A GRAPH ENERGY UPPER BOUND USING SPECTRAL MOMENTS

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ABSTRACT. An upper bounds on the energy of graphs is obtained using the spectral moments of the eigenvalues of adjacency matrix associated to the graph using the method of Lagrange multipliers and properties of cubics.

1. INTRODUCTION

The energy of a graph was introduced by Gutman [5] in connection with the total $\pi-$electron energy of a graph after it was recognised that spectral graph theory can be used in Hückel molecular orbital theory ([4],[6]). The general theory and chemical applications can be found in [7].

Let G be a simple (no loops or repeated edges), connected graph with vertices v_i for $i = 1, ...n$ and m edges. Let $A(G)$ be the nxn adjacency matrix associated with G such that

$$A(G) = \begin{cases} 1 & \text{if } v_i \text{ is connected to } v_j \text{ where } i \neq j \\ 0 & \text{if } v_i \text{ is not connected to } v_j \text{ where } i \neq j. \end{cases}$$

Let $\lambda_1, \lambda_2, ..., \lambda_n$ denote the n eigenvalues of $A(G)$ and the $Spec(A) = \{\lambda_1, \lambda_2, ..., \lambda_n\}$ be the spectrum of A. We note that the $tr(A) = \sum_{i=1}^{n} \lambda_i$ and $\det(A) = \prod_{i=1}^{n} \lambda_i$, and that the $\det(A) = 0$ if and only if there exists at least one eigenvalue equal to zero. In addition, since A is a real, symmetric matrix, its eigenvalues are all real.

In the 1940's, a close correspondence between the graph eigenvalues and the Hückel molecular orbital energy levels E_π of electrons in conjugated

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hydrocarbons was realized. In particular,

$$E_\pi = na + \beta \sum_{i=1}^{n} |\lambda_i|$$

where α, β are constants. Since n is constant in chemical applications, the only non-trivial part of E_π is $\sum_{i=1}^{n} |\lambda_i|$. In practice, the total $\pi-$electron energy of a graph applies only to molecular graphs where the maximm vertex degree of G cannot exceed 3. In the 1978, Gutman [8] expanded the concept to all graphs and defined the energy of any simple graph G on n vertices, as

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

This is a natural extension of this property as crystallographic groups tell us about the structure of matter. Graphs based on groups are used to model individual molecules as well as a variety of chemical systems. In fact, the connection tables used by the Chemicals Abstract Service are essentially adjacency matrices in that the list the atoms in a molecule along with their binding linkages. Broader study of the energy of graphs began in the 2000's and has expanded the field of spectral analysis. Not only does this newer graph invariant allow for a new relation on all graphs, the energy of a graph is related to several other concepts in analysis, linear algebra and spectral graph theory.

McClelland [12] proved the energy of a graph $E(G) \leq \sqrt{2mn}$.

For $2m \geq n$, Koolen et al. [11] improved the bound to

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}.$$

Both of these bounds are very broad. Although Cioslowski [1] presented an improvement for the energy of bipartite graphs using variations of spectral moments and differentiation techniques which provided motivation for this paper, the techniques in [1] do not work for non-bipartite graphs.

2. Definitions

In this paper, we find another bound on the energy of all graphs using spectral moments and properties of cubics. Relations between spectral moments and energy have been studied in several papers in [3],[9], [10] and [13]. Define the δ^{th} spectral moment of a graph G as

$$M_\delta = M_\delta(G) = \sum_{i=1}^{n} \lambda_i^\delta \text{ for } \delta \in \mathbb{Z}^+.$$

From the well-known fact in [2], M_δ is equal to the number of self-returning walks of length δ in the graph G where

$$M_2 = \sum_{i=1}^{n} \lambda_i{}^2 = 2m \qquad \text{and} \qquad M_4 = \sum_{i=1}^{n} \lambda_i{}^4 = \sum_{i=1}^{n} d_i^2 - 2m + 8q$$

where d_i is the degree of each of the vertices of the graph and q is the number of quadrangles in the graph of G.

3. Procedure

The goal is to find bounds on the energy $E(G)$ of graphs by using the second and fourth spectral moments, M_2 and M_4. Since the eigenvalues λ_i of the adjacency matrix associated to the graph are real, set

$$M_2 = \sum_{i=1}^{n} \lambda_i^2 = \sum_{i=1}^{n} |\lambda_i|^2 = A \quad \text{and} \quad M_4 = \sum_{i=1}^{n} \lambda_i^4 = \sum_{i=1}^{n} |\lambda_i|^4 = B.$$

Thus both A and B are real and positive. Note that for a $k-$regular graph, $A > k^2$ and $B > k^4$ as the largest eigenvalue of a $k-$regular graph is k.

Let a, b be real and consider the following equation where a and b are Lagrange multipliers

$$\sum_{i=1}^{n} |\lambda_i| + a\left(\sum_{i=1}^{n} |\lambda_i|^2 - A\right) + b\left(\sum_{i=1}^{n} |\lambda_i|^4 - B\right)$$

and to find the extrema, set

$$\frac{\partial \left[\sum_{i=1}^{n} |\lambda_i| + a\left(\sum_{i=1}^{n} |\lambda_i|^2 - A\right) + b\left(\sum_{i=1}^{n} |\lambda_i|^4 - B\right)\right]'}{\partial \lambda_i} = 0$$

for all $i = 1, ..., n$. Then for each i, we have the equation

$$1 + 2a|\lambda_i| + 4b|\lambda_i|^3 = 0$$

Notice that $|\lambda_i|$ is the root of a cubic whose zeros are of the form $\alpha_i, \beta_i, \gamma_i$ where $\alpha_i + \beta_i + \gamma_i = 0$ and where none of α_i, β_i or γ_i is 0 for each $i = 1, ..., n$. Since $|\lambda_i| \geq 0$ and $|\lambda_i|$ must satisfy A and B, the roots $\alpha_i, \beta_i, \gamma_i$ must be real where two of the three roots are positive. Without loss of generality, assume $\alpha_i \geq \beta_i > 0$ and $\gamma_i < 0$. Then $|\lambda_i| = \alpha_i$ or β_i for each $i = 1, ..., n$. Order $|\lambda_i|$ such that

$$|\lambda_i| = \alpha_i \quad \text{for } 1 \leq i \leq j$$

and

$$|\lambda_i| = \beta_i \quad \text{for } j+1 \leq i \leq n.$$

For each $i = 1, ..., n$, we want to optimize the $j^{th} - term$

$$E(j) = j\alpha_i + (n-j)\beta_i.$$

Solving for the contraints A and B in terms of α_i and β_i, we have

$$A = j\alpha_i^2 + (n-j)\beta_i^2 \qquad \text{and} \qquad B = j\alpha_i^4 + (n-j)\beta_i^4.$$

4. Results

Solving for α_i and β_i using the properties above, we obtain

$$\alpha_i = \sqrt{\frac{1}{n}\left[A + \sqrt{\frac{n-j}{j}}\sqrt{A^2 - nB}\right]}$$

and

$$\beta_i = \sqrt{\frac{1}{n}\left[A - \sqrt{\frac{j}{n-j}}\sqrt{A^2 - nB}\right]}.$$

To verify that α_i and β_i are real, we need to verify that $A - \sqrt{\frac{j}{n-j}}\sqrt{A^2 - nB} \geq 0$.

Lemma 1. *Assume that* $A^2 \geq nB$.

Then inequality $A - \sqrt{\frac{j}{n-j}}\sqrt{A^2 - nB} \geq 0$ *holds for all* $n \geq 2j$.

Proof. Solving the inequality $A - \sqrt{\frac{j}{n-j}}\sqrt{A^2 - nB} \geq 0$, we have

Without loss of generality, remove the subscripts from α_i and β_i and substitute into A and B to obtain

$$A = j\alpha^2 + (n-j)\beta^2 \quad \text{and} \quad B = j\alpha^4 + (n-j)\beta^4.$$

Then we have

$$n\left(j\alpha^2 + (n-j)\beta^2\right)^2 + jn(j\alpha^4 + (n-j)\beta^4) \geq 2(j\alpha^2 + (n-j)\beta^2)^2$$

$$n(j\alpha^4 + 2j(n-j)\alpha^2\beta^2 + (n-j)^2\beta^4) + jn(j\alpha^4 + (n-j)\beta^4) \geq 2j(j\alpha^4 + 2j(n-j)\alpha^2\beta^2 + (n-j)^2\beta^4)$$

$$nj\alpha^4 + 2jn(n-j)\alpha^2\beta^2 + (n-j)^2n\beta^4 + j^2n\alpha^4 + jn(n-j)\beta^4 \geq 2j^2\alpha^4 + 4j^2(n-j)\alpha^2\beta^2 + 2j(n-j)^2\beta^4.$$

Notice that all of the terms on each side of the equation are positive. Comparing the coefficients of each term on the right with the respective terms on the left, at the very least we obtain:

$$\alpha^4 : j^2 n + nj \geq 2j^2$$
$$\alpha^2\beta^2 : 2jn(n-j) \geq 4j^2(n-j)$$
$$\beta^4 : (n-j)^2 n \geq 2j(n-j)^2$$

Simplifying the bounds on these coefficients, at the very least we obtain

$$\alpha^4 : n \geq 1$$
$$\alpha^2\beta^2 : n \geq 2j$$
$$\beta^4 : n \geq 2j.$$

Thus for $n \geq 2j$, $A - \sqrt{\frac{j}{n-j}}\sqrt{A^2 - nB} \geq 0$ whenever $A^2 \geq nB$. □

Recall that we want to optimize the term $E(j)$ where

$E(j) = j\alpha_i + (n-j)\beta_i$.

$$= j\sqrt{\frac{1}{n}\left[A + \sqrt{\frac{n-j}{j}}\sqrt{A^2 - nB}\right]} + (n-j)\sqrt{\frac{1}{n}\left[A - \sqrt{\frac{j}{n-j}}\sqrt{A^2 - nB}\right]}$$

$$= \sqrt{\frac{1}{n}\left[j^2 A + \sqrt{j^3(n-j)}\sqrt{A^2 - nB}\right]}$$

$$+ \sqrt{\frac{1}{n}\left[(n-j)^2 A - \sqrt{j(n-j)^3}\sqrt{A^2 - nB}\right]}$$

Lemma 2. *The values of $E(j)$ decrease as j increases such that*

$$E(1) > E(2) > ... > E(n).$$

Proof. Let $E(j) = j\alpha + (n-j)\beta$. Let

$$E(x) = x\alpha_x + (n-x)\beta_x$$

denote a continuous function in x such that $E(x) = E(j)$ for all $j = 1, ...n$. Also, recall that $\alpha > \beta \geq 0$ and let $\alpha = \alpha_x > \beta = \beta_x \geq 0$ when $x = j$.

Taking the derivative of A_x, B_x and $E(x)$ with respect to x and setting the equations equal to 0, we get

$$A'_x = 2j\alpha_x\alpha'_x + 2(n-x)\beta_x\beta'_x - \beta_x^2 = 0$$

and

$$B'_x = 4j\alpha_x^3\alpha'_x + 4(n-x)\beta_x^3\beta'_x - \beta_x^4 = 0$$

which give

$$\alpha'_x = -\frac{\alpha_x^2 - \beta_x^2}{4x\alpha_x} \quad \text{and} \quad \beta'_x = -\frac{\alpha_x^2 - \beta_x^2}{4(n-x)\beta_x}.$$

Combining with

$$E'(x) = \alpha_x + x\alpha'_x + (n-x)\beta'_x - \beta_x$$

we obtain

$$E'(x) = -\frac{(\alpha_x - \beta_x)^3}{4\alpha_x\beta_x}.$$

which is negative as $\alpha_x > \beta_x \geq 0$. Thus $E(x)$ is a decreasing function in x and $E(1) > E(2) > ... > E(n)$. □

Note that any connected graph has to have at least $n = 2$ vertices, else the graph is simply a single point. Thus $j = 1$ is valid for all connected graphs. By the lemma above, the maximal energy for G at any given eigenvalue occurs at $E(1)$. Since we have n values of $E(j)$, we can now prove the following theorem.

Theorem 1. *For a graph G with spectral moments are M_2 and M_4 such that $M_2^2 \geq nM_4$, the upper bound for the graph energy $E(G)$ is*

$$\sqrt{n\left[M_2 + \sqrt{n-1}\sqrt{M_2^2 - nM_4}\right]} + (n-1)\sqrt{n\left[(n-1)M_2 - \sqrt{(n-1)^3}\sqrt{M_2^2 - nM_4}\right]}.$$

Proof. From above,

$$E(j) = \sqrt{\frac{1}{n}\left[j^2A + \sqrt{j^3(n-j)}\sqrt{A^2 - nB}\right]} + \sqrt{\frac{1}{n}\left[(n-j)^2A - \sqrt{j(n-j)^3}\sqrt{A^2 - nB}\right]}$$

where $A = M_2$ and $B = M_4$.
Since we have n values of $E(j)$ and $E(1) > E(2) > ... > E(n)$ by the above

lemma,

$$\begin{aligned}
E(G) &= E(1) + E(2) + \dots + E(n) \\
&\leq nE(1) \\
&= n\left[\sqrt{\frac{1}{n}\left[M_2 + \sqrt{n-1}\sqrt{nM_4 - M_2^2}\right]}\right. \\
&\left. + (n-1)\sqrt{\frac{1}{n}\left[M_2 - \sqrt{\frac{1}{n-1}}\sqrt{nM_4 - M_2^2}\right]}\right] \\
&= \sqrt{n\left[M_2 + \sqrt{n-1}\sqrt{nM_4 - M_2^2}\right]} \\
&+ (n-1)\sqrt{n\left[M_2 - \sqrt{\frac{1}{n-1}}\sqrt{nM_4 - M_2^2}\right]}.
\end{aligned}$$

□

Unfortunately, the same techinique does not work for lower bounds as the value for β becomes complex when $A^2 - nB < 0$ which occurs at some $j > \frac{n}{2}$.

Additionally, recall that if k is the degree of the vertices of G, then G is called k-regular. We also note that this inequality $M_2^2 \geq nM_4$, will not hold for k-regular graphs. For any $k-$regular graph, it is easy to see that on n vertices and m edges, $2m = kn$. Thus the spectral moments become

$$M_2 = \sum_{i=1}^{n} \lambda_i^2 = kn \qquad \text{and} \qquad M_4 = \sum_{i=1}^{n} \lambda_i^4 = 2nk^2 - kn + 8q$$

If a k-regular graph is not quadrangle-free, then its degree $k = 4$ and the spectral moments are

$$M_2 = \sum_{i=1}^{n} \lambda_i^2 = 4n \qquad \text{and} \qquad M_4 = \sum_{i=1}^{n} \lambda_i^4 = 32n - 4n + 8q.$$

If a k-regular graph is quadrangle-free, then $q = 0$ and the spectral moments are

$$M_2 = \sum_{i=1}^{n} \lambda_i^2 = kn \qquad \text{and} \qquad M_4 = \sum_{i=1}^{n} \lambda_i^4 = 2nk^2 - kn.$$

For $M_2^2 \geq nM_4$ to hold, we would need

$$k^2n^2 \geq 2n^2k^2 - kn^2 + 8qn$$

which would mean that

$$kn^2 \geq k^2n^2 + 8qn.$$

The only solutions to the inequality occur if the graph is quadrangle-free. Then we have that $1 \geq k$ whose solutions are $k = 1$ which is a cycle or $k = 0$ which is a disconnected graph with no edges.

References

[1] Cioslowski, J. Upper bound for total $\frac{1}{4}$-electron energy of benzenoid hydrocarbons, Z. Naturforsch. 40a (1985), 1167-1168.

[2] Cvetkovic, D., Doob, M., Sachs, H., Spectra of Graphs - Theory and Applications, Academic Press, New York, 1980.

[3] de la Pena, J.A., Gutman, I. Rada, J., Zhou, B. On spectral moments and energy of graphs, MATCH Commun. Math. Comput. Chem. 57 (2007), 183-191.

[4] Graovac, A., Gutman, I., Trinajsti, N., Topological Approach to the Chemistry of Conjugated Molecules, Springer, Berlin, 1977.

[5] Gutman, I. The energy of a graph, Ber. Math.-Statist. Sekt. Forshungszentrum Graz 103 (1978) 1–22.

[6] Gutman, I.,Trinajstic N., Topics Curr. Chem. 42 (1973) 49

[7] Gutman, I., Polansky, O.E., Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[8] Gutman, I., The Energy of a Graph, Ber. Math.-Statist. Sekt. Forschungsz. Graz 103, 1-22 (1978)

[9] Gutman, I. On graphs whose energy exceeds the number of vertices, Lin. Algebra Appl. 429 (2008), 2670-2677.

[10] Gutman, I. Remark on the moment expansion of total $\frac{1}{4}$-electron energy, Theor. Chim. Acta 83 (1992) 313-318.

[11] Koolen, J.H.; Moulton, V. Maximal energy graphs. Adv Appl Math 2001, 26, 47–52.

[12] McClelland, B.J. Properties of the latent roots of a matrix: The estimation of π–electron energies. J Chem Phys 1971, 54, 640–643.

[13] Morales, D.A. The total $\frac{1}{4}$-electron energy as a problem of moments: Application of the Backus-Gilbert method, J. Math. Chem. 38 (2005), 389-397.

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