistance R_{ab} between two *arbitrary* nodes a and b in a finite resistor network. We will see that our formula for R_{ab} specializes to that of the effective resistance $r(a, b, G)$ [8] which is valid only for adjacent vertices a and b in a connected graph G. We will also discuss other networks (see e.g. [6]) that are similar to resistor networks.

2. Preliminaries

We will assume basic familiarity with standard terminologies from graph theory. One may refer to most textbooks (e.g., [1] or [9]) for their definitions. The graphs that we consider are finite, unoriented, and loopless, but they may have multiple edges. A *complete graph* has one edge between each pair of vertices. An edge connecting two distinct vertices i and j will be denoted ij.

2.1. Laplacian matrix of a weighted graph. A *weighted graph* G is a loopless graph such that a non-negative weight $w_{ij} = w_{ji}$ is assigned to each edge ij, where i and j are distinct vertices. A weighted graph may be regarded as a complete graph with non-negative weights assigned to its edges. An unweighted graph may be treated as a weighted graph by letting w_{ij} equal the number of edges between i and j. The *adjacency matrix* of G with the vertex set $V(G) = [n] = \{1, 2, \dots, n\}$ is the $n \times n$ symmetric matrix $A = A(G) = (a_{ij})$ whose entries are given by $a_{ij} = w_{ij}$ for $i \neq j$ and $a_{ii} = 0$ for every i. The *degree* d_i of the vertex i is defined by $d_i = \sum_j w_{ij}$ where $w_{ii} = 0$ for every i. We define $D = D(G)$ to be the $n \times n$ diagonal matrix whose diagonal entries are d_i.

The *Laplacian matrix* of a finite weighted graph G is $L = L(G) = D - A$, which is real symmetric. Since the sum of the entries in every row and every column of L is zero, every cofactor of L has the same value. We define the *complexity* $\kappa(G)$ of G to be the value of any cofactor of L. If G is unweighted, $\kappa(G)$ equals the tree number in G by the Matrix-Tree theorem. A weighted graph is defined to be *connected* if $\kappa(G) \neq 0$.

2.2. Contraction of a weighted graph. An important minor of a graph G is the *contraction* G_{a*b} of G that is obtained by shrinking (contracting) the edge ab to a point. We may contract ab by identifying the vertex a with the vertex b so that all edges that were incident to a and b in G are incident to b in G_{a*b} (and a is no longer a vertex of G_{a*b}). As a weighted graph, we define the contraction G_{a*b} of G to be a weighted graph satisfying the following conditions. Let w and ω denote the weights, and let d and δ denote the degrees in G and G_{a*b}, respectively.

- $V(G_{a*b}) = V(G) \setminus \{a\}$,

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- $\omega_{ib} = w_{ia} + w_{ib}$, and $\omega_{ij} = w_{ij}$ if $i, j \neq b$,
- $\delta_b = d_a + d_b - 2w_{ab}$, and $\delta_i = d_i$ if $i \neq b$.

Although the roles of a and b may be switched in defining G_{a*b}, we will not do so in order to avoid confusion in what follows. It is important to note that G_{a*b} is defined as a weighted graph even when $w_{ab} = 0$ in G. Hence, we may have $\kappa(G_{a*b}) > \kappa(G)$. For example, if G has three vertices a, b, and c and $w_{ac} = w_{bc} = 1$ and $w_{ab} = 0$, then $\kappa(G_{a*b}) = 2$ and $\kappa(G) = 1$.

Since a (weighted) graph can be recovered from its Laplacian matrix, we may also define G_{a*b} to be the graph whose Laplacian matrix is obtained from $L = L(G)$ by applying the following sequence of operations: ($R_i(M)$ and $C_j(M)$ denote row i and column j of a matrix M, respectively)

(1) replace $R_b(L)$ by $R_a(L) + R_b(L)$ (denote the result by M_1),
(2) replace $C_b(M_1)$ by $C_a(M_1) + C_b(M_1)$ (denote the result by M_2), and
(3) delete $R_a(M_2)$ and $C_a(M_2)$ (denote the result by M_3).

Clearly, the entries in M_2 except those in $R_a(M_2)$ and $C_a(M_2)$ are the weights and degrees for G_{a*b} as described above. The last operation (3) corresponds to eliminating the vertex a from $V(G)$. It is clear that we have $M_3 = L(G_{a*b})$.

Note that the above three operations may be applied to any square matrix M, and we will denote the resulting matrix by M_{a*b}, called a *contraction* of M. With this notation, we have

$$L(G_{a*b}) = L(G)_{a*b}. \tag{2.1}$$

We note the following useful properties of contractions. If M has the zero sum property for its rows and columns, then so does any contraction of M. If M has rank $\leqslant 1$, then so does any contraction of M. The sum of all entries of M equals that of any contraction of M. We also have

$$(M + N)_{a*b} = M_{a*b} + N_{a*b}. \tag{2.2}$$

Example. This example will be discussed again in Section 4. Let G be a weighted graph with the vertex set $\{1, 2, 3, 4\}$ with the weights $w_{13} = 0$, $w_{24} = 2$, and $w_{ij} = 1$ otherwise. Then

$$L(G) = \begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 4 & -1 & -2 \\ 0 & -1 & 2 & -1 \\ -1 & -2 & -1 & 4 \end{pmatrix}.$$

The following are the Laplacian matrices for various contractions of G:

$$L(G_{1*3}) = \begin{pmatrix} 4 & -2 & -2 \\ -2 & 4 & -2 \\ -2 & -2 & 4 \end{pmatrix} \quad L(G_{2*4}) = \begin{pmatrix} 2 & 0 & -2 \\ 0 & 2 & -2 \\ -2 & -2 & 4 \end{pmatrix} \quad L(G_{1*2}) = \begin{pmatrix} 4 & -1 & -3 \\ -1 & 2 & -1 \\ -3 & -1 & 4 \end{pmatrix}.$$

Lemma 1. *Let $M = (m_{ij})$ be an $n \times n$ matrix, and let μ_{ij} be the (i, j)-cofactor of M, i.e., $\mu_{ij} = (-1)^{i+j} \det M_{ij}$, where M_{ij} is obtained from M by removing $R_i(M)$ and $C_j(M)$. Then the following identity holds for all i and j:*

$$\det M_{i*j} = \mu_{ii} + \mu_{jj} - \mu_{ij} - \mu_{ji}.$$

Proof. First, we will prove the case $i = 1$ and $j = 2$. Note that M_{11} and M_{12} differ only in their first columns. Also, M_{22} and M_{21} differ only in their first columns. By the linearity of determinant on columns, we have

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$$\mu_{11} - \mu_{12} = \det M_{11} + \det M_{12} = \det M' \quad \text{and}$$
$$\mu_{22} - \mu_{21} = \det M_{22} + \det M_{21} = \det M'',$$

where

$$M' = \begin{pmatrix} m_{22} + m_{21} & m_{23} & \cdots & m_{2n} \\ m_{32} + m_{31} & m_{33} & \cdots & m_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{n2} + m_{n1} & m_{n3} & \cdots & m_{nn} \end{pmatrix} \qquad M'' = \begin{pmatrix} m_{11} + m_{12} & m_{13} & \cdots & m_{1n} \\ m_{31} + m_{32} & m_{33} & \cdots & m_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{n1} + m_{n2} & m_{n3} & \cdots & m_{nn} \end{pmatrix}.$$

Note that M' and M'' differ only in their first rows. It is now clear by the linearity of determinant on rows that $\det M' + \det M'' = \det M_{1*2}$.

In general, assume $1 \leqslant i < j \leqslant n$. Let P be the matrix obtained from M by switching row i with row 1, row j with row 2, column i with column 1, and column j with column 2. Let π_{ij} be the (i, j)-cofactor of P. Then $\pi_{11} = \mu_{ii}$ because P_{11} and M_{ii} differ by an even permutation of rows and columns. Similarly, we have $\pi_{22} = \mu_{jj}$, $\pi_{12} = \mu_{ij}$, and $\pi_{21} = \mu_{ji}$. Also it is easily checked that M_{i*j} and P_{1*2} differ by an even permutation of rows and columns. Therefore, $\det M_{i*j} = \det P_{1*2}$, and the result follows. □

3. Main theorems

If an $n \times n$ matrix M satisfies the zero sum condition for its rows and columns, then it is easily checked that every cofactor of M has the same value (see e.g. [4, Lemma 5.6.5] for a proof). For example, we've already seen that every cofactor of the Laplacian matrix $L(G)$ of a finite graph G is $\kappa(G)$. The following is a generalization of Temperley's tree-number formula (1.1).

Theorem 2. *Let M be an $n \times n$ matrix such that the sum of entries in every row and every column is zero, and let μ denote the value of any cofactor of M. Let U be an $n \times n$ rank 1 matrix, and let σ denote the sum of all of its entries. Then the following identity holds*:

$$\mu \cdot \sigma = \det(M + U).$$

Proof. Let $M + U = (C_1 + D_1, C_2 + D_2, \ldots, C_n + D_n)$, where C_i's and D_i's are the columns of M and U, respectively. Given any subset $S \subset [n]$, define $\Delta_S = (X_1, X_2, \ldots, X_n)$, where $X_i = D_i$ if $i \in S$ and $X_i = C_i$ if $i \notin S$. For example, $\Delta_\emptyset = M$ and $\Delta_{[n]} = U$. By the multilinearity of determinant on columns, we have

$$\det(M + U) = \sum_{S \subset [n]} \det \Delta_S$$

where the sum is over all subsets S of $[n]$. Clearly, we have $\det \Delta_\emptyset = \det M = 0$. Also, if $|S| > 1$, then $\det \Delta_S = 0$ because U has rank 1 and every column of U is a multiple of a single column. Furthermore, if we let σ_i be the sum of all entries in D_i, then $\det \Delta_{\{i\}} = \mu \cdot \sigma_i$ for every $i \in [n]$. Therefore, we have

$$\det(M + U) = \sum_{0 \leqslant i \leqslant n} \det \Delta_{\{i\}} = \sum_{0 \leqslant i \leqslant n} \mu \cdot \sigma_i = \mu \cdot \sigma. \qquad \square$$

Recall that for a finite weighted graph G, we *defined* $\kappa(G)$ to be the value of any cofactor of $L(G)$. Let $\mathcal{L}(G) = L(G) + J$. The following is the weighted version of Temperley's tree-number formula (1.1).

Corollary 3. *For a finite weighted graph G with n vertices, we have*

$$n^2 \cdot \kappa(G) = \det \mathcal{L}(G).$$

It follows that $\mathcal{L} = \mathcal{L}(G)$ is non-singular if $\kappa(G) \neq 0$. As in the case of unweighted graphs, we define the combinatorial Green's function of a finite weighted graph G to be $\mathcal{G} = \mathcal{G}(G) = \mathcal{L}^{-1}$. Assume that the rows and columns of $\mathcal{G}$ are indexed by the vertices of G. The following is the main theorem of the paper.

Theorem 4. *Let G be a finite weighted graph with n (> 1) vertices and $\kappa(G) \neq 0$. The entries in $\mathcal{G} = (g_{ij})$ satisfy the following identities*:

$$g_{aa} + g_{bb} - g_{ab} - g_{ba} = \frac{\kappa(G_{a*b})}{\kappa(G)}$$

for any arbitrary pair of distinct vertices a and b of G.

Proof. Let l_{ij} be the (i, j)-cofactor of $\mathcal{L}$. Note that we have $g_{ij} = l_{ij} / \det \mathcal{L}$ because $\mathcal{G} = \mathcal{L}^{-1}$. We also have $\det \mathcal{L} = n^2 \kappa(G)$ by Corollary 3. Therefore,

$$\begin{aligned} g_{aa} + g_{bb} - g_{ab} - g_{ba} &= \frac{1}{n^2 \kappa(G)} (l_{aa} + l_{bb} - l_{ab} - l_{ba}) \\ &= \frac{1}{n^2 \kappa(G)} \det(\mathcal{L}_{a*b}) \quad \text{(by Lemma 1)} \\ &= \frac{1}{n^2 \kappa(G)} \det\bigl(L(G)_{a*b} + J_{a*b}\bigr) \quad \bigl(\text{by (2.2)}\bigr). \end{aligned}$$

Since J has rank 1 and the sum of its entries is n^2, the same is true for J_{a*b}. Also we have $L(G)_{a*b} = L(G_{a*b})$ by (2.1), and every cofactor of $L(G_{a*b})$ equals $\kappa(G_{a*b})$. Therefore, by Theorem 2, we have

$$\det\bigl(L(G)_{a*b} + J_{a*b}\bigr) = n^2 \kappa(G_{a*b}),$$

and the theorem follows. □

4. Applications to networks

In this section, an (undirected) network is represented by a finite connected weighted graph G with n vertices. Its Laplacian matrix L may be regarded as a symmetric linear transformation on $\mathbb{R}^n$ equipped with the standard inner product. Let $\mathbf{1}$ be the column vector each of whose entry is 1, and $\mathbf{0}$ the zero vector in $\mathbb{R}^n$. Since $\mathcal{L} = L + J$ is invertible, let $\mathcal{G} = \mathcal{L}^{-1}$.

Lemma 5. *Suppose $\mathbf{y} \perp \mathbf{1}$. Then, $\mathbf{x} = \mathcal{G}\mathbf{y}$ is a solution to $L\mathbf{x} = \mathbf{y}$.*

Proof. Let $\mathbf{x} = \mathcal{G}\mathbf{y}$. Then we have $\mathcal{L}\mathbf{x} = \mathbf{y}$. Multiplying this equation by J, we get $JL\mathbf{x} + J^2\mathbf{x} = J\mathbf{y}$. Since $JL\mathbf{x} = J\mathbf{y} = \mathbf{0}$ and $J^2 = nJ$, we see that $J\mathbf{x} = \mathbf{0}$. Therefore $L\mathbf{x} = (L + J)\mathbf{x} = \mathcal{L}\mathbf{x} = \mathbf{y}$. □

In what follows, one may refer to [5] for relevant definitions and laws concerning electrical circuits. Our background discussion of a resistor network will follow [10]. Let G represent a finite resistor network consisting of $[n] = \{1, 2, \dots, n\}$ as nodes and a resistor for each pair $i, j \in [n]$ with the resistance $r_{ij} = r_{ji}$. Let the weight of the edge ij in G be the conductance $c_{ij} = c_{ji} = r_{ij}^{-1}$. If i and j are not

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connected by a resistor, then $r_{ij} = \infty$ and $c_{ij} = 0$. Let $\mathcal{G} = (g_{ij})$ be the combinatorial Green's function of G.

The *network resistance* R_{ij} between i and j is what an ohm meter would read if it is connected to i and j. The electrical potential at the node i is denoted by V_i and the net current flowing *into* the network at the node i by I_i with the constraint $\sum_{i=1}^{n} I_i = 0$. The Kirchhoff's law states $\sum_{i=1}^{n} c_{ij}(V_i - V_j) = I_i$ for each i, which is equivalent to

$$L\vec{V} = \vec{I}, \tag{4.1}$$

where $\vec{V}$ and $\vec{I}$ are vectors in $\mathbb{R}^n$ whose components are V_i and I_i, respectively. In order to compute the resistance R_{ab} between two nodes a and b, an external current source with current I is connected to a and b so that $I_a = I$, $I_b = -I$ and $I_i = 0$ for $i \neq a, b$. Then, the network resistance is given by

$$R_{ab} = \frac{V_a - V_b}{I}. \tag{4.2}$$

Since we have $\vec{I} \perp \mathbf{1}$, Lemma 5 implies that $\vec{V} = \mathcal{G}\vec{I}$ is a solution to (4.1). Therefore, we have $V_a = (g_{aa} - g_{ab})I$ and $V_b = (g_{ba} - g_{bb})I$. Now the following theorem is immediate from (4.2) and Theorem 4.

Theorem 6. *The network resistance between two arbitrary nodes a and b in a finite resistor network G is the ratio*

$$R_{ab}(G) = \frac{\kappa(G_{a*b})}{\kappa(G)}.$$

Examples. 1. Let G be the complete graph K_n with every weight equal to 1. Then $\kappa(G_{a*b})$ equals the number of the spanning trees in G that contain the edge ab. Since a spanning tree in G has $n-1$ edges, one obtains the identity $\binom{n}{2}\kappa(G_{a*b}) = (n-1)\kappa(G)$. Hence, $R_{ab} = \kappa(G_{a*b})/\kappa(G) = (n-1)/\binom{n}{2} = 2/n$.

2. Let G be a cycle C_n of length n with every weight equal to a constant w. Given two nodes a and b, suppose G_{a*b} is a one point union of two cycles one of length m and the other of length $(n-m)$. Clearly, we have $\kappa(G) = nw^{n-1}$ and $\kappa(G_{a*b}) = m(n-m)w^{n-2}$. Hence, $R_{ab} = m(n-m)/nw$.

3. Theorem 6 enables relative ranking among R_{ab}'s without knowing their exact values. Referring back to the example in Section 2, we have $\kappa(G_{1*3}) = 12$, $\kappa(G_{2*4}) = 4$, and $\kappa(G_{a*b}) = 6$ for all other pairs a and b. So the network resistances can be ranked in the order of R_{13}, R_{ab}, and R_{24}.

4. If G is a finite graph (unweighted), and if a and b are required to be adjacent in G, then Theorem 6 specializes to the formula for the *effective resistances* $r(a, b, G)$ by Thomassen [8]. It is shown that $r(a, b, G) = \tau_{ab}(G)/\tau(G)$, where $\tau_{ab}(G)$ is the number of spanning trees in G containing the edge ab and $\tau(G) = \kappa(G)$, the tree-number of G. Since $\kappa(G_{a*b}) = \tau_{ab}(G)$ when a and b are adjacent in G, we see that $r(a, b, G) = R_{ab}(G)$ in this case.

5. The network conductance between two arbitrary nodes a and b in a resistor network is defined $C_{ab} = R_{ab}^{-1} = \kappa(G)/\kappa(G_{a*b})$. It is interesting to note that this exact formula appeared in the computation of the amount of information I_{ab} contained in *all* possible paths between two arbitrary nodes a and b in a network [6]. Here, a network is represented by a finite weighted graph G whose weights correspond to, e.g., the frequency of communication. Based on the theory of statistical estimation, it was shown that $I_{ab} = (g_{aa} + g_{bb} - 2g_{ab})^{-1}$, where g_{ij} are the entries in $\mathcal{G}(G)$. Hence, it follows from Theorem 4 that $I_{ab} = \kappa(G)/\kappa(G_{a*b})$.

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