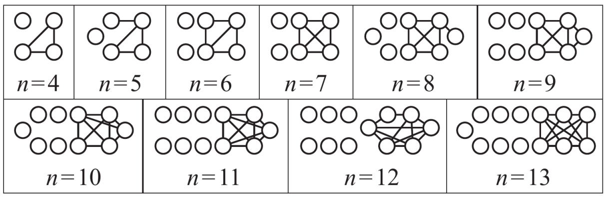

Figure 6: Graphs with minimum Randić index and $n-1$ edges.

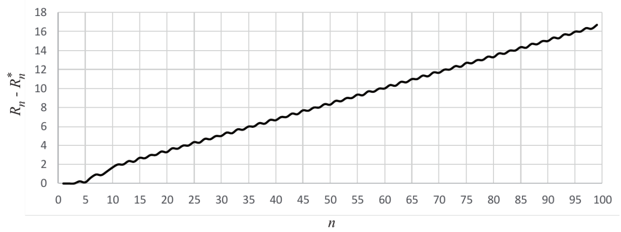

Figure 7: HERE Price of connectivity for the Randić index of chemical trees.

edges, $4 \leq n \leq 13$ vertices, and minimum Randić index.

Let R_n be the minimum Randić index of a chemical tree with n vertices, and let R_n^* be the minimum Randić index of a simple graph with n vertices, $m-1$ edges and maximum degree $r \leq 4$. Clearly, $R_n \geq R_n^*$. The difference $R_n - R_n^*$ is somehow a *price of connectivity* [6] which we represent in Figure 7 for $n \leq 99$. The curve indicates a regular shape for all $n \geq 11$. By analysing the extreme graphs for R_n^*, we have observed that they all have $\frac{n-1}{2}$ vertices of degree 4, and $\frac{n+1}{2}$ isolated vertices if n is odd, and $\frac{n-2}{2}$ vertices of degree 4, 1 vertex of degree 2, and $\frac{n}{2}$ isolated vertices if n is even. The regular shape of the curve in Figure 7 is due to the fact that for all $n \geq 11$, we have

$$R_n - R_n^* = \begin{cases} \frac{n}{6} & \text{if } n \mod 6 = 0 \\ \frac{n-1}{6} + \frac{\sqrt{3}-1}{2} & \text{if } n \mod 6 = 1 \\ \frac{n+4}{6} - \frac{\sqrt{2}}{2} & \text{if } n \mod 6 = 2 \\ \frac{n-3}{6} + \frac{\sqrt{2}}{2} & \text{if } n \mod 6 = 3 \\ \frac{n-4}{6} + \frac{1+\sqrt{3}-\sqrt{2}}{2} & \text{if } n \mod 6 = 4 \\ \frac{n+1}{6} & \text{if } n \mod 6 = 5. \end{cases}$$

As final illustration of the use of the proposed methods, we give in Figure 8 all simple chemical trees with $6 \leq n \leq 12$ vertices having minimum, second-minimum, third-ninimum, fourth-minimum, and fifth-minimum value of the second Zagreb index.

While this was not the case for the Randić index, it happens several times that an extremal value of the second Zagreb index in reached with more than one

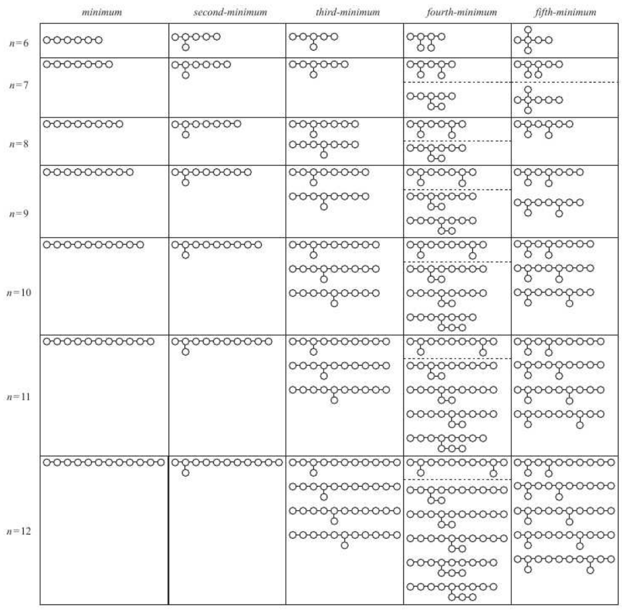

Figure 8: Extremal chemical trees for the second Zagreb index.

M-matrix. Extreme graphs having the same value, but different M-matrices are separated with a dotted line in Figure 8. For example, for $n = 10$, there are 4 graphs with fourth-minimum value of the the second Zagreb index. The first one was obtained from a first M-matrix, while the three others were obtained from a second M-matrix.

Conclusion

We have given necessary and sufficient conditions on the numbers m_{ij} of edges with end-degrees i and j for the existence of a simple graph or a simple connected graph with fixed maximum degree. These conditions can be imposed by an integer programming model, and graphs with these m_{ij} values can be generated using the proposed algorithms.

We have shown that these models and algorithms are very helpful to determine all extremal graphs of Adriatic indices that linearly depend on the the n_i and m_{ij} values.

References:

[1] M. Aouchiche. *Comparaison automatisée d'invariants en théorie des graphes*. PhD Thesis, École Polytechnique de Montréal, February 2006.

[2] M. Aouchiche, J.-M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lacheré and A. Monhait. *Variable neighborhood search*

for extremal graphs. 14. The AutoGraphiX 2 system. In L. Liberti and N. Maculan (editors), Global Optimization: From Theory to Implementation, Springer (2006) 281–310.

[3] M. Aouchiche, G. Caporossi and P. Hansen, *Variable neighborhood search for extremal graphs 20. Automated comparison of graph invariants.* Match Commun. Math. Comput. Chem. 58 (2007) 365–384.

[4] Aouchiche M, Caporossi G, Hansen P, Lucas C (2013) Variable Neighborhood Search for Extremal Graphs. 28: AutoGraphiX After Fifteen Years Les Cahiers du GERAD, G-2013-12.

[5] E. K. Burke and G. Kendall, *Search methodologies. Introductory tutorials in optimization and decision support techniques.* Springer, Berlin, 2005.

[6] E. Camby, J. Cardinal, S. Fiorini, O. Schaudt, The price of connectivity for vertex cover, Discrete mathematics and theoretical computer science 16 (1), 207–224 (2014).

[7] G. Caporossi and P. Hansen, *A learning optimization algorithm in Graph Theory. Versatile Search for extremal graphs using a learning algorithm.* Lecture Notes in Computer Science 7219 (2012) 16–30.

[8] G. Caporossi and P. Hansen. *Variable neighborhood search for extremal graphs: V. Three ways to automate finding conjectures.* Disc. Math, 276 (2004) 81–94.

[9] G. Caporossi and P. Hansen, *Variable neighborhood search for extremal graphs: I. The AutoGraphiX system.* Disc. Math. 212 (2000) 29–44.

[10] G. Caporossi and P. Hansen, *Finding relations in polynomial time*. In Proceedings of the XVIth International Joint Conference on Artificial Intelligence (Stockholm, 1999), vol. 2, 580–585.

[11] J. Christophe, S. Dewez, J.-P. Doignon, G. Fasbender, P. Grégoire, D. Huygens, M. Labbé, S. Elloumi, H. Mélot and H. Yaman, *Linear inequalities among graph invariants: using GraPHedron to uncover optimal relationships.* Networks 52 (2008) 287–298.

[12] F. Glover and G. Kochenberger, (Eds.), *Handbook of metaheuristics.* Kluwer, Amsterdam, 2003.

[13] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total ρ-electron energy of alternant hydrocarbons, Chemical Physics Letters 17 (4) 535–538 (1972).

[14] I. Gutman, O. Miljković, G. Caporossi and P. Hansen, Alkanes with small and large Randić connectivity indices, Chemical Physics Letters 306 (5) 366–372 (1999).

[15] P. Hansen, A. Hertz, C. Sellal, D. Vukičević, M. Aouchiche, G. Caporossi, *Edge Realizability of Connected Simple Graphs.* MATCH Commun. Math. Comput. Chem. 78 (2017) 689–712.

[16] P. Hansen and N. Mladenović, *Variable neighborhood search.* In [12], 145–184.

[17] P. Hansen and N. Mladenović, *Variable neighborhood search: principles and applications.* European Journal of Operational Research, 130 (2001) 449–467.

[18] P. Hansen and N. Mladenović, *Developments of variable neighborhood search.* In C. Ribeiro and P. Hansen (Eds.), *Essays, surveys in metaheuristics.* Kluwer, Amsterdam, 2001, 415–440.

[19] P. Hansen and N. Mladenović, *An introduction to variable neighborhood search.* In S. Voss *et al.* (Eds.), *Metaheuristics, advances, trends in local search paradigms for optimization*. Kluwer, Amsterdam, 1999, 433–458.

[20] P. Hansen, N. Mladenović and J. A. Moreno Pérez, *Variable neighborhood search: methods and applications.* Ann. Oper. Res. 175 (2010) 367–407.

[21] S. C. D. Kirkpatrick, Jr. Gellatt and P. Vecchi, *Optimization by simulated annealing.* Science 220 (1983) 671–680.

[22] X. Li and I. Gutman, Mathematical aspects of Randić-type molecular structure descriptors, *Mathematical Chemistry Monographs*, University of Kragujevac, 2006.

[23] N. Mladenović and P. Hansen, *Variable neighborhood search.* Computers and Operations Research, 24 (1997) 1097–1100.

[24] M. Randić, Characterization of molecular branching, Journal of the American Chemical Society 97 6609–6615 (1975).

[25] C. R. Reeves, (Ed.), *Modern heuristic techniques for combinatorial problems.* Blackwell Scientific, Oxford, 1993.

[26] N. Sloane, The on-line encyclopedia of integer sequences. Available at *http://www.research.att.com/minjas/sequences/.*

[27] D. Vukičević and M. Gašperov, Bond additive modeling 1. Adriatic indices, Croatica Chemica Acta 83 243–260 (2010).