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Calculating Vertex Energies of Graphs – A Tutorial

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Abstract

In 2018, Arizmendi introduced the concept of energy of a vertex of a graph, $\mathcal{E}_G(v)$, i.e., the distribution of graph energy $\mathcal{E}(G)$ over the vertices of the underlying graph G. We now show how $\mathcal{E}_G(v)$ should actually be calculated.

1 Introduction

The energy of a graph G, introduced in the 1970s and defined as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i| \tag{1}$$

is a much studied spectrum-based graph invariant [8] with noteworthy connections to chemistry [6, 7]. Relatively recently, Octavio Arizmendi with various coauthors [1–4] made a significant extension of the theory of graph energy by inventing the concept of energy of a vertex of a graph, defined as

$$\mathcal{E}_G(v_i) = |\mathbf{A}(G)|_{i,i} \tag{2}$$

which, of course, satisfies the relation

$$\mathcal{E}(G) = \sum_{i=1}^{n} \mathcal{E}_G(v_i)$$

and thus implies a distribution of graph energy among the vertices of the underlying graph.

Until now, to this authors' best knowledge, no numerical calculation of vertex energy was reported, see for instance [5,9–11]. The main reason for this may lie in the fact that for calculating $\mathcal{E}_G(v)$ one needs to know not only the graph eigenvalues, but also the graph eigenvectors. The present tutorial is aimed at assisting such calculations in the future.

Throughout this paper, G denotes a simple graph of order n, whose vertices are labeled by $v_1, v_2, \ldots, v_n$. The adjacency matrix of G, denoted by $\mathbf{A}(G)$, is the $n \times n$ matrix, whose (i, j)-element is equal to 1 if the vertices v_i and v_j are adjacent, and equal to zero otherwise. The eigenvalues of $\mathbf{A}(G)$ are $\lambda_1, \lambda_2, \ldots, \lambda_n$, forming the spectrum of G and used in the definition of graph energy, Eq. (1).

The exact meaning of the matrix $|\mathbf{A}(G)|$ in Eq. (2) will be explained later, see Eq. (6).

2 Reminders from linear algebra

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix $\mathbf{A}(G)$, then for $i = 1, 2, \ldots, n$, the following relations holds:

$$\mathbf{C}_i \, \mathbf{A}(G) = \lambda_i \, \mathbf{C}_i \tag{3}$$

where $\mathbf{C}_i$ is an n-tuple of (real or complex) numbers

$$\mathbf{C}_i = (C_{i,1}, C_{i,2}, \ldots, C_{i,n})$$

which can be viewed as an n-dimensional vector or a $(1 \times n)$-matrix. The vectors $\mathbf{C}_i$, $i = 1, 2, \ldots, n$, are the eigenvectors of the adjacency matrix and thus the eigenvectors of the underlying graph G. They can be chosen

so as to be normalized, i.e.,

$$C_{i,1}^2 + C_{i,2}^2 + \cdots + C_{i,n}^2 = 1 \qquad \text{for all } i = 1, 2, \ldots, n$$

and mutually orthogonal, i.e.,

$$C_{i,1}\, C_{j,1} + C_{i,2}\, C_{j,2} + \cdots + C_{i,n}\, C_{j,n} = 0 \qquad \text{for all } 1 \le i < j \le n.$$

Then one speaks of orthonormal eigenvectors.

Eqs. (3) for $i = 1, 2, \ldots, n$, can be combined into

$$\begin{pmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \\ \vdots \\ \mathbf{C}_n \end{pmatrix} \mathbf{A}(G) = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \begin{pmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \\ \vdots \\ \mathbf{C}_n \end{pmatrix}$$

or, simpler as

$$\mathbf{C}\, \mathbf{A}(G) = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \mathbf{C} \tag{4}$$

where $\mathbf{C}$ is the $(n \times n)$ matrix

$$\begin{pmatrix} C_{1,1} & C_{1,2} & \cdots & C_{1,n} \\ C_{2,1} & C_{2,2} & \cdots & C_{2,n} \\ \vdots & \vdots & \vdots & \vdots \\ C_{n,1} & C_{n,2} & \cdots & C_{n,n} \end{pmatrix}.$$

If the eigenvectors are orthonormal, then the matrix $\mathbf{C}$ has the property

$$\mathbf{C}\, \mathbf{C}^t = \mathbf{C}^t\, \mathbf{C} = \mathbf{I}_n$$

where $\mathbf{I}_n$ is the unit matrix of order n, whereas $\mathbf{C}^t$ is the transpose (or, if some matrix elements are complex, the conjugate transpose) of $\mathbf{C}$. This means that $(\mathbf{C}^t)_{i,j} = \mathbf{C}_{j,i}$.

Bearing this in mind, by multiplying Eq. (4) from left-hand side by $\mathbf{C}^t$, we arrive at

$$\mathbf{A}(G) = \mathbf{C}^t \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \mathbf{C}\,.$$

Let $f(x)$ be any function of the variable x, such that $f(\lambda_i)$, $i = 1, 2, \ldots, n$, are well defined quantities. Then the matrix function $f(\mathbf{A}(G))$ is defined as

$$f(\mathbf{A}(G)) = \mathbf{C}^t \begin{pmatrix} f(\lambda_1) & 0 & \cdots & 0 \\ 0 & f(\lambda_2) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & f(\lambda_n) \end{pmatrix} \mathbf{C}\,. \tag{5}$$

Now, $|\mathbf{A}(G)|$ is the special case of Eq. (5), when $f(x) = |x|$, i.e.,

$$|\mathbf{A}(G)| = \mathbf{C}^t \begin{pmatrix} |\lambda_1| & 0 & \cdots & 0 \\ 0 & |\lambda_2| & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & |\lambda_n| \end{pmatrix} \mathbf{C}\,. \tag{6}$$

3 Calculating vertex energy

From Eq. (6), $|\mathbf{A}(G)|_{i,i}$ can be directly calculated. First note that the (k, h)-element of the matrix

$$\begin{pmatrix} |\lambda_1| & 0 & \cdots & 0 \\ 0 & |\lambda_2| & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & |\lambda_n| \end{pmatrix}$$

is equal to $|\lambda_k|$ if $k = h$, and is equal to zero otherwise.

Now, using the laws of matrix multiplication, we get:

$$
\begin{aligned}
|\mathbf{A}(G)|_{i,i} &= \left[\mathbf{C}^t \begin{pmatrix} |\lambda_1| & 0 & \cdots & 0 \\ 0 & |\lambda_2| & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & |\lambda_n| \end{pmatrix} \mathbf{C} \right]_{i,i} \\
&= \sum_{k=1}^{n} \sum_{h=1}^{n} (\mathbf{C}^t)_{i,k} \begin{pmatrix} |\lambda_1| & 0 & \cdots & 0 \\ 0 & |\lambda_2| & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & |\lambda_n| \end{pmatrix}_{k,h} \mathbf{C}_{h,i} \\
&= \sum_{k=1}^{n} (\mathbf{C}^t)_{i,k} \, |\lambda_k| \, \mathbf{C}_{k,i} = \sum_{k-1}^{n} C_{k,i} \, |\lambda_k| \, C_{k,i}
\end{aligned}
$$

which finally yields [1]

$$
|\mathbf{A}(G)|_{i,i} = \sum_{k=1}^{n} |\lambda_k| \, C_{k,i}^2
$$

and

$$
\mathcal{E}_G(v_i) = \sum_{k=1}^{n} |\lambda_k| \, C_{k,i}^2 \, . \tag{7}
$$

Remark. In the exceptional case when $C_{k,i}$ is complex-valued, namely when $C_{k,i} = a_{k,i} + i \, b_{k,i}$, then the term $C_{k,i}^2$ in Eq. (7) and elsewhere needs to be replaced by $a_{k,i}^2 + b_{k,i}^2$.

4 Concluding note

In order to calculate the fraction of the energy of the graph G, associated with the vertex v_i, that is $\mathcal{E}_G(v_i)$, one has to determine the eigenvalues and the orthonormal eigenvectors of this graph, and then apply Eq. (7).

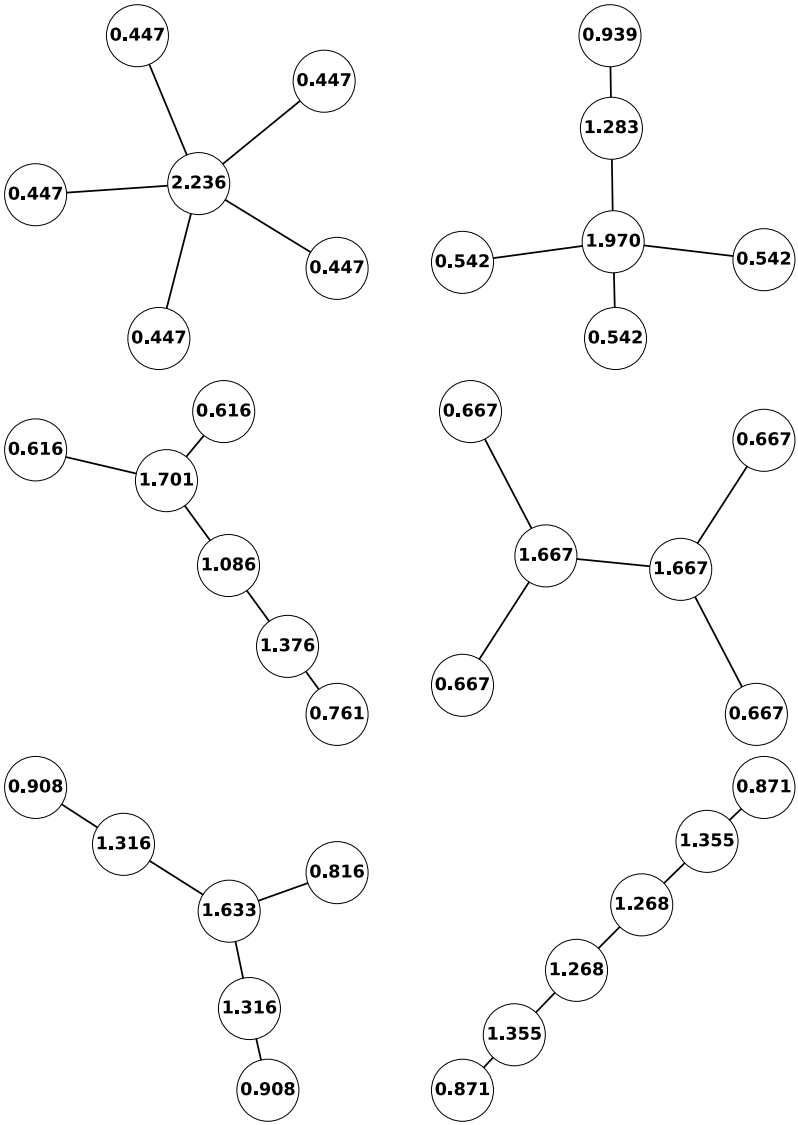

Fig. 1. Energies of vertices of trees of order six.

Graph eigenvalues and eigenvectors should be straightforwardly obtainable by using standard computational software. Therefore, calculations of numerical values of vertex energies, their analysis and possible applications, may follow soon.

In Figure 1 we display the vertex energies of a few trees. These examples may be found useful by those who intend to perform calculations of $\mathcal{E}_G(v_i)$, enabling them to verify the correctness of the results obtained.

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