A combinatorial Laplacian with vertex weights*

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Abstract

One of the classical results in graph theory is the matrix-tree theorem which asserts that the determinant of a cofactor of the combinatorial Laplacian is equal to the number of spanning trees in a graph (see [1, 7, 11, 15]). The usual notion of the combinatorial Laplacian for a graph involves edge weights. Namely, a Laplacian $\mathcal{L}$ for G is a matrix with rows and columns indexed by the vertex set V of G, and the (u, v)-entry of $\mathcal{L}$, for u, v in G, $u \neq v$, is associated with the edge-weight of the edge (u, v). It is not so obvious to consider Laplacians with vertex weights (except for using some symmetric combinations of the vertex weights to define edge-weights). In this note, we consider a vertex weighted Laplacian which is motivated by a problem arising in the study of algebro-geometric aspects of the Bethe Ansatz [8]. The usual Laplacian can be regarded as a special case with all vertex-weights equal. We will generalize the matrix-tree theorem to matrix-tree theorems of counting "rooted" directed spanning trees. In addition, the characteristic polynomial of the vertex-weighted Laplacian has coefficients with similar interpretations. We also consider subgraphs with non-trial boundary. We will shown that the Laplacian with Dirichlet boundary condition has its determinant equal to the number of rooted spanning forests. The usual matrix-tree theorem is a special case with the boundary consisting of one single vertex.

1 Laplacians with vertex weights

Let G denote a graph with vertex set $V = \{v_1, \cdots, v_n\}$ and edge set E. (The general case with edge-weights will be discussed later.) The combinatorial Laplacian L is defined by

$$L(u,v) = \begin{cases} d_v & \text{if } u = v \\ -1 & \text{if } u \text{ and } v \text{ are adjacent } (u_u \sim v_v) \\ 0 & \text{otherwise} \end{cases}$$

where d_v denotes the degree of v. The matrix-tree theorem states that the number of spanning trees of G is equal to the determinant of any cofactor of L.

*Appeared in *Journal of Combinatorial Theory, (A)*, **75** (1996), 316-327.

Suppose vertex v has weight α_v. We define the following matrix:

$$\mathbf{L}(u,v) = \begin{cases} \sum_{z \sim v} \alpha_z & \text{if } u = v \\ -\alpha_v & \text{if } u \sim v \\ 0 & \text{otherwise} \end{cases}$$

For any function $f : V \to \mathbb{R}$, we have

$$\mathbf{L}f(v) = \sum_{\substack{u \\ u \sim v}} \alpha_u (f(v) - f(u))$$

Although $\mathbf{L}$ is not symmetric, it is easy to see that $\mathbf{L}$ is equivalent to the following symmetric matrix $\mathcal{L}$ of G:

$$\mathcal{L}(u,v) = \begin{cases} \sum_{z \sim v} \alpha_v & \text{if } u = v \\ -\sqrt{\alpha_u \ \alpha_v} & \text{if } u \sim v \\ 0 & \text{otherwise} \end{cases}$$

Let W denote the $n \times n$ diagonal matrix with the (v,v)-entry having value α_v. Then we have

$$\mathbf{L} \ = \ W^{-1/2} \ \mathcal{L} \ W^{1/2}$$

We consider the incidence matrix B with rows indexed by vertices and columns indexed by edges as follows:

$$B(v,e) = \begin{cases} \sqrt{\alpha_u} & \text{if } e = \{u,v\}, u = v_i, v = v_j \text{ and } i \leq j \\ -\sqrt{\alpha_u} & \text{if } e = \{u,v\}, u = v_i, v = v_j \text{ and } i > j \\ 0 & \text{otherwise} \end{cases}$$

Although the definition of B might first seem to be somewhat imposing, it is formulated exactly for our need in the generalization of matrix-tree theorem in the next section. We note that

$$\mathcal{L} = B \ B^* \tag{1}$$

where B^* denotes the transpose of B. Therefore, $\mathcal{L}$ is a non-negative matrix. We remark that B^* can be regarded as the weighted coboundary operator from the 0-chains C_0, with vertices as the basis, to 1-chains C_1, with edges as the basis, while the matrix B is just the weighted boundary operator from C_1 to C_0.

$$C_0 \underset{B}{\overset{B^*}{\rightleftarrows}} C_1$$

Suppose we start with a graph G with edge-weights. For each unordered pair $e = \{u,v\}$, there is an associated weight $\omega_e = \omega_{u,v} \geq 0$. Let T denote a diagonal matrix indexed by the edges of G and in which the (e,e)-entry has value w_e. The Laplacian for the graph with edge weights and edge weights is just

$$BTB^*$$

We remark that Lovász [10] considered a version of the Laplacian with vertex-weights, which is equivalent to the special case with edge weights $\omega_e = \alpha_u \alpha_v$ where $e = \{u, v\}$.

2 Rooted directed trees

In the graph G, the vertex v has weight α_v. Let T denote a tree in G. For a vertex v in T, we define the rooted directed tree T_v by orienting every edge of T towards the root v. In other words, the edge set of T_v consists of

$$E(T_v) = \{(x,y) : \{x,y\} \in T \text{ and } d_T(v,x) > d_T(v,y)\}$$

where $d_T(v,x)$ denotes the distance in T between v and x. For each rooted directed tree T_v, we define the weight of T_v as follows:

$$\omega(T_v) = \prod_{(x,y)\in E(T_v)} \alpha_y$$

Also,

$$\kappa_v(G) = \sum_T \omega(T_v)$$

and

$$\kappa(G) = \sum_v \kappa_v(G)$$

We note that for the special case of $\alpha_v = 1$ for all v, $\kappa(G)$ is exactly the number of rooted directed spanning trees.

We will prove a generalization of the matrix-tree theorem as follows:

Theorem 1 *The cofactor of $\mathcal{L}$ obtained by deleting the u-th row and the v-th column has determinant*

$$(\alpha_u \alpha_v)^{1/2} (\sum_z \alpha_z)^{-1} \kappa(G)$$

The proof of Theorem 1 follows from the following facts on the Laplacian:

Fact 1: $W^{1/2}\bar{1}$ is an eigenvector of $\mathcal{L}$ with eigenvalue 0.

Proof: We consider the vector $W^{1/2}\bar{\mathbf{1}}$ where $\bar{\mathbf{1}}$ is the vector all of whose cordinates are 1. It is easy to check that $\mathcal{L}\ W^{1/2}\bar{1} = 0$.

Fact 2: If G is connected, then we have rank $\mathcal{L} = n - 1$.

Proof: Suppose $\mathcal{L}$ has eigenvalues $0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$. We have

$$\begin{aligned}
\lambda_1 &= \min_{\sum_v f(v)\sqrt{\alpha_v} = 0} \frac{\langle f,\ \mathcal{L}\ f\rangle}{\langle f,\ f\rangle} \\
&= \min_{\sum_v g(v)\alpha_v = 0} \frac{\langle W\ g, \mathbf{L}\ g\rangle}{\langle W\ g, g\rangle} \\
&= \min_{\sum_v g(v)\alpha_v = 0} \frac{\sum_{u\sim v} (g(u) - g(v))^2 \alpha_u \alpha_v}{\sum_v g(v)^2 \alpha_v}
\end{aligned}$$

Therefore, the fact that G is connected and $\lambda_1 = 0$ implies that g is a multiple of the all 1's vector, which is a contradiction.

We remark that if G has k connected components, then rank $\mathcal{L} = n - k$. Let *adj* $\mathcal{L}$ denote the matrix of cofactors (adjugate) of $\mathcal{L}$.

Fact 3: If G is connected, then $W^{-1/2}$ *adj* $\mathcal{L}$ $W^{-1/2}$ is a scalar multiple of J, the matrix all of whose entries are 1.
Proof: Since $\mathcal{L}$ *adj* $\mathcal{L} = ($*det* $\mathcal{L})\ I\ = 0$, each column of *adj* $\mathcal{L}$ is in the kernel of $\mathcal{L}$, which is 1-dimensional by Fact 2. So each column of *adj* $\mathcal{L}$ is a multiple of $W^{1/2}\ \bar{1}$. Since $\mathcal{L}$ is symmetric, *adj* $\mathcal{L}$ is symmetric. Therefore we deduce that *adj* $\mathcal{L}$ is a scalar multiple of $W^{1/2}\ J\ W^{1/2}$.

Now, we are ready to prove Theorem 1.

Proof of Theorem 1:
It suffices to show that the cofactor M, which is obtained by deleting the v-th row and v-th column has determinant $\alpha_v(\sum_u \alpha_u)^{-1}\kappa(G)$. Since $\mathcal{L} = B\ B^*$, we have $M = B_0\ B_0^*$ where B_0 denotes the submatrix of B without the v-th column.

By the Binet-Cauchy Theorem [9], we have

$$\det\ B_0\ B_0^* \ = \ \sum_X \det B_X\ \det B_X^*$$

where B_X denotes the square submatrix of B_0 whose $n-1$ columns correspond to the edges in a subset X of $E(G)$ and whose rows are those attached to all the vertices except for v. The sum ranges over all possible choices of X.

Fact 4: If B_X is non-singular, then

$$\det\ B_X \ = \ (\omega(X_v))^{1/2}$$

where X_v is a rooted directed spanning tree formed by edges in X.
Proof: If every column of B_X has two non-zero entries, then B_X has rank no more than $n-2$ and $det\ B_X = 0$. Since B_X is non-singular, X forms a tree T. We consider the set P of columns with exactly one non-zero entry. Since the columns are indexed by edges, we let edges $e_1, \cdots, e_s$ of B_X denote the indices of the columns in P. We note that s is the degree of v in the tree T. Furthermore, we let $X_1, \cdots, X_s$ denote the subtrees obtained by deleting the vertex v (and the adjacent edges) in the tree T. Therefore, we have

$$\det\ B_X \ = \ \alpha_v^{s/2} \det\ B_{X_1} \cdots \det\ B_{X_s}$$

By induction, we have

$$\det\ B_X \ = \ \pm \prod_{(x,y)\in X_v} \alpha_y^{1/2} = (\omega(X_v))^{1/2}$$

As a consequence

$$\begin{aligned} \det\ M \ &= \ \sum_X (\det\ B_X)^2 \\ &= \ \sum_X \omega(X_v) \ = \ \kappa_v(G) \end{aligned}$$

where the sum ranging over all rooted directed spanning trees. Since by Fact 3 , we have $W^{-1/2}\ adj\ \mathcal{L}\ W^{-1/2} \ = \ t\ J$ for a real number t. We conclude that

$$\alpha_v^{-1}\ \kappa_v(G) \ = \ t\ J$$

In general, we have

$$\alpha_v^{-1}\ \kappa_v(G) \ = \ \alpha_u^{-1}\ \kappa_u(G)$$

for any u and v. This implies

$$\begin{aligned} (\sum_v \alpha_v)t \ &= \ \sum_v \kappa_v(G) \\ &= \ \kappa(G) \end{aligned}$$

Hence, we have

$$W^{-1/2}\ adj\ \mathcal{L}\ W^{-1/2} \ = \ (\sum_v \alpha_v)^{-1}\kappa(G)\ J$$

as claimed. Theorem 1 is proved.

3 The characteristic polynomial of $\mathcal{L}$

We consider the characteristic polynomial of $\mathcal{L}$, that is,

$$\det(\lambda I - \mathcal{L}) = \lambda^n + c_1\lambda^{n-1} + \cdots + c_{n-1}\lambda$$

For the case that all vertex-weights are equal to 1, it is known that c_1 is twice the number of edges and c_{n-1} is n-times the number of spanning trees. We will see that the factor of n in c_{n-1} can be explained in the general terms by using the vertex-weights as in Theorem 1. Specifically, $c_{n-1} = \kappa(G)$. In fact, all c_i's have a natural interpretation by considering the following generalization of $\kappa(G)$.

A forest is a subgraph containing no cycle. Let S denote a subset of vertices with $|S| = s$ and X denote a subset of $n - s$ edges. If the subgraph with vertex set $V(G)$ and edge set X is a spanning forest and each of the subtrees contains exactly one vertex in S, we can then define the rooted directed spanning forest X_S which consists of all edges of X oriented toward S. For a rooted directed spanning forest X_S, we define the weight of X_S as follows:

$$\omega(X_S) = \prod_{(x,y)\in E(X_S)} \alpha_y$$

and

$$\kappa_S(G) = \sum_{X_S} \omega(X_S)$$

Also, for an integer s, $1 \leq s \leq n$, we define

$$\kappa_s(G) = \sum_{\substack{S \\ |S|=s}} \kappa_S(G)$$

Theorem 2 *The s-th coefficient of the characteristic polynomial of $\mathcal{L}$ is the sum of weights of all rooted directed spanning forests with s roots, i.e.,*

$$(-1)^s c_s = \kappa_s(G)$$

Proof: First, we note that

$$(-1)^s c_s = \sum_{\substack{S \\ |S|=s}} \det M_S$$

where M_S is an $(n-s) \times (n-s)$ submatrix of L obtained by deleting rows and columns indexed by vertices in S. For each fixed S, we have

$$\det M_S = \sum_X (\det B_X)^2$$

where X ranges over all subsets of $n-s$ edges and B_X denotes the $(n-s)\times(n-s)$ submatrix of B with rows indexed by vertices in $V - S$ and columns indexed by edges in X. If the graph formed by X has a connected component disjoint from S, then we have $\det B_X = 0$. The only case that $\det B_X \neq 0$ is that X defines (as above) a rooted directed spanning forest X_S and

$$\det B_X = (\omega(X_S))^{1/2}$$

This completes the proof of Theorem 2.

Examples

Suppose G is a complete graph K_n on n vertices having vertex weights α_v's. It is easy to check that the characteristic polynomial has one root of 0 and $n-1$ roots of value $\sum_v \alpha_v$. Therefore we have

$$\kappa(G) = (\sum_v \alpha_v)^{n-1}$$

which generalizes the well-known theorem of Cayley [3] that the number of labelled trees on n vertices is n^{n-2}. It is of interest to point out that $f(G) = \kappa(G)$ satisfies the following recurrence which arises in [8]:

$$f(G) = (\sum_v \alpha_v) \; (\sum_{\substack{A,B \\ A\cup B=V}} (\sum_{u\in A} \alpha_u)^{|B|-1} (\sum_{v\in B} \alpha_v)^{|A|-1}$$

where A and B range over all (unordered) partitions of V.

We now consider a complete bipartite graph $K_{m,n}$ with vertex set $X \cup Y$ where $|X| = m$ and $|Y| = n$. It is not difficult to show that the eigenvalues of the Laplacian of the vertex-weighted $K_{m,n}$ are 0, $\sum_{u\in X} \alpha_u$ (of multiplicities $|X|-1$). $\sum_{v\in Y} \alpha_v$ (of multiplicities $|Y|-1$), and $\sum_{v\in X\cup Y} \alpha_v$.

It is also of interest to examine the so-called set-intersection graphs. We consider a graph G with vertex set consisting of all k-subsets of an n-set. Two vertices are adjacent if and only if the intersection of the corresponding k-sets is empty. (In general, adjacency depends only on the cardinalities of the intersections.) Suppose each element x of the n-set is associated with a weight β_x and the weight of a k-set X is the sum $\sum_{x\in X} \beta_x$. This is a generalization of the Gelfand pairs associated with the equal-weighted case which has been extensively studied in the literature ([2][14]). It is not too difficult to check that for the weighted intersection graphs, the spectral decomposition preserves the strong property that the decomposition is multiplicity-free with eigenspaces V_i having $dim\ V_i = \binom{n}{i}$, for $i = 0, \cdots, k$. For the special case with equal weights, the eigenfunctions are classical orthogonal functions, called the Dual Hahn or Eberlein polynomials, with many applications in diverse areas. The eigenfunctions for the weighted generalizations are apparently more complicated and less well understood.

4 Dirichlet eigenvalues and invariant field theory

In this section, we consider another generalization of the matrix-tree theorem, motivated by conformal invariant theory related to the determinant of the Laplacian with Dirichlet boundary conditions (see [5], [8]). For a graph G and a subset X of the vertex set of G, we consider the induced subgraph on X. The vertex boundary δX is defined by

$$\delta X = \{v \in V \ X : v \sim u \in X\}$$

Suppose σ is a function defined on the boundary δX. The "energy" for a function f is related to

$$H(f) = \sum_{\substack{x \sim y \\ x \in X}} [f(x) - f(y)]^2$$

where the x and y range over all edges with at least one endpoint in X. The partition function is

$$Z(\sigma) = \int_f e^{-c\ H(f)}$$

where f ranges over all functions whose restriction to δX is σ.

To compute $Z(\sigma)$, let f_0 denote the function that minimizes $H(f)$ and the restriction of f to δX is σ. We note that f_0 satisfies, for every $x \in X$,

$$\sum_{\substack{y \\ y \sim x}} (f_0(x) - f_0(y)) = 0$$

which can be proved by variation principles. Also, it is not difficult to show that such a function exists if X is connected and is uniquely determined. For any function g whose restriction to δX is σ, we consider

$$f = g - f_0$$

Clearly, f satisfies the Dirichlet condition.

$$f(x) = 0 \text{ for } x \in \delta X$$

We can rewrite $H(g)$ as follows:

$$\begin{aligned} H(g) &= \sum_{x \sim y} (f(x) - f(y))^2 + \sum_{x \sim y} (f_0(x) - f_0(y))^2 \\ &\quad + 2 \sum_{x \sim y} (f(x) - f(y))(f_0(x) - f_0(y)) \\ &= \sum_{x \sim y} (f(x) - f(y))^2 + \sum_{x \sim y} (f_0(x) - f_0(y))^2 + 2 \sum_{x \in X} f_0(x) \sum_{\substack{y \\ x \sim y}} (f(x) - f(y)) \\ &= \sum_{x \sim y} (f(x) - f(y))^2 + \sum_{x \sim y} (f_0(x) - f_0(y))^2 \end{aligned}$$

Therefore, we have

$$Z(\sigma) = e^{-c\ H(f_0)} \int_f e^{-c\ H(f)}$$

where f ranges over all functions satisfying the Dirichlet condition. Then we have

$$\begin{aligned} H(f) &= \sum_{x \sim y} (f(x) - f(y))^2 \\ &= \sum_{x \in X} f(x) \sum_{\substack{y \\ x \sim y}} (f(x) - f(y)) \\ &= \sum_{x \in X} f(x) L f(x) \end{aligned}$$

Suppose we let L_X denote the submatrix of L restricted to columns and rows indexed by vertices in X. Also, we viewed a function f satisfying the Dirichlet boundary condition as a vector indexed by vertices in X. Then we have

$$H(f) = \langle f , L_X f \rangle$$

The dirichlet eigenvalues of X are just the eigenvalues of L_X. If we write f in the basis formed by orthonormal eigenfunctions ϕ_i associated with Dirichlet eigenvalues λ_i, for $i = 1, \ldots, m$ where $m = |X|$.

$$f = \sum_i \alpha_i \phi_i$$

Then we have

$$H(f) = \sum_i \alpha_i^2 \lambda_i$$

and

$$\begin{aligned} Z(\sigma) &= e^{-c\ H(f_0)} \int e^{-c \sum \lambda_i \alpha_i^2} d\alpha_i \\ &= c^{-m/2} (\prod_{i=1}^{m} \lambda_i)^{-1/2} (2\pi)^{m/2} \end{aligned}$$

Therefore the problem is reduced to the problem of evaluating the determinant $\prod_{i=1}^m \lambda_i$ of the Laplacian with the Dirichlet boundary condition.

For an induced subgraph on X with non-empty boundary in a graph G, we define a rooted spanning forest of X to be subgraph F satisfying
(1) F is an acyclic subgraph of G,
(2) F has vertex set $X \cup \delta X$,
(3) Each connected component of F contains exactly one vertex in δX.

The following theorem relates the product of Dirichlet eigenvalues of X with the enumeration of rooted spanning forests of X:

Theorem 3 *For an induced subgraph on X in a graph G with $\delta X \neq \emptyset$, the number of rooted spanning forests of X is the determinant of the Laplacian L_X with Dirichlet boundary conditions.*

We will omit the proof of Theorem 3 since it is quite similar to that of Theorem 1 and the minors matrix-tree theroem by Chaiken [4]. It is worth mentioning that the usual matrix-tree theorem is just a special case of a subgraph with the boundary consisting of a single vertex.

The problem of enumerating forests in a graph is known to be a difficult problem, so-called #P hard. In contrast, the following modified enumeration problem for rooted spanning forests can be computed in polynomial time as a result of Theorem 3.

Theorem 4 *There is a polynomial algorithm to evaluate, for a graph G,*

$$\sum_F \phi(F)$$

where F ranges over all forests in G and $\phi(F)$ denotes the product of the sizes of connected components in a forest F. (The size of a connected component is its number of vertices.)

Proof: For a graph G, we consider a supergraph G' formed by attaching a leaf to each vertex of G. We consider the induced subgraph G in G' and apply Theorem 3. Since each connected component of p vertices in a forest in G corresponds to p rooted trees in G', we have by using Theorem 3

$$\sum_F \phi(F) = \cdot \prod_i \lambda'_i$$

where λ'_i denotes the Dirichlet eigenvalues of G in G'. The theorem follows then from the fact that eigenvalues can be computed in polynomial time.

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