Matrix Tree Theorem for Schrödinger operators on networks

<u>Ángeles Carmona</u>, Andrés M. Encinas and Margarida Mitjana.

Departament Matemàtiques,

Universitat Politècnica de Catalunya, Spain.

This work aims to interpret a family of distances in networks associated with effective resistances with respect to a parameter and a weight in terms of rooted spanning trees. Specifically, we consider the effective resistance distance with respect to a positive parameter and a weight; that is, effective resistance distance associated with an irreducible and symmetric M-matrix. This concept was introduced by the authors in relation with the full extension of Fiedler's characterization of symmetric and diagonal dominant M-matrices as resistive inverses to the case of symmetric M-matrices. The main idea is consider the network embedded in a host network with new edges that reflects the influence of the parameter. Then, we used the all minor tree Theorem to give an expression for the effective resistances in terms of rooted spanning forest.

This work has been partially supported by the Programa Estatal de I+D+i del Ministerio de Economía y Competitividad, Spain, under the project MTM2014-60450-R.

1 Matrix Tree Theorems in the Host Network

In this section we aim to present the matrix tree—theorem for a Schrödinger operator with $\lambda > 0$ and to get the relation between the number of forest and different parameters of the network such as Green function and effective resistance among others. The classical matrix—tree theorem whose first version was proved by G. Kirchhoff in 1847 relates the principal minors of the Laplancian matrix with the total weight of spanning trees of Γ . Since then, many generalization and different proofs have been considered (see for instance [1]). In this work we are going to use an extension of the undirected version of the all-minors theorem by S. Chaiken [9], see also [6] for a beautiful application.

If $\mathcal{T} = (V, E, c)$ is such that for each pair x and y of vertices, there is exactly one path joining x and y, the \mathcal{T} is called a weighted tree. Given $\Gamma = (V, E, c)$ a connected network, we say that \mathcal{T} is a spanning tree of Γ if both networks have the same set of vertices and each edge of \mathcal{T} is also and edge of Γ with the same weight. A forest is a non–necessarily connected network without cycles. A rooted forest is a forest with one vertex marked as a root in each connected component. Moreover a k-rooted forest is a forest with k components and a vertex marked as a root in each connected component. The weight of a forest F is defined as the product of all weights of the edges of F taking into account the weights of the vertices given by ω ; i.e.,

$$w(F) = \frac{\prod_{e \in E(F)} w(e)}{\prod_{x \in V(F)} \omega^{2}(x)},$$

where $e = \{x, y\} \in E(F)$ and $w(e) = c(x, y)\omega(x)\omega(y)$ and we take the convention that empty product equals 1.

We denote by $\mathcal{F} = \mathcal{F}(\Gamma)$ the set of rooted spanning forest of Γ and $\mathcal{F}_k = \mathcal{F}_k(\Gamma)$ the set of k-rooted spanning forest of Γ . Moreover, $\mathcal{F}_x = \mathcal{F}_x(\Gamma)$ denotes the set of rooted spanning forest of Γ such that x is a root and $\mathcal{F}_{k,x} = \mathcal{F}_{k,x}(\Gamma)$ denotes the set of k-rooted spanning forest of Γ such that x is a root. Finally, we denote by $\mathcal{F}_{x,y} = \mathcal{F}_{x,y}(\Gamma)$ the set of rooted spanning forest of Γ such that x is a root and y belong to the same component that x and $\mathcal{F}_{k,x,y} = \mathcal{F}_{k,x,y}(\Gamma)$ the set of k-rooted spanning forest of Γ such that x is a root and y belong to the same component that x. If $F \in \mathcal{F}_k$ we denote by r(F) the set of its roots whereas if $F \in \mathcal{F}_{k,x}$ we denote by $r^*(F)$ the set of roots different from x.

In order to state the matrix notation we need to label the vertices and the edges of the network. So, let $\Gamma = (V, E, c)$ be a network and suppose that $V = \{1, \ldots, n\}$ and $E = \{e_1, \ldots, e_m\}$. Assume that each edge of Γ is assigned an orientation, which is arbitrary but fixed. Then, $e_{\ell} = (i, j)$, for $\ell = 1, \ldots, m$ and $i, j = 1, \ldots, n$, where i is called the *tail* and j is called the *head* of e_{ℓ} . We define the weight of and edge as

 $w(e_{\ell}) = c(i,j)\omega(i)\omega(j)$. Then, the incidence matrix $\mathsf{B} = (b_{\ell i}) \in \mathcal{M}_{m \times n}$ is defined as

$$b_{\ell i} = \begin{cases} 1 & \text{if } i \text{ is the head of } e_{\ell} \\ -1 & \text{if } i \text{ is the tail of } e_{\ell} \\ 0 & \text{otherwise,} \end{cases}$$

and we denote by $W(c, \omega) \in \mathcal{M}_m$, the diagonal matrix whose diagonal elements are given by $w(e_{\ell})$. Using this notation

$$\mathsf{L}_{q_{\omega}} = \left(\mathsf{B}\mathsf{D}_{\omega}^{-1}\right)^{T} \mathsf{W}(c, \omega) \mathsf{B}\mathsf{D}_{\omega}^{-1},\tag{1}$$

where $\mathsf{D}_{\omega}^{-1} \in \mathcal{M}_n$ is a diagonal matrix whose diagonal elements are $\omega(x_i)$. We name matrix $\mathsf{B}_{\omega} = \mathsf{BD}_{\omega}^{-1} \in \mathcal{M}_{m \times n}$ the weighted incidence matrix of Γ . Moreover, the matrix associated with L_q is given by

$$L_a = B_{\omega}^T W(c, \omega) B_{\omega} + \lambda I.$$

The next result, whose proof can be found in [3], establishes the relationship between the original Schrödinger operator L_q and a new semidefinite Schrödinger operator on $\Gamma_{\lambda,\omega}$. From now on, we label the vertex \hat{x} as n+1.

Proposition 1. If $q = q_{\omega} + \lambda$ and we define $\hat{q} = -\frac{1}{\widehat{\omega}} \mathcal{L}^{\lambda,\omega}(\widehat{\omega})$, then $\hat{q}(n+1) = \lambda \left(n - \langle \omega, 1 \rangle\right)$ and $\hat{q} = q - \lambda \omega$ on V. Moreover, for any $u \in \mathcal{C}(V \cup \{n+1\})$ we get that $\mathcal{L}_{\hat{q}}^{\lambda,\omega}(u)(n+1) = \lambda \left(n u(n+1) - \langle \omega, u_{|_{V}} \rangle\right)$ and

$$\mathcal{L}_{\hat{g}}^{\lambda,\omega}(u) = \mathcal{L}_{q}(u|_{V}) - \lambda \,\omega \,u(n+1) \quad on \ V.$$

In matricial terms, the above relation means that

$$\mathsf{L}_q = \mathsf{L}_{\hat{a}}^{\lambda,\omega}(n+1|n+1),\tag{2}$$

where $\mathsf{L}_{\hat{q}}^{\lambda,\omega}(n+1|n+1)$ is the submatrix of $\mathsf{L}_{\hat{q}}^{\lambda,\omega}$ obtained by deleting the (n+1)-th row and column. Moreover, the relation between weighted incidence matrices is the following

$$\mathsf{B}_{\hat{\omega}}^{^{\lambda,\omega}} = \begin{bmatrix} \mathsf{B}_{\omega} & \mathsf{0} \\ D_{\omega}^{-1} & -\mathsf{j} \end{bmatrix} \quad \text{and} \quad \mathsf{W}^{^{\lambda,\omega}}(c,\omega) = \begin{bmatrix} \mathsf{W}(c,\omega) & \mathsf{0} \\ 0 & \lambda D_{\omega}^2 \end{bmatrix},$$

where $\mathsf{B}^{\lambda,\omega}_{\hat{\omega}} \in \mathcal{M}_{(m+n)\times(n+1)}(\mathbb{R})$ and $\mathsf{W}^{\lambda,\omega}(c,\omega) \in \mathcal{M}_{m+n}(\mathbb{R})$. Therefore, if $\mathsf{B}^{\lambda,\omega}_{\hat{\omega}}(n+1)$ denotes the submatrix of $\mathsf{B}^{\lambda,\omega}_{\hat{\omega}}$ obtained by deleting the (n+1)-th column, we get

$$\mathsf{L}_q = \mathsf{B}_{\hat{\omega}}^{\lambda,\omega}(n+1)^T \mathsf{W}^{\lambda,\omega}(c,\omega) \mathsf{B}_{\hat{\omega}}^{\lambda,\omega}(n+1)$$

$$= \begin{bmatrix} \mathsf{B}_\omega^T & D_\omega^{-1} \end{bmatrix} \begin{bmatrix} \mathsf{W}(c,\omega) & 0 \\ 0 & \lambda D_\omega^2 \end{bmatrix} \begin{bmatrix} \mathsf{B}_\omega \\ D_\omega^{-1} \end{bmatrix} = \mathsf{B}_\omega^T \mathsf{W}(c,\omega) \mathsf{B}_\omega + \lambda \mathsf{I}.$$

Note, that the above matrices are similar to the ones introduced in [12] in relation with the normalized Laplacian. Notice that with our interpretation these matrices acquire a real meaning.

Observe that if \hat{F} is an spanning tree on $\Gamma_{\lambda,\omega}$ with n+1 as a root and k edges of type $\{n+1,i\}$, the forest generated in Γ , F, has k connected components and each i belongs to a different component and hence it can be considered as a root of the forest. With this interpretation of $\hat{\Gamma}$, we can estate some generalization of the matrix-tree Theorem. This extension considers not only weights in the edges, as in the previous works, but also weights on the vertices. We omit the proof because it is a simple consequence of the above results.

Call a subset $J = \{(i_1, j_1), \dots, (i_\ell, j_\ell)\} \subset V \times V$ component–disjoint if $i_p \neq i_q$ and $j_q \neq j_q$ for every $p \neq q$ and $i_1 < i_2 < \dots < i_\ell$; denote $\sum J = \sum_{p=1}^{\ell} (i_p + j_p)$. Denote by τ_J

the permutation of $\{1, 2, \dots, \ell\}$ defined by the condition $j_{\tau_J(1)} < j_{\tau_J(2)} < \dots < j_{\tau_J(\ell)}$. A spanning forest is called J-admisible if it has ℓ connected components, and every component contains exactly one vertex from the set $\{i_1, \dots, i_\ell\}$, and exactly one, from $\{j_1, \dots, j_\ell\}$ (the two may coincide if the sets intersect). The vertices from i_1, \dots, i_ℓ will be considered as roots. Denote by σ_J^F a permutation of V such that i_p and $j_{\sigma_J^F(p)}$ lie in the same component of F, for every $p = 1, 2, \dots, \ell$.

For a n-matrix M and a component-disjoint set J, denote by M(J) the submatrix of M obtained by deletion of the rows i_1, \ldots, i_ℓ and the columns j_1, \ldots, j_ℓ . For any permutation ϵ will denote its sign.

Theorem 1. [9] For any component-disjoint subset $J \subset V \times V$ it is verified

$$(-1)^{\sum J} \det(\mathsf{L}_{q_{\omega}})(J) = \sum_{F} \epsilon(\tau_{J} \circ \sigma_{J}^{F}) w(F) \prod_{p=1}^{\ell} \omega(i_{p}) \omega(j_{p})$$

where the sum is taken over the set of all J-admissible forest F of Γ .

The cases in which $\ell = 0, 1, 2$ have an special meaning.

Proposition 2. Let $\lambda > 0$ and $\omega \in \Omega(V)$. Then, the determinant of the matrix associated with a positive semi-definite Schrödinger operator, L_q , is given by

$$\det(\mathsf{L}_q) = \sum_{k=1}^n a_k \lambda^k,$$

with

$$a_k = \sum_{F \in \mathcal{F}_k} w(F) \prod_{i_p \in r(F)} \omega(i_p)^2.$$

Proof. From Equation (2) and Theorem 1 taking $J = \{(n+1, n+1)\}$ and keeping in mind that $\omega(n+1) = 1$, we get that

$$\det(\mathsf{L}_q) = \det\left(\mathsf{L}_{\hat{q}}^{\lambda,\omega}(J)\right) = \sum_{\widehat{r}} \widehat{w}(\widehat{r}),$$

where \hat{F} is a J-admisible forest in $\Gamma_{\lambda,\omega}$ rooted at n+1. Notice that in this case the permutations are the identity. Moreover, if k is the number of edges of the form $e_p = \{n+1, i_p\}, \ p=1, \ldots, k$, in \hat{F} and F is the induced k-rooted spanning forest in $\Gamma, k=1,\ldots,n$ with $r(F)=\{i_1,\ldots,i_k\}$ as set of roots, we have that

$$\widehat{w}(\widehat{F}) = \frac{\prod_{e_p} \lambda \omega(i_p)^2 \prod_{e \in E(F)} w(e)}{\prod_{j \in V(F)} \omega(j)^2} = \lambda^k w(F) \prod_{p=1}^k \omega(i_p)^2. \quad \Box$$

Observe that

$$\det(\mathsf{L}_q) = \det(\mathsf{L}_{q_\omega} + \lambda \mathsf{I}),$$

and hence a_n must equal 1 and $a_{n-1} = \operatorname{tr}(\mathsf{L}_{q_\omega}) = \sum_{x,y \in V} c(x,y) \frac{\omega(x)}{\omega(y)}$. This values can also be deduced from the fact that there is only one forest with n connected components and there are 2m rooted forest with n-1 components. Moreover, notice that the above result is also valid for $\lambda = 0$, since in this case $\det(\mathsf{L}_q) = 0$.

References

- [1] A. Abdesselam, The Grassmann–Berezin calculus and theorems of the matrix–tree type, Ad. Appl. Math. 33 (2004) 51–70.
- [2] E. Bendito, A. Carmona and A. M. Encinas, Potential theory for Schrödinger operators on finite networks, *Rev. Mat. Iberoamericana* **21** (2005) 771–818.
- [3] E. Bendito, A. Carmona, A.M. Encinas and J.M. Gesto. Characterization of symmetric *M*-matrices as resistive inverses. *Linear Algebra Appl.*, **430** (2009) 1336–1349.
- [4] E. Bendito, A. Carmona, A.M. Encinas, J.M. Gesto and M. Mitjana. The Kirchhoff indices of join networks. in *Linear Algebra Appl.*, **432** (2010) 2278–2292.
- [5] T. Biyikoğlu, J. Leydold and P.F. Stadler. *Laplacian Eigenvectors of Graphs*. LNM 1915, Springer, Berlin, 2007.
- [6] Y. Burman and B. Shapiro. Around matrix-tree theorem. Math. Res. Lett., 13 (2006) 761–774.
- [7] A. Carmona, A.M. Encinas and M. Mitjana. Discrete elliptic operators and their Green operators. *Linear Algebra Appl.*, **442** (2014) 115–134.
- [8] A. Carmona, A.M. Encinas and M. Mitjana. Star—mesh transforms on networks. *submitted*.
- [9] S. Chaiken. A combinatorial proof of the all minors matrix tree theorem. SIAM J. Alg. Disc. Meth., 3 (1982) 319–329.

- [10] P. Chebotarev and E. Shamis. On proximity measures for graphs vertices. *Automat. Remote Control*, **59** (1998) 1443–1459.
- [11] P. Chebotarev and E. Shamis, The Forest Metrics for Graph Vertices, *Electron. Notes Discrete Math.*, **11** (2002) 98-107.
- [12] F. Chung, and W. Zhao, PageRank and random walks on graphs. Fete of combinatorics and computer science, Bolyai Soc. Math. Stud., 20, Jnos Bolyai Math. Soc., Budapest, 2010, 43–62.
- [13] C. Dellacherie, S. Martínez and J. San Martín, Ultrametric matrices and induced Markov Cjains, Adv. Appl. Math., 17 (1996) 169–183.
- [14] C. Dellacherie, S. Martínez and J. San Martín, Description of the sub–Markov kernel associated to generalized ultrametric matrices. An algorithm approach, *Linear Algebra Appl.*, **318** (2000) 1–21.
- [15] W. Ellens, F.M. Spieksma, P. Van Mieghem, A. Jamakovic, R.E. Kooij, Effective graph resistance, *Linear Algebra Appl.* **435** (2011) 2491–2506.
- [16] M. Fiedler, Some characterizations of symmetric M-matrices , $Linear\ Algebra\ Appl.\ 275-276\ (1998)\ 179-187.$
- [17] Y. Yang and D.J. Klein, A recursion formula for resistance distances and its applications, *Discrete Appl. Math.* **161** (2013) 2702–2715.