

## MAJORIZATION UNDER CONSTRAINTS AND BOUNDS ON THE SECOND ZAGREB INDEX

MONICA BIANCHI, ALESSANDRA CORNARO AND ANNA TORRIERO

*Abstract.* In this paper we present a theoretical analysis in order to establish maximal and minimal vectors with respect to the majorization order of particular subsets of  $\mathfrak{R}^n$ . Afterwards we apply these issues to the calculation of bounds for a topological descriptor of a graph known as the second Zagreb index. Finally, we show how our bounds may improve the results obtained in the literature, providing some theoretical and numerical examples.

*Mathematics subject classification (2010):* 05C35, 05C05, 05C50.

*Keywords and phrases:* Majorization, Schur-convex functions, graphs, second Zagreb index.

### REFERENCES

- [1] D. L. ALDERSON AND L. LI, *Diversity of graphs with highly variable connectivity*, Physical Review E **75**(046102) (2007), 1–11.
- [2] B. C. ARNOLD, *Majorization and Lorenz Order: A Brief Introduction*, Lectures Notes in Statistics 43, Springer Verlag, Berlin, 1980.
- [3] A. B. ATKINSON, *On the Measurement of Inequality*, Journal of Economic Theory **2** (1970), 224–263.
- [4] M. BIANCHI AND A. TORRIERO, *Some localization theorems using a majorization technique*, Journal of Inequalities and Applications **5** (2000), 433–446.
- [5] B. BOLLOBAS AND P. ERDŐS, *Graphs of extremal weights*, Ars Combinatoria **50** (1998), 225–233.
- [6] K. CH. DAS, I. GUTMAN AND B. ZHOU, *New upper bounds on Zagreb indices*, J. Math. Chem. **46** (2009), 514–521.
- [7] R. GRASSI, S. STEFANI AND A. TORRIERO, *Extremal Properties of Graphs and Eigencentality in Trees with a Given Degree Sequence*, The Journal of Mathematical Sociology **34-2** (2010), 115–135.
- [8] I. GUTMAN AND B. FURTULA, *Recent Results in the Theory of Randic*, Mathematical Chemistry, Monograph No. 6, University of Kragujevac, Serbia, 2008.
- [9] I. GUTMAN, B. RUŠIĆ, N. TRINAJSTIĆ AND C. F. WILCOX, *Graph Theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. **62** (1975), 3399–3405.
- [10] I. GUTMAN AND N. TRINAJSTIĆ, *Graph Theory and molecular orbitals. Total  $\pi$ -electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), 535–538.
- [11] P. ERDŐS AND T. GALLAI, *Graphs with prescribed degrees of nodes*, Hungarian Matematikai Lapok **11** (1960), 264–274.
- [12] G. H. HARDY, E. LITTLEWOOD AND G. POLYA, *Some simple inequalities satisfied by convex functions*, Messenger of Math. **58** (1929), 145–152.
- [13] J. KARAMATA, *Sur une inégalité ré lative aux fonctions convexes* (in French), Publ. Math. Univ. Belgrade **1** (1932), 145–148.
- [14] L. LI, D. ALDERSON, J. C. DOYLE AND W. WILLINGER, *Supplemental material: the  $S(G)$  metric and assortativity*, Internet Mathematics **2**, 4 (2005a), 1–6.
- [15] L. LI, D. ALDERSON, J. C. DOYLE AND W. WILLINGER, *Toward a theory of scalefree graphs: definitions, properties and implications*, Internet Mathematics **2**, 4 (2005b), 431–523.
- [16] L. LOVÁSZ, *Combinatorial Problems and Exercises* (2nd ed.), Amsterdam: North-Holland, 1993.
- [17] M. LU, H. LIU AND F. TIAN, *The connectivity index*, MATCH Communications in Mathematical and Computer Chemistry **51** (2004), 149–154.

- [18] A. W. MARSHALL AND I. OLKIN, *Inequalities: Theory of Majorization and Its Applications*, Academic Press, London, 1979.
- [19] S. NIKOLIĆ, G. KOVAČEVIĆ, A. MILIČEVIĆ AND N. TRINAJSTIĆ, *The Zagreb indices 30 years after*, Croat. Chem. Acta. **76** (2003), 113–124.
- [20] C. T. PAN, *A Vector Majorization Method for Solving a Nonlinear Programming Problem*, Linear Algebra and its Applications **119** (1989), 129–139.
- [21] I. SCHUR, *Über ein Klass von Mittelbindungen mit Anwendungen auf Determinantentheorie*, Sitzber. Berl. Math. Ges. **22** (1923), 9–20.
- [22] P. TARAZAGA, *Eigenvalue Estimate for Symmetric Matrices*, Linear Algebra and its Applications **135** (1990), 171–179.
- [23] P. TARAZAGA, *More Estimate for Eigenvalues and Singular Values*, Linear Algebra and its Applications **149** (1991), 97–110.
- [24] R. TODESCHINI AND V. CONSONNI, *Handbook of Molecular Descriptor*, Wiley-VHC, Weinheim, 2000.
- [25] Z. YAN, H. LIU AND H. LIU, *Sharp bound for the second Zagreb index of unicyclic graphs*, Journal of Mathematical Chemistry **42**, 3 (2007), 565–574.
- [26] Q. ZHAO, S. LI, *Sharp bounds for the Zagreb indices of bicyclic graphs with  $k$ -pendant nodes*, Discrete Applied Mathematics **158**, 17 (2010), 1953–1962.