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UPPER BOUND FOR THE ENERGY OF GRAPHS WITH FIXED SECOND AND FOURTH SPECTRAL MOMENTS

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Abstract. A method, earlier put forward for estimating from above the energy of a bipartite graph is modified so as to be applicable to any graph. The upper bound thus obtained is a function of the second and fourth spectral moments, whose dependence on graph structure is well known.

1. INTRODUCTION

Let G be a graph on n vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues (or, more precisely, the eigenvalues of the adjacency matrix of G) [3]. The energy of G is defined as

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

Details of the theory of this, currently much studied, graph invariant can be found in the reviews [5, 6, 8].

The k-th spectral moment of the graph G is defined as

$$M_k = M_k(G) = \sum_{i=1}^{n} \lambda_i^k \ . \tag{2}$$

¿From the well-known fact [3] that $M_k(G)$ is equal to the number of self–returning walks of length k in the graph G, we readily obtain explicit combinatorial expressions for the first few spectral moments. In particular,

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

where m is the number of edges, d_i the degree of the i-th vertex, and q the number of quadrangles.

If the graph G has no edges ($m = 0$), then both spectral moments M_2 and M_4 are zero. Otherwise, they are strictly greater than zero. In what follows all graphs are assumed to have at least one edge.

Relations between spectral moments and energy were much investigated in the past, see for instance [4, 7, 9, 10].

In 1985 Cioslowski [1] proposed an upper bound for the energy of a special (chemically important) class of bipartite graphs, the so-called benzenoid systems. He used for this a peculiar version of variational calculus, with M_2 and M_4 as constrains. The complete solution of this problem, obtained by using standard methods, was communicated a year later by Cioslowski and one of the present authors [2].

The results obtained in [2] were formulated so as to apply to benzenoid systems. It is, however, easy to see that these are valid for all bipartite graphs. On the other hand, the results obtained in [2] are not applicable to non-bipartite graphs. The aim of the present note is to offer an analogous approach that would embrace all graphs, and that would result in an upper bound for the energy of all graphs. We shall then see that the results from [2] happen to be a pertinent special case of what we obtain here.

2. FORMULATING THE PROBLEM

Our aim is to find an extremal (maximal and, perhaps, minimal) value for the right–hand side of Eq. (1), requiring that the second and fourth spectral moments M_2 and M_4 have some fixed values, say P and Q, respectively. The standard procedure to achieve this goal is to replace $|\lambda_i|$, $i = 1, 2, \ldots, n$, by some non-negative real numbers x_i , $i = 1, 2, \ldots, n$, such that the constraints

$$\sum_{i=1}^{n} x_i^2 = P \qquad \text{and} \qquad \sum_{i=1}^{n} x_i^4 = Q \tag{3}$$

are obeyed. As before, we assume that $P > 0$ and $Q > 0$. Then, by the method of Lagrange multipliers we consider the expression

$$\sum_{i=1}^{n} x_i + \alpha \left(\sum_{i=1}^{n} x_i^2 - P \right) + \beta \left(\sum_{i=1}^{n} x_i^4 - Q \right)$$

and equate with zero its derivatives w. r. t. x_i , $i = 1, 2, \ldots, n$. This leads to a series of equations:

$$1 + 2\alpha\, x_i + 4\beta\, x_i^3 = 0 \ , \ i = 1, 2, \ldots, n$$

implying that any x_i is a zero of the cubic polynomial

$$\phi(\lambda) = 1 + 2\alpha\,\lambda + 4\beta\,\lambda^3 \ .$$

Denote the zeros of $\phi(\lambda)$ by x, y, z.

Because $\phi(\lambda)$ has no quadratic term, it must be $x + y + z = 0$. Because the free term of $\phi(\lambda)$ is non-zero (equal to 1), none of x, y, z can be equal to zero. Therefore, only the following possibilities may occur:

Case 1: two zeros are real and positive whereas one is real and negative.
Case 2: two zeros are real and negative whereas one is real and positive.
Case 3: one zero is real, whereas two zeros are mutually conjugated complex numbers.

Because our assumption was that the x_i's are real and non-negative, and because they must satisfy two independent constraints, Eqs. (3), only Case 1 is acceptable.

We thus assume that $\phi(\lambda)$ has two distinct positive zeros, say x and y, and that $x > y$. If so, then $x_i \in \{x, y\}$ holds for all $i = 1, 2, \ldots, n$. Without loss of generality we may choose

$$x_i = x \quad \text{for} \quad 1 \leq i \leq t$$
$$x_i = y \quad \text{for} \quad t+1 \leq i \leq n$$

for some t, $1 \leq t \leq n-1$.

Then the quantity we are maximizing (or, perhaps, minimizing) is

$$E^* = E^*(t) = t\,x + (n-t)\,y \tag{4}$$

and the constraints (3) become

$$t\,x^2 + (n-t)\,y^2 = P \qquad \text{and} \qquad t\,x^4 + (n-t)\,y^4 = Q\ . \tag{5}$$

3. THE SOLUTION

From Eqs. (5) we directly obtain

$$x = \sqrt{\frac{1}{n}\left[P + \sqrt{\frac{n-t}{t}}\,\sqrt{n\,Q - P^2}\right]} \tag{6}$$

$$y = \sqrt{\frac{1}{n}\left[P - \sqrt{\frac{t}{n-t}}\,\sqrt{n\,Q - P^2}\right]} \tag{7}$$

from which

$$E^* = t\sqrt{\frac{1}{n}\left[P + \sqrt{\frac{n-t}{t}}\,\sqrt{n\,Q - P^2}\right]} + (n-t)\sqrt{\frac{1}{n}\left[P - \sqrt{\frac{t}{n-t}}\,\sqrt{n\,Q - P^2}\right]}\ . \tag{8}$$

We now need to check if the above determined quantities x and y are indeed real–valued, as required by our model. Unfortunately, y fails to be real–valued for all t, $1 \leq t \leq n-1$.

Lemma 1. *For all graphs, the expression* $n\,Q - P^2$ *, occurring in formulas (6), (7), and (8) is non-negative.*

Proof. In view of (2),

$$n\,Q - P^2 = n^2 \left[\frac{1}{n}\,Q - \left(\frac{1}{n}\,P \right)^2 \right] = n^2\,Var(x_i^2)$$

which evidently is non-negative. □

As a consequence of Lemma 1, x is real–valued for all t , $1 \leq t \leq n-1$. Unfortunately, y is not. By requiring that

$$P - \sqrt{\frac{t}{n-t}}\,\sqrt{n\,Q - P^2} \geq 0$$

we arrive at:

Lemma 2. *The expression on the right–hand side of Eq. (7) is real–valued if and only if* $P^2 \geq t\,Q$ *.* □

Corollary 3. *If* $t = 1$ *, then* y *in formula (7) is real–valued. Therefore* $E^*(1)$ *is real–valued for all graphs with at least one edge.*

Corollary 4. *If* $t \leq P^2/Q$ *, that is* $t \leq (M_2)^2/M_4$ *, then* y *and therefore also* $E^*(t)$ *are real–valued. If* $t > P^2/Q$ *, that is* $t > (M_2)^2/M_4$ *, then* y *and therefore also* $E^*(t)$ *are complex–valued and thus useless for the model considered in this paper.*

Remark 5. *The quotient* P^2/Q *assumes different values for different graphs. For instance, for the complete graph* K_n *, its is equal to* $n(n-1)/(n^2-3n+3)$ *, which for all values of* n *is smaller than 2. Consequently, for the complete graph already* $E^*(2)$ *is complex–valued.*

Lemma 6. *If the parameter* t *in formulas (4)–(8) is viewed as a continuous variable, then for* t *belonging to the interval* $(1\,,\,P^2/Q)$ *, the function* $E^*(t)$ *monotonically decreases.*

Proof. Denote by x' , y' , and $E^*(t)'$ the first derivatives of x , y , and $E^*(t)$, respectively, w. r. t. the variable t. Then by (5),

$$x^2 + 2t\,x\,x' - y^2 + 2(n-t)\,y\,y' = 0$$

$$x^4 + 4t\,x^3\,x' - y^4 + 4(n-t)\,y^3\,y' = 0$$

from which it follows

$$x' = -\frac{x^2 - y^2}{4tx} \qquad \text{and} \qquad y' = -\frac{x^2 - y^2}{4(n-t)y} \ . \tag{9}$$

¿From (4) we have

$$E^*(t)' = x + t\,x' - y + (n-t)\,y'$$

which combined with (9) yields

$$E^*(t)' = -\frac{(x-y)^3}{4xy} \ . \tag{10}$$

Bearing in mind that by Corollary 4, y is real–valued for $t \in (1\,,\,P^2/Q)$, and thus $x > y > 0$ holds, it is evident that the right–hand side of (10) is negative–valued. □

Corollary 7.

$$E^*(1) > E^*(2) > \cdots > E^*(\lfloor P^2/Q \rfloor) \ .$$

Corollary 8. *The expression* $E^*(1)$, *namely,*

$$\sqrt{\frac{1}{n}\left[P + \sqrt{(n-1)(n\,Q - P^2)}\right]} + (n-1)\sqrt{\frac{1}{n}\left[P - \sqrt{(n\,Q - P^2)/(n-1)}\right]} \tag{11}$$

is an upper bound for the energy of any n-vertex graph whose second and fourth spectral moments are equal to P and Q, respectively.

4. DISCUSSION

If the graph G is bipartite, then its eigenvalues satisfy $\lambda_i = -\lambda_{n-i+1}$, $i = 1, 2, \ldots, \lfloor n/2 \rfloor$, see [3]. With this detail in mind, in addition to the constraints

(3), one may require that the variational parameters obey a third condition, namely $x_i = x_{n-i+1}$, $i = 1, 2, \ldots, \lfloor n/2 \rfloor$. This is precisely what (tacitly) has been done in Ref. [2]. As a consequence, the upper bound deduced in [1, 2] is just $E^*(2)$.

Lemma 9. *If G is a bipartite graph, then the quotient P^2/Q is greater than 2.*

Proof.

$$P^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i^2 \, \lambda_j^2 = \sum_{i=1}^{n} \lambda_i^4 + \sum_{i \neq j} \lambda_i^2 \, \lambda_j^2 = Q + \sum_{i \neq j} \lambda_i^2 \, \lambda_j^2 \, . \tag{12}$$

For each $i = 1, 2, \ldots, n$, the right–hand side summation in (12) contains the term $\lambda_i^2 \, \lambda_j^2$ for $j = n - i + 1$, equal to λ_i^4 . The sum of these terms is Q . Since this summation includes also other (non-negative) terms, we have that

$$\sum_{i \neq j} \lambda_i^2 \, \lambda_j^2 \geq Q$$

which together with (12) yields $P^2 > 2Q$. □

Corollary 10. *If G is a bipartite graph, then $E^*(2)$ is real–valued.*

Corollary 11 [1, 2]. *The expression $E^*(2)$, namely,*

$$2\sqrt{\frac{1}{n}\left[P + \sqrt{\frac{n-2}{2}}\sqrt{n\,Q - P^2}\right]} + (n-2)\sqrt{\frac{1}{n}\left[P - \sqrt{\frac{2}{n-2}}\sqrt{n\,Q - P^2}\right]} \tag{13}$$

is an upper bound for the energy of any n-vertex bipartite graph whose second and fourth spectral moments are equal to P and Q , respectively.

Corollary 7 implies:

Corollary 12. *The upper bound (13) is better than the upper bound (11).*

This is no surprise whatsoever, since (11) and (13) are obtained by imposing on the variational parameters two and three constraints, respectively. On the other hand, the domain of applicability of (11) is much wider that that of (13).

Concluding this paper we wish to point out that the variational method employed by us could, in favorable cases, lead also to a lower bound. The evident candidates for such a lower bound would be $E^*(n-1)$ (for all n-vertex graphs) and $E^*(n-2)$ (for bipartite n-vertex graphs). However, as specified in Corollary 4 and Remark 5, for such high values of the parameter t, $E^*(t)$ is complex–valued. In other words, the model elaborated in [1, 2] and in the present work is not suitable for designing lower bounds for graph energy.

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