

Green's kernel of Schrödinger operators on generalized subdivision networks

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Abstract

In the present work, we define a *generalized subdivision network* Γ^S of a given network Γ , by inserting a new vertex in some selected edges of Γ , so that each of these edges is replaced by two new edges with conductances that fulfill the Kirchhoff series law on the new network. Then, we obtain an expression for the Green kernel of Schrödinger operators on generalized subdivision networks in terms of the Green kernel of a Schrödinger operator of the base network. For that, we show the relation between Poisson problems on a generalized subdivision network and Poisson problems on the base network. Moreover, we also obtain the effective resistance and the Kirchhoff index of a generalized subdivision network in terms of the corresponding parameters on the base network. Finally, as an example, we carry out the computations in the case of a star network in which we have subdivided the even edges.

Keywords: Resistance distance, Green kernel, Kirchhoff Index, generalized subdivision network

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1 Introduction

In the whole work, a *network* is the triplet $\Gamma = (V, E, c)$ where (V, E) stands for a finite and connected graph, without loops nor multiple edges; and $c: V \times V \rightarrow [0, +\infty)$ is a symmetric function called *conductance* satisfying $c(x, y) > 0$ iff $x \sim y$ which means that $\{x, y\} \in E$. Let n be the number of nodes and m the number of edges.

On the other hand, $\mathcal{C}(V)$ is the set of real functions on V . For any vertex $x \in V$, $\varepsilon_x \in \mathcal{C}(V)$ is the Dirac function at x and $k \in \mathcal{C}(V)$ defined as $k(x) = \sum_{y \in V} c(x, y)$, is the *degree* of x . The standard inner product in $\mathcal{C}(V)$ is denoted by $\langle \cdot, \cdot \rangle$; that is, if $u, v \in \mathcal{C}(V)$ then, $\langle u, v \rangle = \sum_{x \in V} u(x)v(x)$. A real-valued function $\omega \in \mathcal{C}(V)$ is called *weight* if $\omega(x) > 0$ for any $x \in V$ and in addition $\|\omega\| = 1$. The sets of weights on V is denoted by $\Omega(V)$. Clearly the unique constant weight on V assigns $\frac{1}{\sqrt{n}}$, to any vertex of V .

The *combinatorial Laplacian* or simply the *Laplacian* of the network Γ is the endomorphism

of $\mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function

$$\mathcal{L}(u)(x) = \sum_{y \in V} c(x, y) (u(x) - u(y)), \quad x \in V. \quad (1)$$

Given $q \in \mathcal{C}(V)$, the *Schrödinger operator* on Γ with *potential* q is the endomorphism of $\mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function $\mathcal{L}_q(u) = \mathcal{L}(u) + qu$, where $qu \in \mathcal{C}(V)$ is defined as $(qu)(x) = q(x)u(x)$; see for instance [1, 3]. If ω is a weight, then the potential $q_\omega = -\omega\mathcal{L}^{-1}(\omega)$ is called *potential determined by ω* . The *Doob transform* consists in the identity

$$\mathcal{L}_{q_\omega}(u)(x) = \frac{1}{\omega(x)} \sum_{y \in V} c(x, y) \omega(x) \omega(y) \left(\frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right), \quad x \in V, \quad u \in \mathcal{C}(V).$$

It is well-known that any Schrödinger operator is self-adjoint and moreover it is positive semi-definite iff there exist $\omega \in \Omega(V)$ and $\lambda \geq 0$ such that $q = q_\omega + \lambda$; see [1]. In addition, \mathcal{L}_q is singular iff $\lambda = 0$, in which case $\langle \mathcal{L}_{q_\omega}(v), v \rangle = 0$ iff $v = a\omega$, $a \in \mathbb{R}$. In any case, λ is the lowest eigenvalue of \mathcal{L}_q and its associated eigenfunctions are multiple of ω .

Throughout this work we will consider only positive semi-definite and singular Schrödinger operator, \mathcal{L}_{q_ω} . Then, the operator that assigns to each function $f \in \mathcal{C}(V)$ the unique $u \in \mathcal{C}(V)$ such that $\mathcal{L}_{q_\omega}(u) = f - \langle \omega, f \rangle \omega$ and $\langle u, \omega \rangle = 0$ is called *Green's operator*. The Green operator is denoted by \mathcal{G}_{q_ω} , see [2]. Moreover, the function $G_{q_\omega} : V \times V \rightarrow \mathbb{R}$, defined as $G_{q_\omega}(x, y) = \mathcal{G}_{q_\omega}(\varepsilon_y)(x)$, for any $x, y \in V$, is called *Green's function*. Observe that $\mathcal{G}_{q_\omega}(\omega) = 0$, and moreover, \mathcal{G}_{q_ω} is self-adjoint as a consequence of the Fredholm Alternative and \mathcal{G}_{q_ω} is a symmetric function.

In [2], the authors introduced a generalization of the concept of effective resistance with respect to a weight $\omega \in \Omega(V)$. Specifically, from the functional on $\mathcal{C}(V)$ defined as

$$\mathfrak{J}_{x,y}(u) = 2 \left[\frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right] - \langle \mathcal{L}_{q_\omega}(u), u \rangle, \quad (2)$$

we defined the generalization of the effective resistance.

Definition 1.1. *Given $x, y \in V$, the effective resistance between x and y with respect to ω , is the value*

$$R_\omega(x, y) = \max_{u \in \mathcal{C}(V)} \{ \mathfrak{J}_{x,y}(u) \}.$$

When ω is constant we omit the subindex ω . Therefore, R is nothing else than a multiple of the standard effective resistance of the network.

The following result can be found in [2] and allows us to express the effective resistances in terms of the solution of a Poisson equation. In particular, these expressions will be useful to prove the main properties of the effective resistances.

Proposition 1.2. *If $u \in \mathcal{C}(V)$ is a solution of the Poisson equation $\mathcal{L}_{q_\omega}(u) = \omega^{-1}(\varepsilon_x - \varepsilon_y)$, then*

$$R_\omega(x, y) = \langle \mathcal{L}_{q_\omega}(u), u \rangle = \frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)}.$$

Therefore, R_ω is symmetric, non-negative and moreover $R_\omega(x, y) = 0$ iff $x = y$. In addition,

$$R_\omega(x, y) = \frac{G_{q_\omega}(x, x)}{\omega^2(x)} + \frac{G_{q_\omega}(y, y)}{\omega^2(y)} - \frac{2G_{q_\omega}(x, y)}{\omega(x)\omega(y)}.$$

Notice that, if we label the vertices of Γ , both the Schrödinger operator and the Green operator can be interpreted as singular matrices and hence, the Green kernel can be identified as the group inverse of the matrix associated with the Schrödinger operator.

The *Kirchhoff Index* of a network Γ with respect to a weight is defined as

$$k_\omega(\Gamma) = \frac{1}{2} \sum_{x,y \in V} R_\omega(x,y) \omega^2(x) \omega^2(y) = \sum_{x \in V} G_{q_\omega}(x,x) \quad (3)$$

and gives a measure of the global connectivity of the network. The Kirchhoff index is a descriptor of the structure of the network and exhibits many interesting interpretations, see [10, 14].

A *partial subdivision network* $\Gamma^S = (V^S, E^S, c^S)$ of a given network $\Gamma = (V, E, c)$, is obtained by inserting a new vertex in some edges of Γ , we denote the set of subdivided edges by E' , so that each edge $\{x, y\} \in E'$ is replaced by two new edges, say $\{x, v_{xy}\}$ and $\{y, v_{xy}\}$ where v_{xy} is the new inserted vertex. We denote by V' the new vertex set assuming that, $v_{xy} = v_{yx}$. Thus, $V^S = V \cup V'$, the order of the subdivision network is $n + |E'|$, whereas the size is $m + |E'|$. When, $E' = E$, the partial subdivision network is nothing else but the so-called *subdivision network*; see [6]. Given $x \in V$ we denote by $S(x)$ the set of adjacent vertices to x such that $\{x, y\} \in E'$.

Given $\omega : V \rightarrow \mathbb{R}^+$ a weight; that is, $\omega(x) > 0$ and $\sum_{x \in V} \omega^2(x) = 1$ in the base network, we now define an extension of this weight function, $\omega^S : V \cup V' \rightarrow \mathbb{R}^+$ in such a way that $\omega^S(x) = \alpha \omega(x)$ when $x \in V$ and $\omega^S(v_{xy}) = \alpha \omega(v_{xy})$, where $\omega(v_{xy})$ is absolutely arbitrary, except for positivity, for $v_{xy} \in V'$ and

$$\alpha^2 = \frac{1}{1 + \sum_{x \in V'} \omega(v_{xy})^2}.$$

Moreover, according to the well-known rule that express the equivalent resistance of two resistors connected in series and the expression for the Schrödinger operator, we define the conductance function $c^S : V^S \times V^S \rightarrow [0, +\infty)$ by choosing, for every edge in E' , $\{x, y\}$, non-null values $c^S(x, v_{xy})$ and $c^S(y, v_{xy})$ such that

$$\frac{1}{\omega(x)\omega(y)} \frac{1}{c(x,y)} = \frac{1}{\omega(x)\omega(v_{xy})} \frac{1}{c^S(x, v_{xy})} + \frac{1}{\omega(y)\omega(v_{xy})} \frac{1}{c^S(y, v_{xy})}, \quad (4)$$

whereas for every edge in $E^S \setminus E'$ we define $c^S(x, y) = c(x, y)$. The definition of c^S cannot be misunderstood as all the edges in E' have both kind of vertices, one in V and the other in V' . Hence, by the sake of simplicity, it will be denoted as c . Moreover for each edge, there exist infinitely many different choices of conductances fulfilling (4), so that different choices will lead to different partial subdivision networks.

In the literature it has been studied the case of subdivision networks for the combinatorial Laplacian when $c(x, y) = c(x, v_{xy}) = c(y, v_{xy}) = 1$, that not fulfills the electrical compatibility condition (4), see ([7, 9, 13, 15]); and the case of arbitrary conductances when all the edges have been divided, see [6].

Observe that Γ^S is also a connected, finite, with no loops, nor multiple edges network.

2 The Poisson Problem on Partial Subdivision Networks

If \mathcal{L}^S denotes the combinatorial Laplacian of Γ^S , then for any $u \in \mathcal{C}(V^S)$ we have that

$$\begin{aligned}\mathcal{L}^S(u)(x) &= \sum_{y \in V \setminus S(x)} c(x, y) (u(x) - u(y)) + \sum_{y \in S(x)} c(x, v_{xy}) (u(x) - u(v_{xy})), \quad \text{for any } x \in V; \\ \mathcal{L}^S(u)(v_{xy}) &= c(x, v_{xy}) (u(v_{xy}) - u(x)) + c(y, v_{xy}) (u(v_{xy}) - u(y)), \quad \text{for any } v_{xy} \in V'.\end{aligned}$$

On the other hand, we consider the potential determined by ω^S ,

$$q' = -(\omega^S)^{-1} \mathcal{L}^S(\omega^S) = -\omega^{-1} \mathcal{L}^S(\omega),$$

and hence

$$\begin{aligned}\mathcal{L}_{q'}^S(u)(v_{xy}) &= \frac{c(v_{xy}, x)\omega(x) + c(v_{xy}, y)\omega(y)}{\omega(v_{xy})} u(v_{xy}) - c(v_{xy}, x)u(x) - c(v_{xy}, y)u(y), \quad v_{xy} \in V' \\ \mathcal{L}_{q'}^S(u)(x) &= \frac{1}{\omega(x)} \sum_{y \in S(x)} c(x, v_{xy})\omega(x)\omega(v_{xy}) \left[\frac{u(x)}{\omega(x)} - \frac{u(v_{xy})}{\omega(v_{xy})} \right] \\ &\quad + \frac{1}{\omega(x)} \sum_{y \in V \setminus S(x)} c(x, y)\omega(x)\omega(y) \left[\frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right], \quad x \in V.\end{aligned}$$

Therefore, for any $v_{xy} \in V'$ and $u \in \mathcal{C}(V^S)$ we have that

$$\frac{u(v_{xy})}{\omega(v_{xy})} = \frac{\mathcal{L}_{q'}^S(u)(v_{xy}) + c(x, v_{xy})u(x) + c(y, v_{xy})u(y)}{c(x, v_{xy})\omega(x) + c(y, v_{xy})\omega(y)}.$$

Keeping in mind the compatibility equation (4) we can rewrite the expression for $\mathcal{L}_{q'}^S(u)(x)$ as

$$\mathcal{L}_{q'}^S(u)(x) = \mathcal{L}_{q_\omega}(u)(x) - \sum_{y \in S(x)} \frac{c(x, v_{xy})\omega(v_{xy})}{c(x, v_{xy})\omega(x) + c(y, v_{xy})\omega(y)} \mathcal{L}_{q'}^S(u)(v_{xy}). \quad (5)$$

This expression suggests to call *contraction* of $h \in \mathcal{C}(V^S)$ the function of $\mathcal{C}(V)$, \underline{h} , defined as

$$\underline{h}(x) = h(x) + \sum_{y \in S(x)} \alpha(x, y)h(v_{xy}),$$

where

$$\alpha(x, y) = \frac{c(x, v_{xy})\omega(v_{xy})}{c(x, v_{xy})\omega(x) + c(y, v_{xy})\omega(y)}.$$

Observe that,

$$\alpha(x, y)\omega(x) + \alpha(y, x)\omega(y) = \omega(v_{xy}).$$

Moreover, we call *extension* of $u \in \mathcal{C}(V)$ with respect to $h \in \mathcal{C}(V^S)$, the function of $\mathcal{C}(V^S)$, u^h , defined as

$$u^h(v_{xy}) = \frac{h(v_{xy})c(x, y)}{c(x, v_{xy})c(y, v_{xy})} + \alpha(x, y)u(x) + \alpha(y, x)u(y), \quad v_{xy} \in V'$$

$$u^h(x) = u(x), \quad x \in V$$

Using these definitions we obtain from (5) that for any $u \in \mathcal{C}(V)$ and $x \in V$,

$$\mathcal{L}_{q_\omega}(u)(x) = \underline{\mathcal{L}_{q'}^S(u)}(x).$$

This relation allows us to obtain the following result.

Theorem 2.1. *Given $h \in \mathcal{C}(V^S)$ such that $\langle h, \omega^S \rangle = 0$, then $\langle \underline{h}, \omega \rangle = 0$. Moreover, $\bar{u} \in \mathcal{C}(V^S)$ is a solution of the Poisson equation $\mathcal{L}_{q'}^S(\bar{u}) = h$ in V^S iff $u = \bar{u}|_V$ is a solution of the Poisson equation $\mathcal{L}_{q_\omega}(u) = \underline{h}$ in V . In this case, the identity $\bar{u} = u^h$ holds.*

Next result shows how to obtain the unique solution of a Poisson problem on the partial subdivision network Γ^S orthogonal to ω^S .

Corollary 2.2. *Given $h \in \mathcal{C}(V^S)$, such that $\langle h, \omega^S \rangle = 0$, let $\underline{h} \in \mathcal{C}(V)$ be its contraction to V , $u \in \mathcal{C}(V)$ be the unique solution of $\mathcal{L}_{q_\omega}(u) = \underline{h}$ that satisfies $\langle u, \omega \rangle = 0$ and the constant*

$$\lambda = - \sum_{\{x,y\} \in E'} \frac{c(x,y)\omega^S(v_{xy})}{c(x,v_{xy})c(y,v_{xy})} (h(v_{xy}) + c(x,v_{xy})u(x) + c(y,v_{xy})u(y))$$

Then, $u^\perp = u^h + \lambda\omega^S$ is the unique solution of $\mathcal{L}_{q'}^S(u^\perp) = h$ that satisfies $\langle u^\perp, \omega^S \rangle = 0$.

The preceding results allows us to obtain the expression for the Green kernel of a generalized subdivision network in terms of the Green kernel of the base network and some other parameters.

If we let

$$\pi^S(x) = \sum_{y \sim S(x)} \frac{c(x,y)\omega^S(v_{xy})}{c(y,v_{xy})} = \sum_{y \sim S(x)} \alpha(x,y)\omega^S(v_{xy})$$

and

$$\beta = \sum_{r,s \in V} G_{q_\omega}(s,r)\pi^S(r)\pi^S(s) + \sum_{\{r,s\} \in E'} \frac{c(r,s)\omega^S(v_{rs})^2}{c(r,v_{rs})c(s,v_{rs})},$$

we get, in the next result, the desired expression.

Proposition 2.3. *Let Γ^S be a generalized subdivision network of Γ , then for any $x, z \in V$ and*

$v_{xy}, v_{zt} \in V'$, the Green kernel of Γ^S is given by

$$\begin{aligned}
G_{q'}^S(x, z) &= G_{q_\omega}(x, z) - \sum_{\ell \in V} \left[\omega^S(z)G_{q_\omega}(x, \ell) + \omega^S(x)G_{q_\omega}(z, \ell) \right] \pi^S(\ell) + \beta \omega^S(x)\omega^S(z), \\
G_{q'}^S(v_{xy}, z) &= \alpha(x, y)G_{q_\omega}(x, z) + \alpha(y, x)G_{q_\omega}(y, z) \\
&\quad - \sum_{\ell \in V} \left(\omega^S(z)\alpha(x, y)G_{q_\omega}(x, \ell) + \omega^S(z)\alpha(y, x)G_{q_\omega}(y, \ell) + \omega^S(v_{xy})G_{q_\omega}(z, \ell) \right) \pi^S(\ell) \\
&\quad + \left(\beta - \frac{c(x, y)}{c(x, v_{xy})c(y, v_{xy})} \right) \omega^S(v_{xy})\omega^S(z), \\
G_{q'}^S(v_{xy}, v_{zt}) &= \frac{\varepsilon_{zt}(v_{xy})c(x, y)}{c(x, v_{xy})c(y, v_{xy})} + \omega^S(v_{zt})\omega^S(v_{xy}) \left(\beta - \frac{c(x, y)}{c(x, v_{xy})c(y, v_{xy})} - \frac{c(z, t)}{c(z, v_{zt})c(t, v_{zt})} \right) \\
&\quad - \omega^S(v_{zt}) \sum_{\ell \in V} \left(\alpha(x, y)G_{q_\omega}(x, \ell) + \alpha(y, x)G_{q_\omega}(y, \ell) \right) \pi^S(\ell) \\
&\quad - \omega^S(v_{xy}) \sum_{\ell \in V} \left(\alpha(z, t)G_{q_\omega}(z, \ell) + \alpha(t, z)G_{q_\omega}(t, \ell) \right) \pi^S(\ell) \\
&\quad + \alpha(x, y)(\alpha(z, t)G_{q_\omega}(x, z) + \alpha(t, z)G_{q_\omega}(x, t)) \\
&\quad + \alpha(y, x)(\alpha(z, t)G_{q_\omega}(y, z) + \alpha(t, z)G_{q_\omega}(y, t)).
\end{aligned}$$

If we consider $E' = E$; that is, the case of subdivision networks, the above result coincides except for a constant with [6, Proposition 3.1]. The scalar is due to the fact that in the mentioned work, we were considering no weights in the vertex set; *i.e.*, $\omega(x) = 1$ for any $x \in V$ and hence the normalization factor appears.

3 Resistance distances and Kirchhoff index

In this section we aim at obtaining the expression for the effective resistances on a generalized subdivision network of a given network Γ . The expression will follow by taking into account the expression for the effective resistances in terms of Green's function as stated in Proposition 1.2. Again, the results coincide except for a constant with [6, Proposition 4.1].

Proposition 3.1. *Let Γ^S be a partial subdivision network of Γ , then for any $x, z \in V$ and $v_{xy}, v_{zt} \in$*

V' , the Effective resistances of Γ^S are given by

$$\begin{aligned}
R_{\omega^S}^S(x, z) &= \frac{1}{\alpha^2} R_\omega(x, y), \\
R_{\omega^S}^S(v_{zt}, x) &= \frac{c(z, t)}{\alpha^2 c(z, v_{zt}) c(t, v_{zt}) \omega(v_{zt})^2} \\
&\quad + \frac{\omega(z) \omega(t)}{\alpha^2 \omega(v_{zt})} \left(\frac{\alpha(z, t) R_\omega(x, z)}{\omega(t)} + \frac{\alpha(t, z) R_\omega(x, t)}{\omega(z)} - \frac{\alpha(t, z) \alpha(z, t) R_\omega(z, t)}{\omega(v_{zt})} \right), \\
R_{\omega^S}^S(v_{xy}, v_{zt}) &= \frac{c(x, y)}{\alpha^2 c(x, v_{xy}) c(y, v_{xy}) \omega(v_{xy})^2} + \frac{c(z, t)}{\alpha^2 c(z, v_{zt}) c(t, v_{zt}) \omega(v_{zt})^2} \\
&\quad + \frac{1}{\alpha^2 \omega(v_{xy}) \omega(v_{zt})} \left[\alpha(x, y) \alpha(z, t) \omega(x) \omega(z) R_\omega(x, z) + \alpha(x, y) \alpha(t, z) \omega(x) \omega(t) R_\omega(x, t) \right. \\
&\quad \left. + \alpha(y, x) \alpha(z, t) \omega(y) \omega(z) R_\omega(y, z) + \alpha(y, x) \alpha(t, z) \omega(y) \omega(t) R_\omega(y, t) \right] \\
&\quad - \frac{\alpha(x, y) \alpha(y, x) \omega(x) \omega(y)}{\alpha^2 \omega(v_{xy})^2} R_\omega(x, y) - \frac{\alpha(z, t) \alpha(t, z) \omega(z) \omega(t)}{\alpha^2 \omega(v_{zt})^2} R_\omega(z, t), \text{ for any } v_{xy} \neq v_{zt}.
\end{aligned}$$

Proposition 3.2. Let Γ^S be the partial subdivision network of Γ , then the Kirchhoff index of Γ^S is given by

$$\begin{aligned}
k_{\omega^S}^S(\Gamma^S) &= k_\omega(\Gamma) + \sum_{x \in V} \frac{\pi^S(x)}{\omega^S(x)} G_{q_\omega}(x, x) - \sum_{\{x, y\} \in E'} \alpha(x, y) \alpha(y, x) \omega(x) \omega(y) R_\omega(x, y) \\
&\quad + \sum_{\{x, y\} \in E'} \frac{c(x, y)}{c(x, v_{xy}) c(y, v_{xy})} - \beta.
\end{aligned}$$

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