My Favorite Application Using Graph Eigenvalues: Graph Energy

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Abstract

The energy of a graph G, often denoted $\mathcal{E}(G)$, is defined to be the sum of the absolute value of the eigenvalues of its adjacency matrix. This graph invariant is very closely connected to a chemical quantity known as the total π-electron energy of conjugated hydrocarbon molecules. Very recently graph energy has become a quantity of interest to mathematicians, and several variations have been introduced. Here we present some of the history, basic definitions, and proof techniques used to study energy. We also list a few basic results of the field.

1   History

The energy of a graph was first defined by Ivan Gutman in 1978 [5]. However, the motivation for his definition appeared much earlier, in the 1930's, when Erich Hückel proposed the famous Hückel Molecular Orbital Theory. Hückel's method allows chemists to approximate energies associated with π-electron orbitals in a special class of molecules called conjugated hydrocarbons. The method assumes that the Hamiltonian operator is a simple linear combination of certain orbitals, and uses the time-independent Schrödinger equation to solve for the energies desired [8].

As late as 1956, Günthard and Primas realized that the matrix used in the Hückel method is a first-degree polynomial of the adjacency matrix of a certain graph related to the molecule being studied [4]. Moreover, under certain reasonable assumptions about the molecule, its "total π-electron energy" can be written as the sum of the absolute eigenvalues of this graph.

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According to Gutman, Klobučar, and Majstorović [7], chemists studying total π-electron energy were aware of this graph theoretic connection but did not consider graphs that did not arise from purely chemical origins.

Gutman introduced his definition of the energy of a general simple graph in his paper "The energy of a graph." He notes that at first, very few mathematicians seemed to be attracted to the definition [7]. In the past decade, interest in graph energy has increased and many different versions have been conceived. In 2006, Gutman and Zhou defined the Laplacian energy of a graph as the sum of the absolute deviations (i.e., distance from the mean) of the eigenvalues of its Laplacian matrix [9]. Similar variants of graph energy were developed for the signless Laplacian [1], the distance matrix [6], the incidence matrix [10], and even for a general matrix not associated with a graph [12]. In 2010, Cavers, Fallat, and Kirkland first studied the Normalized Laplacian energy of a graph, also known as the Randić energy for its connection to the Randić index [2].

In 2012, Gutman, Li, and Shi published a book summarizing the main applications, theorems, and methods regarding the adjacency energy of a graph [8]. This books also contains a chapter on other types of energy, as well as a nearly exhaustive list of references of results on graph energy. Interested readers are encouraged to see this book, and especially its bibliography, for more information.

2 Motivation

The time-independent Schrödinger equation, often written as

$$H\Psi = E\Psi,$$

is used to predict the energy of a system when the Hamiltonian operator H of the system is not dependent on time. Here Ψ is a wave function known as a stationary state, and E is the energy of that state. One can easily see that in this situation (E, Ψ) is just an eigenpair of H.

Hückel Molecular Orbital Theory gives chemists a way to approximate π-electron energies when the H above is the Hamiltonian operator of a single conjugated hydrocarbon molecule. In this case it has been determined that $H = \alpha I + \beta A$, where A is the adjacency matrix of a graph representing the carbon skeleton of the molecule, and α and β are constants. It follows that

solving the eigenvalue problem for H is equivalent to solving the eigenvalue problem for A. Eigenvectors of H correspond to orbitals of the molecule, which may contain 0, 1, or 2 π-electrons. It is noted that most frequently an orbital contains two π-electrons exactly when the corresponding E value is positive, and no π-electrons when E is negative. Since the trace of an adjacency matrix is 0, which implies the sum of the positive eigenvalues equals the sum of the negative ones, it turns out that total π-electron energy is largely concerned with the quantity

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

where n is the number of carbon atoms in the molecule, and λ_i is the ith eigenvalue of the adjacency matrix of the graph G corresponding to the carbon skeleton [8].

There is no reason that one cannot study this quantity for an arbitrary graph, and so Gutman defines the energy of a graph to be the sum of the absolute values of its eigenvalues. Formulae and bounds for this expression are useful for theoretical chemists, for whom this value can take on physical significance. For mathematicians, the concept leads to many interesting problems which are not necessarily identical to determining the spectrum of a graph.

Similar definitions have been formulated for other matrices associated with a graph, such as the Laplacian, normalized Laplacian, and distance matrices. For some of these matrices, eigenvalues are always non-negative and so expression (1) is just the trace. The natural way to adapt the definition for these matrices is

$$\sum_{i=1}^{n} |\lambda_i - \overline{\lambda}|, \tag{2}$$

where $\overline{\lambda}$ is the average of all of the eigenvalues $\lambda_1, \ldots, \lambda_n$.

Nikiforov suggested the definition of a matrix, not necessarily associated with any graph, to be

$$\mathcal{E}(M) = \sum_{i=1}^{n} \sigma_i, \tag{3}$$

where $\sigma_1, \ldots, \sigma_n$ are the singular values of the matrix M. It is worth noting that definition (2) does not agree with definition (3) for all graph matrices.

3 Methods

It is obvious that given the eigenvalues of a graph one can calculate its energy. However, if we are not interested in the individual eigenvalues but merely the sum of their absolute deviations then there are less direct methods that we may utilize.

One such method takes advantage of one version of the Cauchy Residue Theorem, which states that the contour integral of a meromorphic function along a simple closed curve is equal to the sum of the residues of the poles contained in the curve. Given a graph G on n vertices, if we choose our poles to be at the positive eigenvalues of G and our contour to be a sufficiently large semicircle growing in the direction of the positive real axis, then we should retrieve $\frac{1}{2}\mathcal{E}(G)$. A careful treatment produces what is known as the Coulson Integral Formula:

$$\mathcal{E}(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(n - \frac{ix\phi'(G, ix)}{\phi(G, ix)} \right) dx,$$

where $\phi(G, x)$ is the characteristic polynomial of the adjacency matrix of G [8, 3].

Another useful result is the Ky Fan Inequality of Linear Algebra. It states that for $n \times n$ matrices A, B, and C such that $A + B = C$, we have

$$\sum_{i=1}^{n} \sigma_i(C) \leq \sum_{i=1}^{n} \left(\sigma_i(A) + \sigma_i(B) \right),$$

where $\sigma_1, \ldots, \sigma_n$ are the singular values of the appropriate matrix. Notice that this is suited very well for the energy of a general square matrix. Moreover, many of the graph energies that have been defined can be rewritten as the sum of the singular values of some matrix. In particular, the adjacency energy of a graph is equal to the sum of the singular values of the adjacency matrix itself. Because the sum of the adjacency matrices of a graph and its complement give us the adjacency matrix of a complete graph, whose spectrum is well-known, the Ky Fan Inequality is very useful for obtaining Nordhaus-Gaddum type bounds [8].

The definition of graph energy is also reminiscent of the so-called spectral moments of the form $\sum_{i=1}^{n} \lambda_i^k$ for a given integer k. By clever applications of the Cauchy-Schwarz inequality, it is possible to derive bounds on graph energy in terms of spectral moments. One example is the following [13, 14]:

Theorem. *Let G be a nontrivial bipartite graph with adjacency eigenvalues $\lambda_1, \ldots, \lambda_n$, and let r, s, and t be even positive integers such that $4r = s+t+2$. Then*

$$\mathcal{E}(G) \geq \frac{\left(\sum_{i=1}^n \lambda_i^r\right)^2}{\sqrt{\left(\sum_{i=1}^n \lambda_i^s\right)\left(\sum_{i=1}^n \lambda_i^t\right)}}.$$

4   Some Results

Some of the standard goals for those who study graph energy are to find formulae or bounds for energy, as well as extremal examples. Understanding how graph operations (like standard products or edge deletion) affect the energy of a graph can aid in this, and has also become a popular area of research. [8].

A very simple upper bound for graph energy is demonstrated below.
Theorem. *For a graph G with n vertices and m edges, we have*

$$\mathcal{E}(G) \leq \sqrt{2mn}.$$

Proof. By the Cauchy-Schwarz inequality,

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

$$\leq \sqrt{n \sum_{i=1}^n \lambda_i^2}$$

$$= \sqrt{n \operatorname{Tr}(A^2)}$$

$$= \sqrt{2mn}.$$

$\square$

It is known that equality is achieved exactly in the cases where G is either an empty graph or a 1-regular graph. Despite the tightness of this upper bound, more precise bounds can be obtained by determining special classes of graphs. For example [11],
Theorem. *If G is a bipartite graph on n vertices, where $n > 2$, then*

$$\mathcal{E}(G) \leq \frac{n(\sqrt{n} + \sqrt{2})}{\sqrt{8}}.$$

The question of how small the energy of a bipartite graph can be has been partially answered via an extremal example [8]. If G is bipartite with n vertices and m edges satisfying $n \leq m \leq 2n - 4$, then

$$\mathcal{E}(G) \geq 2\sqrt{m + 2\sqrt{(m - n + 2)(2n - m - 4)}}.$$

This is achieved by the bipartite graph with parts $|A| = 2$ and $|B| = n - 2$. We join one vertex in A to every vertex in B, and then finish the construction by connecting the remaining vertex in A to $m - n + 2$ vertices in B.

Another fundamental result is:
Theorem. *If H is a subgraph of G, let G' be the graph obtained by removing all edges of H from G. Then*

$$\mathcal{E}(G) - \mathcal{E}(H) \leq \mathcal{E}(G') \leq \mathcal{E}(G) + \mathcal{E}(H).$$

This can be easily proved using the Ky Fan inequality, once we notice that the adjacency matrix of G is exactly the sum of the adjacency matrices of G' and H.

Gutman, Li, and Shi's book on graph energy contains a large variety of other results, a majority with proofs.

References

[1] N.M.M. de Abreu, I. Gutman, M. Robbiano, and W. So, Applications of a theorem by Ky Fan in the theory of graph energy, *Lin. Algebra Appl.*, **432** (2010) 2163–2169.

[2] M. Cavers, S. Fallat, and S. Kirkland, On the normalized laplacian energy and general Randić index R_{-1} of graphs, *Lin. Algebra Appl.*, **443** (2010) 172–190.

[3] C. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, *Proc. Cambridge Phil. Soc.*, **36** (1940) 201–203.

[4] H. H. Günthard and H. Primas, Zusammenhang von Graphentheorie und MO-Theorie von Molekeln mit Systemen konjugierter Bindungen, *Helv. Chim. Acta*, **39** (1956) 1645–1653.

[5] Ivan Gutman, The energy of a graph, *10. Steiermärkisches Mathematisches Symposium (Stift Rein, Graz, 1978)*, **103** (1978) 1–22.

[6] I. Gutman, G. Indulal, and A. Vijayakumar, On distance energy of graphs, *MATCH Commun. Math. Comput. Chem.*, **60** (2008) 461–472.

[7] Ivan Gutman, Antoaneta Klobučar, and Snježana Majstorović, Selected Topics from the Theory of Graph Energy: Hypoenergetic Graphs, *Applications of Graph Spectra (Mathematical Institution, Belgrade)* (2009) 65–105.

[8] I. Gutman, X. Li, and Y. Shi. *Graph Energy.* New York: Springer, 2012.

[9] Ivan Gutman and B. Zhou, Laplacian energy of a graph, *Lin. Algebra Appl.*, **414** (2006) 29–37.

[10] M. R. Jooyandeh, D. Kiani, and M. Mirzakhah, Incidence energy of a graph, *MATCH Commun. Math. Comput. Chem.*, **62** (2009) 561–572.

[11] J. H. Koolen and V. Moulton, Maximal energy bipartite graphs, *Graphs Combin.*, **19** (2003) 131–135.

[12] V. Nikiforov, The energy of graphs and matrices, *J. Math. Anal. Appl.*, **326** (2007) 1472–1475.

[13] J. A. de La Peña and L. Mendoza, Comparing momenta and π-electron energy of benzenoid molecules, *Discr. Math.*, **302** (2005) 77–84.

[14] J. Rada and A. Tineo, Upper and lower bounds for the energy of bipartite graphs, *J. Math. Anal. Appl.*, **289** (2004) 446–455.