MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **80** (2018) 459-465

ISSN 0340 - 6253

Lower Bounds for the Resolvent Energy

Monica Bianchi[a], **Alessandra Cornaro**[a], **José Luis Palacios**[b], **Anna Torriero**[a]

[a] *Department of Mathematics and Econometrics, Catholic University, Milan, Italy*

monica.bianchi@unicatt.it, alessandra.cornaro@unicatt.it, anna.torriero@unicatt.it

[b] *Electrical and Computer Engineering Department, The University of New Mexico, Albuquerque, USA.*

jpalacios@unm.edu

(Received August 3, 2017)

Abstract

Using majorization, we give new bounds for the resolvent energy of general bipartite graphs. We also find more specific lower bounds in the particular case of trees.

1 Introduction

Let $G = (V, E)$ be a finite simple graph with vertex set $V = \{1, 2, \dots, n\}$ and degrees d_i for $1 \le i \le n$, with $d_G = \frac{2|E|}{n}$ the *average degree*. We consider A to be the adjacency matrix of G, with eigenvalues $\lambda_1 \ge \lambda_2 \ge \dots \ge \lambda_n$. There are several descriptors in Mathematical Chemistry defined in terms of these eigenvalues; among them we will work with the *resolvent energy*, defined in [6] (see also [5]) as

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n - \lambda_i}.$$

In [6], Theorem 11, it is shown that

$$ER(G) \ge \frac{n^3}{n^3 - 2|E|}, \tag{1}$$

where the equality is attained by the graph on n vertices without any edges $\overline{K_n}$ or (provided n is even) by the graph obtained by the union of $n/2$ complete graphs of order two.

Moreover, for bipartite graphs with an odd number of vertices, the following inequality was also proved in [6]:

$$ER(G) \geq \frac{1}{n} + \frac{n(n-1)^2}{n^2(n-1) - 2|E|}. \tag{2}$$

More recently, this index has been investigated in several works (see [3] and [4]).

In what follows, we improve these lower bounds whenever the average degree d_G lies in certain intervals described below. We focus first on simple connected bipartite graphs and then on trees, which are a particular case of bipartite graphs. The main technique used in this note is majorization.

2 Preliminaries and notations

The main references about majorization order and Schur convexity are the classical book [8] and the paper [1] for the notations and techniques. We briefly recall some basic facts.

Definition 1. *Given two vectors* $\mathbf{y}$, $\mathbf{z} \in D = \{\mathbf{x} \in \mathbb{R}^n : x_1 \geq x_2 \geq ... \geq x_n\}$, *the majorization order* $\mathbf{y} \trianglelefteq \mathbf{z}$ *means:*

$$\begin{cases} \langle \mathbf{y}, \mathbf{s^k} \rangle \leq \langle \mathbf{z}, \mathbf{s^k} \rangle, \; k = 1, ..., (n-1) \\ \langle \mathbf{y}, \mathbf{s^n} \rangle = \langle \mathbf{z}, \mathbf{s^n} \rangle \end{cases}$$

where $\langle \cdot, \cdot \rangle$ *is the inner product in* $\mathbb{R}^n$ *and* $\mathbf{s^j} = [\underbrace{1, 1, \cdots, 1}_{j}, \underbrace{0, 0, \cdots 0}_{n-j}], \quad j = 1, 2, \cdots, n.$

Given a closed subset $S \subseteq \Sigma_a = D \cap \{\mathbf{x} \in \mathbb{R}^n_+ : \langle \mathbf{x}, \mathbf{s^n} \rangle = a\}$, where a is a positive real number, let us consider the following optimization problem

$$\mathrm{Min}_{\mathbf{x} \in S}\; \phi(\mathbf{x}). \tag{3}$$

If the objective function ϕ is Schur-convex, i.e. $\mathbf{x} \trianglelefteq \mathbf{y}$ implies $\phi(\mathbf{x}) \leq \phi(\mathbf{y})$, and the set S has a minimal element $\mathbf{x}_*(S)$ with respect to the majorization order, then $\mathbf{x}_*(S)$ solves problem (3), that is

$$\phi(\mathbf{x}) \geq \phi(\mathbf{x}_*(S)) \quad \text{for all } \mathbf{x} \in S.$$

It is worthwhile to notice that if $S' \subseteq S$ the inequality $\mathbf{x}_*(S) \trianglelefteq \mathbf{x}_*(S')$ holds and thus

$$\phi(\mathbf{x}) \geq \phi(\mathbf{x}_*(S')) \geq \phi(\mathbf{x}_*(S)) \text{ for all } \mathbf{x} \in S'. \tag{4}$$

On the other hand, if the objective function ϕ is Schur-concave, i.e. $-\phi$ is Schur-convex, then

$$\phi(\mathbf{x}) \leq \phi(\mathbf{x}_*(S')) \leq \phi(\mathbf{x}_*(S) \text{ for all } \mathbf{x} \in S'. \tag{5}$$

A very important class of Schur-convex (Schur-concave) functions can be built adding convex (concave) functions of one variable. Indeed, given an interval $I \subset \mathbb{R}$, and a convex function $g : I \to \mathbb{R}$, the function $\phi(\mathbf{x}) = \sum_{i=1}^{n} g(x_i)$ is Schur-convex on $I^n = \underbrace{I \times I \times \cdots \times I}_{n-times}$. The corresponding result holds if g is concave on I^n.

In [1] some of the authors derived the maximal and minimal elements, with respect to the majorization order, of the set

$$S_a = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_i \geq x_i \geq m_i, i = 1, \cdots, n\}$$

where $M_1 \geq M_2 \geq \cdots \geq M_n$, $m_1 \geq m_2, \cdots \geq m_n$.

In particular, in the sequel, we need the following result.

Theorem 1. *(see [1], Theorem 8) Let $k \geq 0$ and $d \geq 0$ be the smallest integers such that*

1) $k + d < n$

2) $m_{k+1} \leq \rho \leq M_{n-d}$ where $\rho = \dfrac{a - \sum_{i=1}^{k} m_i - \sum_{i=n-d+1}^{n} M_i}{n-k-d}$.

Then

$$\mathbf{x}_*(S_a) = [m_1, \cdots, m_k, \rho^{n-d-k}, M_{n-d+1} \cdots, M_n].$$

3 Lower bounds for bipartite graphs

The resolvent energy is defined as

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n - \lambda_i}.$$

We consider the Schur-convex function $\Phi(\mathbf{x}) = \displaystyle\sum_{i=1}^{n} \frac{1}{x_i}$, where $x_i = n - \lambda_{n-i+1}$ with $i = 1, \cdots, n$. Since the sum of the eigenvalues of the adjacency matrix is zero, we have $\sum_{i=1}^{n} x_i = a = n^2$. Moreover, for bipartite graphs we know that the eigenvalues of the adjacency matrix are symmetric around 0, that is, $\lambda_1 = -\lambda_n$, $\lambda_2 = -\lambda_{n-1}$, etc., and the numbers

$$n - \lambda_n \geq n - \lambda_{n-1} \geq \cdots \geq n - \lambda_2 \geq n - \lambda_1,$$

are actually

$$n + \lambda_1 \geq n + \lambda_2 \geq \cdots \geq n + \lambda_{n-1} \geq n + \lambda_n,$$

therefore $x_i = n + \lambda_i$. We consider the following general constraints $n - 1 \geq \lambda_1 \geq \alpha$ and $\gamma \geq \lambda_2 \geq \beta$ on λ_1 and λ_2. Since the spectrum is symmetric around zero, we also obtain the restrictions $1 - n \leq \lambda_n \leq -\alpha$ and $-\gamma \leq \lambda_{n-1} \leq -\beta$ on λ_n and $\lambda_n - 1$.

By using well-known results we can set

$$\alpha = d_G \ \text{(see [7])},$$

$$\beta = -1 \ \text{(see [2])},$$

$$\gamma = \left\lfloor \frac{n}{2} \right\rfloor - 1 \ \text{(see Corollary 1 in [10])}.$$

In order to apply Theorem 1, in the following table we summarize the lower and upper bounds on the variables x_i, $i = 1, \cdots, n$:

$m_1 = n + d_G$	$M_1 = 2n - 1$
$m_2 = n - 1$	$M_2 = n + \lfloor \frac{n}{2} \rfloor - 1$
$m_k = n - \lfloor \frac{n}{2} \rfloor + 1$	$M_k = n + \lfloor \frac{n}{2} \rfloor - 1$ with $k = 3, \cdots, n-2$.
$m_{n-1} = n - \lfloor \frac{n}{2} \rfloor + 1$	$M_{n-1} = n + 1$
$m_n = 1$	$M_n = n - d_G$

Theorem 2. *The following lower bound holds:*

$$ER(G) \geq \frac{2n}{n^2 - d_G^2} + \frac{n-2}{n}. \tag{6}$$

Proof. The smallest integers k and d satisfying the assumptions of Theorem 1 are $k = d = 1$. Thus the minimal element of S_{n^2} is given by

$$\left(n + d_G, \underbrace{n, n, \cdots, n}_{n-2}, n - d_G \right)$$

and we get the lower bound (6). ∎

We now compare our result with those in [6]; by simple algebra it is easy to verify that:

1) bound (6) performs better than (1)

   (a) for $d_G \in I_1 = \left(\frac{-2n^2 + \sqrt{8n^4 - 8n^3}}{2(n-2)}; \frac{n}{2} \right)$ for bipartite graphs with $n > 3$ even;

   (b) for $d_G \in I_2 = \left(\frac{-2n^2 + \sqrt{8n^4 - 8n^3}}{2(n-2)}; \frac{n^2-1}{2n} \right)$ for bipartite graphs with $n > 3$ odd.

2) bound (6) is sharper than (2) for $d_G \in I_3 = \left(\frac{n\left(1 - n + \sqrt{2(n^2 - 3n + 2)}\right)}{n-3}; \frac{n^2-1}{2n} \right)$ for bipartite graphs with $n > 3$ odd.

Some examples of bipartite graphs whose average degrees are in the intervals I_1, I_2 and I_3, for selected values of n, are provided in table (1) and (2) (notice that graphs have been randomly derived by using the i-graph R package):

n	d_G	I_1	bound (1)	bound (6)
10	4.4	(4.27051;5)	1.046025	1.048016
20	8.8	(8.408997;10)	1.022495	1.024008
50	20.92	(20.83333;25)	1.008439	1.008488
100	41.68	(41.54334;50)	1.004185	1.004205

Table 1. Bipartite graphs with $n > 3$ even

n	d_G	I_2	I_3	bound (1)	bound (2)	bound (6)
15	6.428571	(6.339117;7.466667)	(6.34848;7.466667)	1.027397	1.027451	1.03
25	10.66667	(10.47937;12.48)	(10.48465;12.48)	1.016657	1.016668	1.017805
55	22.96296	(20.83333;27.49091)	(22.90657;27.49091)	1.007509	1.00751	1.007677
105	47.23077	(43.61438;52.49524)	(43.61555;52.49524)	1.004261	1.004261	1.004832

Table 2. Bipartite graphs with $n > 3$ odd

4 Lower bounds for trees

It is worthwhile to note that if G is a tree T, then $d_G = \frac{2(n-1)}{n}$ and this value lies outside the intervals $I_i, i = 1, 2, 3$. Therefore in the sequel we keep focused on trees, and in order to get a bound sharper than (6), we look for a more binding constraint on λ_2.

Suppose it is known that $\lambda_2(T) \geq \beta \geq 0$; then the bounds on the variables x_i, $i = 1, \cdots, n$ can be summarized in the table below:

$m_1 = \frac{n^2+2n-2}{n}$	$M_1 = 2n - 1$
$m_2 = n + \beta$	$M_2 = n + \lfloor \frac{n}{2} \rfloor - 1$
$m_k = n - \lfloor \frac{n}{2} \rfloor + 1$	$M_k = n + \lfloor \frac{n}{2} \rfloor - 1$ with $k = 3, \cdots, n-2$.
$m_{n-1} = n - \lfloor \frac{n}{2} \rfloor + 1$	$M_{n-1} = n - \beta$
$m_n = 1$	$M_n = \frac{n^2-2n+2}{n}$

Theorem 3. *The following lower bound holds for trees:*

$$ER(T) \geq \frac{2n^3}{(n^2+2n-2)(n^2-2n+2)} + \frac{2n}{n^2-\beta^2} + \frac{n-4}{n}. \tag{7}$$

Proof. In this case the smallest integers k and d required by Theorem 1 are $k = d = 2$. Hence the minimal element of the set S_{n^2} is given by

$$\left(\frac{n^2+2n-2}{n}, n+\beta, \underbrace{n, n, \cdots, n}_{n-4}, n-\beta, \frac{n^2-2n+2}{n}\right)$$

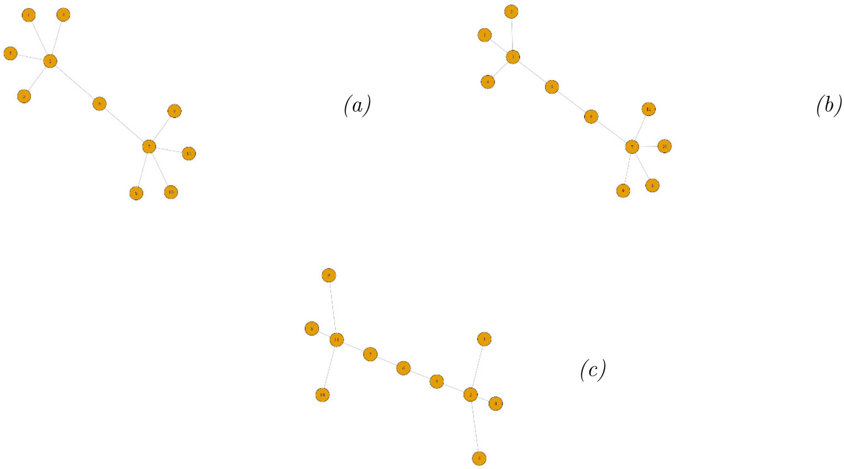
and the corresponding lower bound is (7). ■

Some basic algebra shows that bound (7) performs better than (2), if $\beta > \gamma$, considering $n \geq 11$ and odd, where

$$\gamma = \sqrt{\frac{n^2\,(n^2-8n+6)\,(n^2-2)}{(24n+12n^2-16n^3+3n^4+2n^5-20)}}.$$

In the following example we will show a class of trees for which $\lambda_2 = \beta > \gamma$.

Example. *We deal with a special class of trees studied in [9] (see Theorem 4.7, (ii)). For these trees we have* $\lambda_2 = \beta = \sqrt{\frac{n-3}{2}}$ *and the above inequality is satisfied. Figure 1 shows the class of graphs for* $n = 11$.



(a) *(b)* *(c)*

Figure 1. Special trees with $\lambda_2 = \beta = 2$.

5 Conclusions

We have applied majorization in this note, which is an important tool in Mathematical Chemistry used frequently to obtain upper and lower bounds of molecular descriptors. In the particular case of the resolvent energy the technique seems to work better than other approaches only in the case of bipartite graphs and under the condition that the average degree belong to certain interval in the real line. In the case of trees this condition is vacuous, but under a different condition on the second eigenvalue of the adjacency matrix - which is shown to be satisfied by a previously studied family of trees - we find a new and improved lower bound for trees.

References

[1] M. Bianchi, A. Cornaro, A. Torriero, Majorization under constraints and bounds of the second Zagreb index, *Math. Ineq. Appl.* **16** (2013) 329–347.

[2] D. Cvetković, S. Simić, The second largest eigenvalue of a graph (a survey), *Filomat* **9** (1995) 449–472.

[3] Z. Du, Asymptotic expressions for resolvent energies of paths and cycles, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 85–94.

[4] M. Ghebleh, A. Kanso, D. Stevanović, On trees with smallest resolvent energy, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 635–654.

[5] I. Gutman, E. Furtula, E. Zogić, E. Glogić, Resolvent energy in: I. Gutman, X. Li (Eds.), *Energies of Graphs – Theory and Applications*, Univ. Kragujevac, Kragujevac, 2016, pp. 277–290.

[6] I. Gutman, E. Furtula, E. Zogić, Glogić, Resolvent energy of graphs, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 163–174.

[7] L. Lovász, *Eigenvalues of Graphs*, Eotvos Lorand Univ., 2007.

[8] A. W. Marshall, I. Olkin, B. Arnold, *Inequalities: Theory of Majorization and Its Applications*, Springer, New York, 2011.

[9] A. Neumaier, The second largest eigenvalue of a tree, *Lin. Algebra Appl.* **46** (1982) 9–25.

[10] D. L. Powers, Graph partitioning by eigenvectors, *Lin. Algebra Appl.* **101** (1988) 121–133.