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ON THE CALCULATION OF THE LARGEST EIGENVALUE OF MOLECULAR GRAPH

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Abstract

The iterative procedure for the calculation of the largest eigenvalue λ_1 of a graph based on eq. (4) cannot be applied to all graphs. It is shown that eq. (4) converges to λ_1 if the graph is non-bipartite or if it is bipartite and possesses an automorphism group of the form $S_2[B]$.

The largest eigenvalue λ_1 of a graph is a quantity of some importance in theoretical chemistry and was subject of several recent investigations [1]. Therefore, one might be interested in techniques for its evaluation which are not based on a proper diagonalization of the adjacency matrix. In matrix calculus there exists a suitable iterative procedure for estimating the largest eigenvalue of a matrix [2].

Thus let a square matrix $\underline{\underline{M}}$ of order n fulfil the equations $\underline{\underline{M}}\ \underline{c}_i = \lambda_i\ \underline{c}_i$, with $\lambda_1 \geq \lambda_2 \ldots \geq \lambda_n$ being its eigenvalues and $\underline{c}_1, \underline{c}_2, \ldots, \underline{c}_n$ the corresponding eigenvectors. Let $\underline{x} = \underline{x}_0$ be an arbitrary vector of the same dimension as $\underline{c}_i$'s. Then $\underline{x}$ can be expanded as

$$\underline{x} = \sum_{i=1}^{n} \alpha_i\ \underline{c}_i \qquad (1)$$

with the scalars α_i being given as

$$\alpha_i = \underline{c}_i^T\ \underline{x} \qquad (2)$$

Let us now define the vectors $\underline{x}_m$ (m = 1,2, ...) as

$$\underline{x}_m = \underline{\underline{M}}\ \underline{x}_{m-1}$$

Of course, $\underline{\underline{x}}_m = \underline{\underline{M}}^m \underline{\underline{x}}$. Then the sequence of numbers L_m

$$L_m = \frac{\underline{\underline{x}}_m^T \underline{\underline{M}} \underline{\underline{x}}_m}{\underline{\underline{x}}_m^T \underline{\underline{x}}_m} = \frac{\underline{\underline{x}}^T \underline{\underline{M}}^{2m+1} \underline{\underline{x}}}{\underline{\underline{x}}^T \underline{\underline{M}}^{2m} \underline{\underline{x}}} \tag{3}$$

convergs to λ_1 with increasing m, provided that both $\underline{\underline{x}}$ and the eigenvalues and eigenvectors of $\underline{\underline{M}}$ fulfil certain conditions [2]. Therefore, for sufficiently large m, L_m can be used as a satisfactory approximation for λ_1. On the other hand, however, L_m is a lower bound for λ_1 [1d].

If we are interested in the largest eigenvalue of a graph, we have to calculate

$$L = \lim_{m\to\infty} L_m = \lim_{m\to\infty} \frac{\underline{\underline{x}}^T \underline{\underline{A}}^{2m+1} \underline{\underline{x}}}{\underline{\underline{x}}^T \underline{\underline{A}}^{2m} \underline{\underline{x}}} \tag{4}$$

where $\underline{\underline{A}}$ is the corresponding adjacency matrix. In the general case, however, the value of L is not equal to λ_1. The aim of the present work is to determine those graphs for which $L = \lambda_1$, that is those graphs for which eq. (4) can be used for evaluation of λ_1.

The number of vertices of the graphs considered is n. It is natural to restrict our discussion to connected graphs only (i.e. graphs containing exactly one component).

For these graphs it is $\lambda_1 \neq \lambda_2$ and $|\lambda_1| \geq |\lambda_i|$ $(i = 2,3,\ldots,n)$. Moreover, if $|\lambda_1| = |\lambda_n|$ (that is, $\lambda_1 + \lambda_n = 0$), it must be necessarily $\lambda_n \neq \lambda_{n-1}$ [3,4].

Proposition 1. If $\underline{x}$ is an arbitrary vector with the property $\underline{c}_1^T \underline{x} \neq 0$, $L = \lambda_1$ for all (connected) non-bipartite graphs.

Proof. By substituting (1) back into (3) we get

$$L_m = \frac{\sum_i \sum_j \alpha_i \alpha_j \underline{c}_i^T \underline{A}^{2m+1} \underline{c}_j}{\sum_i \sum_j \alpha_i \alpha_j \underline{c}_i^T \underline{A}^{2m} \underline{c}_j} = \frac{\sum_i \lambda_i^{2m+1} \alpha_i^2}{\sum_i \lambda_i^{2m} \alpha_i^2}$$

since $\underline{c}_i^T \underline{A}^m \underline{c}_j = \lambda_j^m \delta_{ij}$. From eq. (2) it follows that $\alpha_1 \neq 0$ and therefore

$$L_m = \lambda_1 \frac{1 + \sum_{i=2}^{n} \left(\frac{\alpha_i}{\alpha_1}\right)^2 \left(\frac{\lambda_i}{\lambda_1}\right)^{2m+1}}{1 + \sum_{i=2}^{n} \left(\frac{\alpha_i}{\alpha_1}\right)^2 \left(\frac{\lambda_i}{\lambda_1}\right)^{2m}} \qquad (5)$$

It is known [3] that a (connected) graph is bipartite if and only if $\lambda_1 + \lambda_n = 0$. Hence, for non-bipartite graphs it is $|\lambda_i/\lambda_1| < 1$ for all $i = 2,3,\ldots,n$, and from eq. (5) it follows simply that $L = \lambda_1$. //

Note that bipartite and non-bipartite graphs re-

present alternant and non-alternant molecules, respectively [4].

In the case of bipartite graphs it is $\lambda_n/\lambda_1 = -1$ and eq. (5) yields

$$L = \lambda_1 \frac{1 - (\alpha_n/\alpha_1)^2}{1 + (\alpha_n/\alpha_1)^2} \tag{6}$$

Since both $\alpha_1 = \underline{c}_1^T \underline{x}$ and $\alpha_n = \underline{c}_n^T \underline{x}$ depend on the actual choice of the vector $\underline{x}$, the result of the iterative estimation of λ_1 will also depend on $\underline{x}$. In particular, $\underline{x}$ can be always chosen in such a manner that $\alpha_n = 0$ and thus $L = \lambda_1$. If $\underline{x}$ is not chosen in an appropriate way, i.e. $\alpha_n \neq 0$, L can take any value between λ_1 and $-\infty$.

Let us now consider a special case when $\underline{x} = (1,1,\ldots,1)^T$, which implies $\alpha_1 \neq 0$ for all graphs. Eqs. (5) and (6) are then transformed into

$$L_m = \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} (\underline{A}^{2m+1})_{ij}}{\sum_{i=1}^{n} \sum_{j=1}^{n} (\underline{A}^{2m})_{ij}} \tag{7}$$

and

$$L = \lambda_1 \frac{\left(\sum_{i=1}^{n} c_{1i}\right)^2 - \left(\sum_{i=1}^{n} c_{ni}\right)^2}{\left(\sum_{i=1}^{n} c_{1i}\right)^2 + \left(\sum_{i=1}^{n} c_{ni}\right)^2}$$

Proposition 2. If $\underline{x} = (1,1,\ldots,1)^T$, the equality $L = \lambda_1$ holds exactly for those bipartite graphs for which the sum of the components of the eigenvector $\underline{c}_n$ is zero.

Corollary. Regular bipartite graphs have $L = \lambda_1$.

Proof. Regular graphs (i.e. graphs, all vertices of which are of equal valency) have $\underline{c}_1 = n^{-1/2}\ (1,1,\ldots,1)^T$. From the orthogonality of eigenvectors, $\underline{c}_1^T\underline{c}_j = 0$ it follows that $\sum_{i=1}^{n} c_{ji} = 0$ for all $j = 2,3,\ldots,n$.//

Regular bipartite graphs are for example the cycles of even length and the path P_2 with two vertices.

Proposition 3. Bipartite graphs, the automorphism group of which possesses an element π which interchanges all vertices of one colour with vertices of the other colour, have the property $L = \lambda_1$.

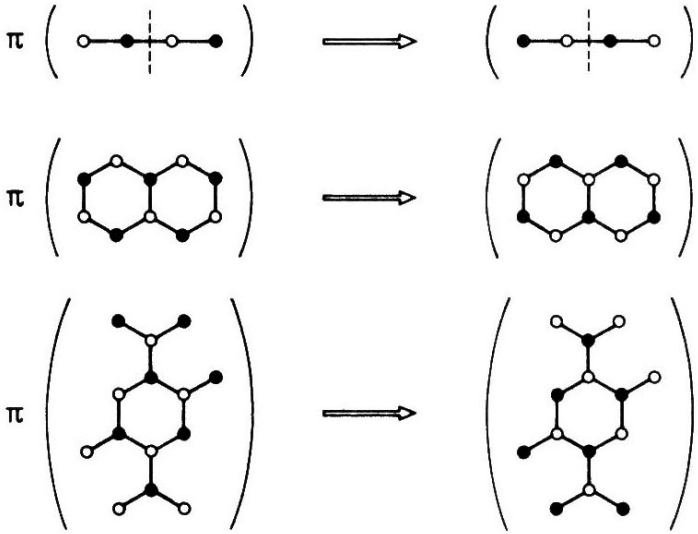
Proof. Let us consider two vertices p and q which are interchanged by means of π. Since p and q are of different colour, the components of $\underline{c}_1$ belonging to p and q are c_{1p} and c_{1q}, while the corresponding components of $\underline{c}_n$ are $c_{np} = c_{1p}$ and $c_{nq} = -c_{1q}$. Moreover, because of symmetry, $c_{1p} = c_{1q}$ and consequently, $c_{np} + c_{nq} = 0$. All vertices of the graph can be grouped into

such pairs, which finally gives $\sum_{i=1}^{n} c_{ni} = 0$.//

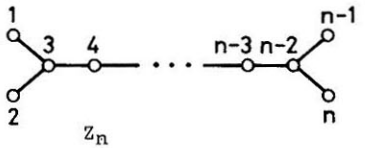
The requirements of proposiition 3 mean that the automorphism group is of the wreath product $S_2[B]$. Where B is the group of the automorphic mapping of vertices of the same colour and S_2 the symmetric group of degree 2. In the point group of the corresponding molecule the operation π may be represented for example by:

a) Reflecting in a plane which contains no vertex of the graph;

b) Inversion with respect to the center of a 4m+2 membered cycle.



Proposition 3 seems to give not only the sufficient but also the necessary conditions for a bipartite graph having the property $L = \lambda_1$. For example let us consider the graphs Z_n of the form



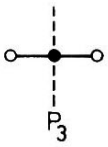
Z_n

which all have $\lambda_1 = 2$. Besides, $c_{1,1} = c_{1,2} = c_{1,n-1} = c_{1,n} = 1$ and $c_{1,3} = c_{1,4} = \ldots = c_{1,n-2} = 2$, from which one can calculate straightforwardly

$$L(Z_n) = \begin{cases} 2 & \text{for even } n \\ 2\,\dfrac{n^2 - 4n + 3}{n^2 - 4n + 5} & \text{for odd } n \end{cases}$$

On the other hand, the graphs Z_n fulfil the symmetry requirements of Proposition 3 only if n is even.

As another example we mention the graph P_3



For this graph

$$\underline{\underline{A}} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \underline{\underline{A}}^2 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \quad \underline{\underline{A}}^3 = 2\,\underline{\underline{A}} \text{ etc.}$$

Using eq. (7) we deduce $L_m = 4/3$ and hence $L = 4/3$, which is in disagreement with the value of $\sqrt{2}$ for the maximal eigenvalue of P_3. More generally, for all stars[*)] one gets $\underline{\underline{A}}^3 = (n-1)\,\underline{\underline{A}}$ etc., and therefore from eqn. (7) we deduce $L_m = L = 2(n-1)/n$; the largest eigenvalue of a star with n vertices is $\sqrt{n-1}$.

In the absence of an appropriate group operation, there is no reason why the sum of the components of $\underline{c}_n$ should be equal to zero. If graphs of this kind do exist

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*) Stars are graphs having (n-1) vertices of degree 1 and 1 vertex of degree (n-1); P_3 is the star with 3 vertices.

at all, they are certainly rather rare. Therefore we conclude our considerations with the following statement, which we cannot prove at present.

Proposition 4. Bipartite graphs which possess no group element described in Proposition 3 have $L \neq \lambda_1$.

Corollary. If in a bipartite graph the number of vertices of one colour differs from the number of vertices of the other colour, $L \neq \lambda_1$. In particular, all bipartite graphs with odd number of vertices have the above property.

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