Spectral Graph Theory – From Practice to Theory

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Abstract

Graph theory is the area of mathematics that studies networks, or graphs. It arose from the need to analyse many diverse network-like structures like road networks, molecules, the Internet, social networks and electrical networks. In spectral graph theory, which is a branch of graph theory, matrices are constructed from such graphs and analysed from the point of view of their so-called eigenvalues and eigenvectors. The first practical need for studying graph eigenvalues was in quantum chemistry in the thirties, forties and fifties, specifically to describe the Hückel molecular orbital theory for unsaturated conjugated hydrocarbons. This study led to the field which nowadays is called chemical graph theory. A few years later, during the late fifties and sixties, graph eigenvalues also proved to be important in physics, particularly in the solution of the membrane vibration problem via the discrete approximation of the membrane as a graph. This paper delves into the journey of how the practical needs of quantum chemistry and vibrating membranes compelled the creation of the more abstract spectral graph theory. Important, yet basic, mathematical results stemming from spectral graph theory shall be mentioned in this paper. Later, areas of study that make full use of these mathematical results, thus benefitting greatly from spectral graph theory, shall be described. These fields of study include the P versus NP problem in the field of computational complexity, Internet search, network centrality measures and control theory.

Keywords: *spectral graph theory, eigenvalue, eigenvector, graph.*

Introduction: Spectral Graph Theory

Graph theory is the area of mathematics that deals with networks. In its simplest form, a graph, or network, is a set of points called vertices, connected to each other by edges (Wilson, 1996). Such a graph may represent things as diverse as, but not limited to, molecules, road networks, computer networks, interconnections of a brain, electrical networks and social networks. This vast array of representations

allows graph theory to be applied in virtually all areas related to science, technology, engineering and mathematics.

Spectral graph theory is a subfield of graph theory in which a matrix is used to represent the underlying graph, then the graph is studied using the eigenvalues and eigenvectors of this matrix. (Cvetković et al., 2009). The simplest graph matrix representation is the so-called adjacency matrix $\mathbf{A}$, which is the $n \times n$ matrix (n being the number of vertices in the graph) whose entry in its jth row and kth column is 1 if vertices j and k are connected by an edge in the graph and is 0 otherwise. But other matrices are possible, for example the Laplacian matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where $\mathbf{D}$ is the diagonal matrix of vertex degrees of the graph (by degree is meant the number of vertices that are incident to a particular vertex) and the generalized adjacency matrix $\mathbf{A} + y\mathbf{J}$, where $\mathbf{J}$ is the matrix of all ones and y is any real number (Cvetković et al., 2009).

If, for some $n \times n$ matrix $\mathbf{M}$, there exists a nonzero vector $\mathbf{x}$ (an $n \times 1$ matrix) that satisfies the following equation:

$$\mathbf{M}\mathbf{x} = \lambda\mathbf{x} \qquad [1]$$

then λ is called an eigenvalue of $\mathbf{M}$ and $\mathbf{x}$ is called an eigenvector associated with the eigenvalue λ. The set of all the n eigenvalues obtained in this way is called the spectrum of $\mathbf{M}$ (Horn & Johnson, 2012).

Spectral graph theory deals with discovering properties of a graph from the spectrum (and, sometimes, the eigenvectors) of some matrix representing it. Doing this may seem unnecessary and devoid of any applications at this point, but this couldn't be further from the truth.

Hückel Molecular Orbital Theory

In 1926, the Austrian Erwin Schrödinger (1926) published what would later be called the Schrödinger equation. The time-independent version of this equation is of the form

$$\hat{H}\,\Psi = \mathcal{E}\,\Psi \qquad [2]$$

where Ψ is the wave function of the system modelled by the partial differential equation above, $\hat{H}$ is the Hamiltonian operator of the system and $\mathcal{E}$ is the energy of the system. If the Schrödinger equation is applied to a molecule and is solved, then its solutions end up describing the behaviour of the electrons in the molecule, as well as their energies (Majstorović et al., 2009). Unfortunately, solving the Schrödinger equation proved difficult.

In 1931, Erich Hückel, a German scholar, proposed the following method to approximate solutions of [2], the Schrödinger equation for unsaturated conjugated hydrocarbons. Hückel's approach (1931), nowadays called the Hückel Molecular Orbital theory (HMO) was to express Ψ as a linear combination of a finite number of suitably chosen basis functions. This transforms [2] into

$$\boldsymbol{H}\,\Psi = E\,\Psi \qquad [3]$$

so that the Hamiltonian operator $\mathbf{H}$ is now a finite matrix. The similarity of equations [1] and [3] is apparent.

The matrix $\mathbf{H}$ was defined such that its diagonal entries are all equal to a constant α and any entry in the jth row and kth column is equal to a constant β if the (carbon) atoms j and k are chemically bonded and is equal to 0 otherwise. In other words, $\mathbf{H} = \alpha\mathbf{I} + \beta\mathbf{A}$, where $\mathbf{I}$ is the identity matrix and $\mathbf{A}$ is the adjacency matrix of the graph corresponding to the carbon-atom skeleton of the conjugated molecule. Interestingly, this relation became known only in 1956, a full 25 years after Hückel proposed his HMO theory (Majstorović et al., 2009).

This means that the energy levels of the π-electrons are $E_j = \alpha + \beta\lambda_j$ for all $j = 1,2,\dots,n$, where λ_j is the jth eigenvalue of the adjacency matrix $\mathbf{A}$. The eigenvectors, in turn, were taken as discrete approximations to the molecular orbitals $\Psi_1,\dots,\Psi_n$. Thus, a clear association between the π-electron energy levels of the hydrocarbon, the molecular orbitals and the eigenvalues and eigenvectors of the adjacency matrix of the underlying graph has been established. The area of spectral graph theory was born.

From here, Ivan Gutman deduced the total π-electron energy as being

$$E_\pi = \alpha n + \beta(|\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|).$$

Because of this, he called the expression in brackets $|\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$ the energy of the graph (Gutman, 1978). Researchers ignored this achievement until around the turn of this century, when suddenly the graph energy concept started to attract attention. This resulted in what Gutman himself called an 'energy deluge' of papers! (Gutman, 2017, pers. comm., 17 April).

Vibrating Membranes

Another problem that contributed to the birth of spectral graph theory was the study of vibrating membranes. It is assumed that a vibrating membrane is held fixed along its boundary, which may have any shape. A simple example of such a membrane is a drumhead, which is hit by hands or sticks to produce certain frequencies. Its displacement $F(x,y,t)$ orthogonal to the (x,y) plane at time t is given by the wave equation (Cvetković et al., 1978; Cvetković et al. 2009). When the harmonic vibrations, given by solutions of the form $F(x,y,t) = z(x,y)\,e^{i\omega t}$ are substituted in this wave equation, a partial differential equation of the following form is obtained:

$$\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2} + \lambda z = 0, \qquad z(x,y) = 0 \text{ at boundary.}$$

Solutions to the above equations are approximated by forming a regular lattice, for example a square lattice, and only considering the z coordinates that lie on this

lattice. The lattice, of course, is a graph. The value of $\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2}$ at the point (x_0, y_0) can be approximated by

$$\frac{1}{h^2}\big(z(x_0 + h, y_0) + z(x_0 - h, y_0) + z(x_0, y_0 + h) + z(x_0, y_0 - h) - 4\, z(x_0, y_0)\big).$$

By substituting this in the partial differential equation and summing up over all internal points z_j (points within the boundary) that neighbour the point z_i, the following equation is obtained:

$$(4 - \lambda h^2) z_i = \sum_{j \sim i} z_j.$$

Considering the subgraph of the lattice induced by the internal vertices, the above equation is just the eigenvalue equation for this graph, which are then used to obtain approximate solutions to the original partial differential equation (Cvetković et al, 2009).

This led to Mark Kac (1966) asking the question "Can we hear the shape of a drum?". In other words, if the vibrating frequencies of a drum are heard, can the shape of the drum be reconstructed uniquely? Or are there two different drum shapes that produce the same frequencies? In spectral graph theory terms, this question asks whether one can reconstruct a graph uniquely given its spectrum. As shall be presented in the subsequent sections, the answer is, in general, no.

Back to Spectral Graph Theory

Research in spectral graph theory thus began roughly in the late fifties. In 1978, the very first monograph on spectral graph theory called *Spectra of Graphs: Theory and Application* (Cvetković, Doob & Sachs, 1978) was published. This book attempted, and largely succeeded, to serve "as a unifying collection of material in the subject" of spectral graph theory. Its bibliography contains 683 papers on different aspects of this topic, which the authors claimed to comprise most papers written in this area up to that point in time. A survey of the important mathematical results stemming from spectral graph theory, taken from this monograph and its modern follow-up *An Introduction to the Theory of Graph Spectra* (Cvetković et al., 2009), shall now be presented.

One important aspect of spectral graph theory is discovering what information of the graph can be extracted from the eigenvalues of the adjacency matrix. Early on, researchers, including the notable Frank Harary, thought that the eigenvalues characterize the graph completely, that is, no two graphs share the same eigenvalues. This was shown to be incorrect by several researchers, the earliest of whom can be traced back to 1957 (Collatz & Sinogowitz, 1957). Thus, from a set of eigenvalues, one cannot, in general, uniquely reconstruct the original graph.

Researchers thus turned their attention to what aspects of the graph can be deduced from its spectrum.

It is assumed henceforth that the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ are in non-increasing order, so that λ_1 is the largest and λ_n is the smallest among the n eigenvalues. The kth spectral moment s_k is defined as the sum ${\lambda_1}^k + {\lambda_2}^k + \cdots + {\lambda_n}^k$. A closed walk of length k in a graph is a sequence of vertices $v_1, v_2, \ldots, v_k, v_1$ having $(k+1)$ vertices where the first and last vertex are identical and every two consecutive vertices in the sequence are connected by an edge. An early result states that s_k is precisely the number of closed walks of length k in the graph (Cvetković et al., 2009). There is also the reverse result that states that if the spectral moments $s_0, s_1, s_2, \ldots, s_n$ are known, without prior knowledge of the eigenvalues, then the n eigenvalues themselves can be extracted uniquely. Thus, knowledge of the spectrum of a graph is equivalent to the knowledge of the number of closed walks of length $0,1,2, \ldots, n$ in the graph (Cvetković et al., 2009).

For any graph, the number of closed walks of length zero is n, while the number of closed walks of length one is 0. The number of closed walks of length two is equal to twice the number of edges – this tells us that the number of edges of a graph is deducible from its spectrum. The number of closed walks of length three is equal to six times the number of triangles – cycles of length three – in the graph. This implies that the number of triangles is also recognisable from the spectrum.

A graph is regular if its vertices have the same degree, that is, if each vertex has the same number of edges incident to it. Collatz and Sinogowitz (1957) proved that the largest eigenvalue λ_1 is at least equal to the average degree and at most equal to the maximum degree in the graph. This immediately implies that λ_1 is equal to the (common) degree of the graph if the graph is regular. Remarkably, this condition is also sufficient. Thus, a graph is regular exactly when $n\lambda_1 = s_2$, showing that whether a graph is regular or not is also recognisable from its spectrum (Cvetković et al., 2009).

A graph is k-colourable if it is possible to assign k colours to the vertices of the graph such that adjacent vertices have different colours. If a graph is 2-colourable, then it is said to be bipartite. Many hydrocarbons studied by chemical graph theorists are, in fact, bipartite. Whether a graph is bipartite or not is also deducible from the spectrum; indeed, a graph is bipartite if and only if $\lambda_1 = -\lambda_n$. Moreover, when this is true, the other eigenvalues would also share a similar trait; $\lambda_2 = -\lambda_{n-1}$, $\lambda_3 = -\lambda_{n-2}$, and so on (Cvetković et al. 1978). (It is known that $\lambda_1 > -\lambda_n$ except when the graph is bipartite.)

The chromatic number of a graph is the smallest possible k such that the graph is k-colourable. For example, bipartite graphs have chromatic number 2. The calculation of the chromatic number is, in general, an NP-complete problem – see the next section. However, Wilf (1986) showed that the chromatic number is at most equal to $1 + \lambda_1$, while Hoffman (1970) showed that it is at least equal to $1 -$

$\frac{\lambda_1}{\lambda_n}$. These results are striking, because even though determining the chromatic number is NP-complete, spectral graph theory provides bounds for what it can be, and clearly determining the spectrum of a graph can be performed in polynomial time.

Recent Applications of Spectral Graph Theory

Computer Science: the P versus NP problem

The P versus NP problem in computer science asks, informally, whether any problem that can be *verified* in polynomial time (NP) can also be *solved* in polynomial time (P) (Cook, 1971). This question is made relevant by quite a few problems that can be verified in polynomial time but that, so far, their solution does not seem to be possible in polynomial time. Some of these problems are also known to be NP-complete; this means that any NP problem can be transformed to an NP-complete problem in polynomial time (van Leeuwen, 1998). Examples of NP-complete problems include the games of Sudoku, Rubik's Cube and Lemmings (Kendall et al., 2008). There are many problems related to graph theory that are also NP-complete; as mentioned earlier, finding the chromatic number of a graph is one of them. Many experts believe the answer to the P versus NP problem is "no".

Some NP problems are not known whether they are also NP-complete. One of them is the graph isomorphism problem, which asks whether two graphs are isomorphic, or essentially the same (Schöning, 1988). There is a class of graphs called strongly regular graphs for which deducing whether two such graphs are isomorphic is particularly hard. However, spectral graph theory characterizes strongly regular graphs completely – they are the regular graphs whose spectrum contains three distinct numbers only (Shrikhande & Bhagwandas, 1965). Thus, a strongly regular graph cannot share its spectrum with another regular graph that is not strongly regular, and this provides a way of recognising that two such graphs are non-isomorphic in polynomial time. Moreover, if two graphs have different spectra, then they must clearly be non-isomorphic, irrespective of whether they are strongly regular or not.

We have already mentioned, however, that two graphs may share the same spectrum without being isomorphic. Such pairs of graphs are called cospectral. Sometimes, such graphs are distinguished by using a more general matrix, different from the adjacency matrix $\mathbf{A}$, to represent them. A popular choice is the generalized adjacency matrix $\mathbf{A} + y\mathbf{J}$ described in the introduction (Abiad & Haemers, 2012; Farrugia, 2019a). Unfortunately, some graphs are cospectral with respect to this matrix for all real numbers y (called *generalized cospectral*), even though they are not isomorphic! Indeed, the author of this paper recently

described a method to generate thousands of pairs of non-isomorphic, generalized cospectral graphs from just one pair of such graphs (Farrugia, 2019a).

Internet Search – The Google PageRank Algorithm

It is perhaps surprising that spectral graph theory is at the heart of the PageRank algorithm, which millions of people use every day to perform Google searches (Brin & Page, 1998). It assumes a directed graph on n web pages, with an arrow from web page x to web page y if x contains a link to y. The adjacency matrix $\mathbf{A}$ is, as usual, the matrix containing an entry 1 at the xth row and yth column if x is a web page linking to web page y. Note that, for this application, it's not always the case that the reverse arrow exists. The algorithm uses matrix $\mathbf{M}$, equal to $\frac{1-\alpha}{n}\mathbf{J} + \alpha\mathbf{D}^{-1}\mathbf{A}$, where $\mathbf{D}$ is the matrix where each diagonal entry contains the number of links that web page links to externally and α is some constant between 0 and 1 (the authors suggest $\alpha = 0.85$). If some web page has no external links, the relevant diagonal entry of $\mathbf{D}$ is 1 instead of 0 (otherwise $\mathbf{D}^{-1}$ would not exist). The spectrum of $\mathbf{M}$ is then found and the eigenvector $\mathbf{u}$ of the largest eigenvalue λ_1 is focused upon. The web pages displayed in the search are then ordered according to the entries of $\mathbf{u}$. Intuitively, each entry of $\mathbf{u}$ represents the expectation of finding oneself at that web page, either by clicking on a random link on the current page, with probability α, or by selecting an Internet web page at random, with probability $1 - \alpha$ (Brouwer & Haemers, 2012).

Network Centrality Measures

In many networks, measuring which vertices are deemed more important than others is paramount. This is what we mean by network centrality. The Google PageRank algorithm measures the more important web pages on the Internet that correspond to the user's search query; in this sense, the PageRank algorithm can be understood as pertaining to this section as well.

There are various other ways to measure network centrality. One of them, due to Estrada (2000) calculates the number of closed walks of the graph and then combines them together by assigning a weighting to each of them, giving priority to the shortest walks, and adding them up. The vertices that score highest are deemed more important. Note that, as was mentioned earlier, the number of closed walks of any length in a graph is obtained from the knowledge of the n eigenvalues of matrix $\mathbf{A}$.

The Estrada index (Estrada, 2000) is a way of totalling these network centralities to give an overall score to the graph. Its initial application was in biochemistry, to quantify the degree of folding in proteins (Deng et al., 2009). Only later was the Estrada index used to measure the centrality of complex networks like metabolic, communication and social networks (Estrada, 2007). The Estrada index has also

found utility in statistical thermodynamics (Estrada & Hatano, 2007) and information theory (Carbó-Dorca, 2008), so much so that its importance is now widely accepted and used by scientists, not just mathematicians.

Another way to interpret network centrality is as clustering a large data set given as a graph. An effective way of doing this is by using the eigenvectors associated with the m smallest eigenvalues of the Laplacian matrix $\mathbf{L}$ (or a normalised version) and producing an m-dimensional plot of points obtained from these eigenvectors, to obtain a visual clue as to which data points 'cluster' together (Brouwer & Haemers, 2012).

Control Theory

A control system is represented by a diagram showing how several agents are linked together, exchanging information to move from one state to another. This is akin to a graph where the agents are represented by the vertices and edges are represented by their interconnections. The controllability, or otherwise, of such a system can be investigated by considering the eigenvectors of the matrix associated with the underlying graph and applying the Popov-Belevitch-Hautus (PBH) test (Kailath, 1980). Since spectral graph theory deals with the revealing of the structure of a graph from its eigenvalues and eigenvectors, control system theory has recently received much research attention from leading graph theorists such as Cvetković (2011) and Godsil (2012). Their research has applications in the control of biological systems (Julius et al, 2008) and quantum spin networks (Christiandl et al., 2005).

Another way to check for the controllability of a system is by using Kalman's controllability criterion – a system is controllable if and only if its controllability matrix has an inverse (Kailath, 1980). It so happens that the controllability matrix is precisely the same as the matrix containing the enumeration of walks in the underlying graph, called a walk matrix in the graph-theoretical literature. This adds to the value of using spectral graph theory to analyse the controllability of systems. The graph theory community defined a controllable graph as one that represents interconnected agents that can be controlled by an external agent that can communicate with all agents with equal sensitivity (Cvetković et al., 2011). The author of this paper has also contributed to the research of controllable graphs and has recently generalised the concept of a walk matrix to one where the starting and ending points of walks is arbitrary (Farrugia, 2019b). This allows the future study of controllability of systems whose control requirements do not necessarily start and end at the same set of vertices.

Conclusion

With this paper, the reader has gone through the history of the practical needs of what required the introduction of the theoretical subject of spectral graph theory, to the subsequent applications of this theory to other fields. Together, we have thus progressed from practice to theory, and then from theory back to practice again.

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Bio-note

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