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Green matrices associated with generalized linear polyominoes ☆

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A polyomino is an edge-connected union of cells in the planar square lattice. Here we consider generalized linear polyominoes; that is, the polyominoes supported by an $n \times 2$ lattice. In this paper, we obtain the Green function and the Kirchhoff index of a generalized linear polyomino as a perturbation of a $2n$-path by adding weighted edges between opposite vertices. This approach deeply links generalized linear polyomino Green functions with the inverse M-matrix problem, and especially with the so-called Green matrices.

1. Introduction

A polyomino is an edge-connected union of cells in the planar square lattice. Quoting [8, Chapter 15], “Polyominoes have a long history, going back to the start of the 20th

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century, but they were popularized in the present era initially by Solomon Golomb, then by Martin Gardner in his *Scientific American* columns "Mathematical Games". They now constitute one of the most popular subjects in mathematical recreations, and have found interest among mathematicians, physicists, biologists, and computer scientists as well." Because the chemical constitution of a molecule is conventionally represented by a molecular graph or network, the polyominoes have attracted the attention of the organic chemistry community. So, several molecular structure descriptors based on network structural parameters have been introduced, see for instance [13]. In particular, in the last decade a great amount of work devoted to calculating the Kirchhoff index of linear polyominoes-like networks have been published, see [12] and references therein. In this work, we deal with this class of polyominoes, referred to here as generalized linear polyominoes, which besides including the most popular class of linear polyomino chains, also includes cycles, phenylenes and hexagonal chains, to name only a few. Since the Kirchhoff index is the trace of the Green function of the network, see [3], here we obtain the Green function of such networks. To do this, we understand a polyomino as a perturbation of a path by adding weighted edges between opposite vertices. Therefore, unlike the techniques used in [12], which are based on the decomposition of the combinatorial Laplacian in structured blocks, here we obtain the Green function of a linear polyomino from a perturbation of the combinatorial Laplacian. This approach deeply links linear polyomino Green functions with the inverse M-matrix problem, and especially with the so-called Green matrices, see [7].

The oldest class of symmetric, inverse M-matrices is the class of positive *type D* matrices defined by Markham [9]. An $s \times s$ matrix $\Sigma = (\sigma_{ij})$ is of type D if there exist real numbers $\{\sigma_i\}_{i=1}^s$, with $\sigma_s > \sigma_{s-1} > \cdots > \sigma_1$, such that $\sigma_{ij} = \sigma_{\min\{i,j\}}$. In the same work, it was proved that if $\sigma_1 > 0$ then Σ^{-1} is a tridiagonal M-matrix. The matrix Σ is named of *weak type D* if there are no constrains on the parameters $\{\sigma_i\}_{i=1}^s$.

On the other hand, an $s \times s$ *flipped weak type D* matrix with parameters $\{\sigma_i\}_{k=1}^s$ is the matrix $\Sigma = (\sigma_{ij})$ whose entries satisfy $\sigma_{ij} = \sigma_{\max\{i,j\}}$. When, in addition, the parameters satisfy $\sigma_1 > \cdots > \sigma_s$, then Σ is named a *flipped type D* matrix. In this work, we use the following result about flipped weak type D matrices, see [10].

Lemma 1.1. *Consider Σ the $s \times s$ flipped weak type D matrix with parameters $\sigma_1, \dots, \sigma_s$ and define $\sigma_{s+1} = 0$. Then Σ is invertible iff the parameters satisfy $\sigma_j \neq \sigma_{j+1}$, $j = 1, \dots, s$, and when this condition holds, Σ^{-1} is the tridiagonal matrix*

$$\Sigma^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 & 0 \\ -\gamma_1 & \gamma_1+\gamma_2 & -\gamma_2 & \cdots & 0 & 0 \\ 0 & -\gamma_2 & \gamma_2+\gamma_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \gamma_{s-2}+\gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1}+\gamma_s \end{bmatrix},$$