THE MINIMUM 3-COVERING ENERGY OF COMPLETE GRAPHS

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ABSTRACT: In this paper we introduce a different kind of graph energy, the minimum 3-covering energy of a graph, and determine the minimum 3-covering energy of complete graphs.

1. INTRODUCTION

The Huckel Molecular Orbital theory provided the motivation for the idea of the energy of a graph – the sum of the absolute values of the eigenvalues associated with the graph (see [1]). This resulted in the idea of the minimum 2-covering energy of a graph in [1]. This idea is generalized to the minimum 3-covering energy of a graph in this paper.

All graphs which we shall consider will be finite, simple, loopless and undirected. Let G be such a graph of order n with vertex set \( \{v_1, v_2, \ldots, v_n\} \). A covering (2-covering) of a graph G is a set S of vertices of G of such that every edge of G has at least one vertex in S (see [1]). Since an edge is a path length 1 on 2 vertices (a 2-path) we generalize this to a 3-covering of a graph G as being set Q of vertices of G such that every path of G of length 2 (or 3-path) has at least one vertex in Q (see [2]). Any 3-covering set of G of minimum cardinality is called a minimum 3-covering of G.
2. THE MINIMUM 3-COVERING ENERGY OF A GRAPH

A minimum 3-covering matrix of \( G \) with a minimum 3-covering set \( Q \) of vertices is a matrix:

\[
A_Q^3(G) = (a_{i,j})
\]

where

\[
a_{ij} = \begin{cases} 
1 & \text{if } v_i v_j \in E(G) \\
1 & \text{if } i = j \text{ and } v_i \in Q \\
0 & \text{otherwise}
\end{cases} \tag{*}
\]

The middle condition (*) is equivalent to loops of weight 1 being attached to the vertices of \( Q \).

The characteristic polynomial of \( A_Q^3(G) \) is then denoted by

\[
f_n(G, \lambda) := \det(\lambda I - A_Q^3(G))
\]

The minimum 3-covering energy is then defined as:

\[
E_Q(G) = \sum_{i=1}^{n} |\lambda_i|
\]

Where \( \lambda_i \) (the minimum 3-covering eigenvalues) are the \( n \) real roots of the characteristic polynomial.
3. MOLECULAR STRUCTURES AND ENERGY

The minimum 2-covering energy of molecular structures involves the smallest set of atoms, such that every atom of the structure, is either in the set, or is connected (via bonding) directly to at least one vertex of the set. This is generalized to a minimum 3-covering energy of molecular structures, where the smallest set of atoms is considered, such that every path of 3 atoms has at least one atom in this set, so that no atom is more than a distance 2 from this set.

4. EXAMPLES

For example, consider the path $P_3$ on vertices $v_1, v_2, v_3$ where the first and the last listed vertices are end (pendant) vertices.

A minimum 3-covering is $\{v_1\}$ so that:

$$A^3_{Q}(P_3) = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} Q = \{ v_1 \}$$

The characteristic polynomial is therefore:

$$\det(\lambda I - A^3_{Q}(P_3)) = \begin{vmatrix} \lambda -1 & -1 & 0 \\ -1 & \lambda & -1 \\ 0 & -1 & \lambda \end{vmatrix}$$

$$= (\lambda -1) \begin{vmatrix} \lambda -1 & -1 \\ 0 & \lambda \end{vmatrix} + \begin{vmatrix} \lambda -1 & -1 \\ -1 & \lambda \end{vmatrix} = 1 - \lambda + \lambda(\lambda^2 - \lambda - 1) = \lambda^3 - \lambda^2 - 2\lambda + 1$$

The eigenvalues are (to 5 decimal places – online bluebit matrix calculator):
0.44504; -1.24698; 1.80134 so that the minimum 3-covering energy of this path is:

3.49396

If we take \{v_2\} as another minimum 3-covering of the same path then:

\[
A_3^Q(P_3) = \begin{bmatrix}
0 & 1 & 0 \\
1 & 1 & 1 \\
0 & 1 & 0
\end{bmatrix} \quad Q = \{v_2\}
\]

The characteristic polynomial is therefore:

\[
\det(\lambda I - A_3^Q(P_3)) = \begin{vmatrix}
\lambda & -1 & 0 \\
-1 & \lambda - 1 & -1 \\
0 & -1 & \lambda
\end{vmatrix}
\]

\[
= \begin{vmatrix}
\lambda & 0 \\
-1 & -1
\end{vmatrix} + \begin{vmatrix}
\lambda & -1 \\
-1 & \lambda - 1
\end{vmatrix} = -\lambda + \lambda \left(\lambda^2 - \lambda - 1\right) = \lambda^3 - \lambda^2 - 2\lambda = \lambda(\lambda^2 - \lambda - 2)
\]

\[
\lambda(\lambda - 2)(\lambda + 1).
\]

The minimum 3-covering eigenvalues are therefore: 0, 2 and -1 so that the minimum 3-covering energy of this path is 3.

The above examples illustrate that, in case of a path on 3 vertices, the minimum 3-covering energy of a graph depends on the choice of the 3-covering set.

However, consider the completer graph on 3 vertices, vertices labeled \(v_1, v_2, v_3\). We take our 3-covering set as \(v_1\).
The characteristic polynomial is therefore:

\[ \det(\lambda I - A_Q^3(K_3)) = \begin{vmatrix} \lambda - 1 & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{vmatrix} \]

\[ = \begin{vmatrix} \lambda - 1 & -1 \\ -1 & \lambda \end{vmatrix} + \begin{vmatrix} \lambda - 1 & -1 \\ 0 & -1 - \lambda \end{vmatrix} \]

\[ = (1 + \lambda) \begin{vmatrix} \lambda - 1 & -1 \\ -1 & -1 \end{vmatrix} + (1 + \lambda) \begin{vmatrix} \lambda - 1 & -1 \\ -1 & \lambda \end{vmatrix} \]

\[ = (1 + \lambda)(-\lambda) + (1 + \lambda)(\lambda^2 - \lambda - 1) = (1 + \lambda)(\lambda^2 - 2\lambda - 1) \]

So that eigenvalues are \(-1, \frac{2 \pm \sqrt{8}}{2}\) so that the minimum 3-covering energy of the complete graph is \(1 + \sqrt{8}\).

If we take our minimum 3-covering as \(v_2\) instead of \(v_1\) then we have:

\[ A_Q^3(K_3) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix} \quad Q = \{v_2\} \]
the characteristic polynomial is:

$$\det(\lambda I - A^3_Q(P_4)) = \begin{vmatrix} \lambda & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{vmatrix} = -1 \begin{vmatrix} \lambda & -1 \\ -1 & \lambda \end{vmatrix} - 1 \begin{vmatrix} \lambda & 1 \\ -1 & \lambda \end{vmatrix} + 1 \begin{vmatrix} 1 & 1 \\ -1 & \lambda \end{vmatrix}$$

$$= \lambda(-1 - \lambda) + (1 + \lambda)(\lambda^2 - \lambda - 1)$$

$$(1 + \lambda)(\lambda^2 - 2\lambda - 1)$$

Which is the same as when Q was a different vertex.

5. THE MIMIMUM 3-COVERING ENERGY OF COMPLETE GRAPHS

Generally, the minimum 2-covering of a complete graph G on n vertices is any set of (n-1) vertices of G (see 1). The minimum 3-covering of a complete graph G on n vertices is any set of (n-2) vertices. Thus:

$$A^3_Q(K_n) = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & : & 1 \\ : & 1 & : & 1 & 1 \\ 1 & : & 1 & 1 & 0 \\ 1 & 1 & : & 1 & 1 \end{bmatrix}_{nxn}$$

; Hence the characteristic equation:
\[
\det(\lambda I - A_Q^3(K_n)) = \det \begin{bmatrix}
\lambda - 1 & -1 & -1 & : & -1 & -1 \\
-1 & \lambda - 1 & -1 & : & -1 & -1 \\
-1 & -1 & : & -1 & -1 & : \\
: & -1 & -1 & \lambda - 1 & : & -1 \\
-1 & : & -1 & -1 & \lambda & -1 \\
-1 & -1 & : & -1 & -1 & \lambda
\end{bmatrix}
\]

Subtracting the last row from the second to last row:

\[
= \det \begin{bmatrix}
\lambda - 1 & -1 & -1 & : & -1 & -1 \\
-1 & \lambda - 1 & -1 & : & -1 & -1 \\
-1 & -1 & : & -1 & -1 & : \\
: & -1 & -1 & \lambda - 1 & : & -1 \\
-1 & : & -1 & -1 & \lambda & -1 \\
0 & 0 & : & 0 & -1-\lambda & \lambda + 1
\end{bmatrix}^n_{n \times n}
\]

Expanding this determinant using the last row yields:

\[
(1 + \lambda) \begin{vmatrix}
\lambda - 1 & -1 & : & -1 & -1 \\
-1 & \lambda - 1 & -1 & : & -1 \\
: & : & -1 & \lambda - 1 & -1 \\
-1 & -1 & -1 & : & -1
\end{vmatrix}_{((n-1)(n-1))}
\]

\[
(\lambda + 1) \begin{vmatrix}
\lambda - 1 & -1 & : & -1 & -1 \\
-1 & \lambda - 1 & -1 & : & -1 \\
-1 & : & -1 & \lambda - 1 & -1 \\
-1 & -1 & : & -1 & \lambda
\end{vmatrix}_{(n-1)(n-1)}
\]
The first determinant is $-\lambda^{n-2}$, and we subtract the last row of the second determinant from the second to last row:

$$
= -(1 + \lambda)\lambda^{n-2} + (\lambda + 1) \left|\begin{array}{ccc}
\lambda - 1 & -1 & -1 \\
-1 & \lambda - 1 & -1 \\
-1 & -1 & \lambda - 1 \\
0 & 0 & -\lambda & \lambda + 1
\end{array}\right|_{(n-1)(n-1)}
$$

Expandint the determinat using the last row yields:

$$
= -(1 + \lambda)\lambda^{n-2} + (\lambda + 1)\lambda \left|\begin{array}{ccc}
\lambda - 1 & -1 & -1 \\
-1 & -1 & \lambda - 1 \\
-1 & -1 & \lambda - 1 \\
0 & 0 & -\lambda & \lambda + 1
\end{array}\right|_{(n-2)(n-2)}
$$

+ $(\lambda + 1)(1 + \lambda) \left|\begin{array}{ccc}
\lambda - 1 & -1 & -1 \\
-1 & \lambda - 1 & -1 \\
-1 & -1 & \lambda - 1 \\
-1 & -1 & \lambda - 1
\end{array}\right|_{(n-2)(n-2)}$
The first determinant is \(-\lambda^{n-3}\) while the second determinant yields
\[\lambda^{n-3}(\lambda - (n - 2))\] so that we have:

\[-(1 + \lambda)\lambda^{n-2} - (1 + \lambda)\lambda^{n-2} + (1 + \lambda)^2(\lambda^{n-3}(\lambda - (n - 2)))\]
\[-2(1 + \lambda)\lambda^{n-2} + (1 + \lambda)^2\lambda^{n-2} - \lambda^{n-3}(1 + \lambda)^2(n - 2)\]
\[= (1 + \lambda)\lambda^{n-3}(-2\lambda + (1 + \lambda)\lambda - (1 + \lambda)(n - 2))\]
\[= (1 + \lambda)\lambda^{n-3}(\lambda^2 - (n - 1)\lambda - (n - 2))\]

Eigenvalues are 0 \((n-3)\) times, -1 and the conjugate pairs:

\[
\frac{(n-1) \pm \sqrt{(n-1)^2 + (4n - 8)}}{2} = \frac{(n-1) \pm \sqrt{n^2 + 2n - 7}}{2}
\]

Thus we have the following theorem:

**THEOREM**

The minimum 3-covering energy of a complete graph on \(n \geq 3\) vertices is:

\[1 + \sqrt{n^2 + 2n - 7}\]
REFERENCES

1. Adiga C., Bayad, A., Gutman, I., Srinivas, S. A. THE MINIMUM COVERING ENERGY OF A GRAPH. Kragujevac J. Sci. 34, 39-56. (2012).
2. Bresar, B., Kardos F., Katrenic J., Semanisin, G. MINIMUM K-PATH VERTEX COVER. Discrete Applied Mathematics 159, 12, 1189-1195 (2011)