Contribuţii la teoria indicilor topologici
- Rezumat -

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Capitolul 1

Introducere

Descriptorii moleculari sunt valori numerice ce caracterizează diferite proprietăţi ale moleculelor. Sunt utilizaţi în principal în construirea modelelor Quantitative Structure-Activity Relationship (QSAR) sau Quantitative Structure-Property Relationship (QSPR) pentru a genera predicţii asupra activităţii biologice sau a proprietăţilor fizico-chimice ale noilor substanţe.

O familie specială de descriptori moleculari este reprezentată de indicii topologici (IT), invarianţi ce caracterizează topologia unui graf, indicând ramificarea sa. IT sunt studiaţi în principal în strânsă legătură cu grafurile chimice - grafuri conexe, neorientate ce modelează componente organice în care considerăm numai legături de tip carbon-carbon şi carbon-hidrogen. Analizaţi în acest context, IT au apărut din dorinţa de a studia proprietăţi fizico-chimice ale componentelor chimice. Cum structurile substanţelor, chiar modelate ca grafuri, nu pot fi analizate direct, trebuie găsite cantităţi numerice asociate acestor structuri pentru a întreprinde cu succes studii în acest domeniu.

Teoria grafurilor extremale pentru indici topologici a intrat într-o nouă fază, ca urmare a articolului de referinţă (vezi [2]). Din acest punct, pentru fiecare indice topologic cunoscut sau nou introdus a fost dedicat un nou segment de cercetare determinării grafurilor extremale (minimale şi maximale) pentru diferite clase, precum grafuri chimice (fulerene, nanotuburi, sisteme şi lanţuri hexagonale, fenilene, etc.) sau arbori oarecare, grafuri cacti şi uni/bi/triciclice. Monografii dedicate integral sau parţial acestui subiect au fost scrise pentru IT dintr ecei mai reprezentativi ([10, 11]). O parte considerabilă a acestui segment de cercetare este dedicată determinării grafurilor extremale pentru IT în condiţii restrictive suplimentare precum gradul minim/maxim dat, cardinalul maxim al unui cuplaj, diametru fixat, număr dat de noduri pendante, grosime sau număr fixat de cicluri.

Din cauza proliferării acestor indici, a fost propusă în literatura de specialitate o schemă de clasificare. Principalele două categorii ale acestei scheme sunt cele ale IT bazaţi pe grade şi IT bazaţi pe distanţe. Această teză vizează studiul extremal pentru diverşi IT bazaţi pe grade. Mai exact, au fost detectate grafurile extremale cacti şi biciclice cu număr dat de noduri pedante, diametru şi/sau număr de cicluri fixate pentru *indicele sumă conectivitate generalizat cu* $\alpha > 1$, *indicele Randić general zeroth-order*, *primul indice Zagreb*, *indicii Zagreb multipcativi* şi *indicele (modificat) Narumi-Katayama*.

În prezent, din ce în ce mai mulţi indici topologici sunt creaţi, în încercarea de a oferi instrumente cât mai bune modelării QSAR/QSPR pentru a rezolva diverse probleme precum distingerea între izomerii unei subtanţe date sau prezicerea gradului de toxicitate pentru o anumită substanţă. Un exemplu bun în acest sens este crearea unor modele pentru a prezice efectul diverselor medicamente asupra unor anumite specii de viruşi conoscute pentru agresivitatea lor, precum hepatita B şi C, Papillomavirus, Citomegalovirus sau HIV-1. Astfel de modele au o acurateţe de până la 90 %, iar importanţa lor este amplificată de faptul că anumite boli severe precum HIV sau anumite tipuri de cancer sunt generate de viruşi ([8]).

Un alt exemplu este dat de construirea unui model QSAR pe baza a 27 de descriptori moleculari, din care 13 sunt indici topologici (unul dintre ei fiind indicele J al lui Alexandru T. Balaban), pentru a obţine un nou imunosupresor. Astfel, dintr-o bază de date de 250000 de compuşi chimici, au fost selectate 25 de peptide pe baza acestui model. După trieri suplimentare, cinci dintre acestea au fost sintetizate, cea mai bună dintre ele dovedindu-se în urma testelor clinice a fi de 100 de ori mai activ decât cel mai bun imunosupresor deja existent.

Capitolul 2

Scopul şi structura tezei

Una dintre cele mai investigate categorii de indici topologici folosiţi în chimia matematică este cea a *indicilor topologici bazaţi pe grade*, a căror definiţie este dată în funcţie de gradele nodurilor grafului de investigat. Putem scrie definiţia unui astfel de TI în forma dată de Gutman în [9] prin

$$TI(G) = \sum_{uv \in E(G)} F(d(u), d(v)), \tag{2.1}$$

unde $G = (V(G), E(G))$ este un graf simplu, neorientat şi conex, $d(u)$ reprezintă gradul unui nod u, iar F este o funcţie reală.

În cele ce urmează, vom împărţi categoria sus-menţionată a indicilor topologici bazaţi pe grade în două subcategorii. Prima este alcătuită din acei indici în a căror definiţie se găseşte o sumă sau un produs luat după nodurile grafului, în timp ce a doua este alcătuită din acei indici pentru care suma sau produsul din definiţie se formează după muchiile grafului. În această lucrare, vom numi prima subcategorie *indici topologici bazaţi pe noduri* şi a doua *indici topologici bazaţi pe muchii*.

Enumerăm în continuare principalele direcţii de cercetare în domeniul teoriei grafurilor chimice, dând în fiecare caz exemple pentru câţiva dintre IT importanţi şi intens studiaţi:

- determinarea relaţiilor matematice între diferiţi IT (spre exemplu, între indicii Szeged şi Wiener [3], între indicii Wiener şi Zagreb [22]);
- determinarea inegalităţilor de tip Nordhaus-Gaddum - în care se consideră sume şi produse ale IT pentru un graf şi complementarul său (pentru indicele sumă-conectivitate generalizat [1], pentru indicele polaritate Wiener [24], pentru indicii Zagreb [5]);

- determinarea unor inegalităţi de tip Nordhaus-Gaddum - în care sunt considerate sume sau produse pentru un IT ale unui graf şi complementului său (pentru indicele sumă conectivitate generalizat [1], pentru indicele de polaritate Wiener [24], pentru indicii Zagreb [5]);
- problema inversă: verificarea dacă un număr poate reprezenta valoarea unui anumit TI ([12]);
- determinarea de limite superioare şi inferioare pentru IT în funcţie de anumite concepte numerice din teoria grafurilor precum grad minim/maxim, grosime, număr cromatic, rază, diametru sau distanţă medie (pentru indicele Randić [2, 4, 6, 7, 13, 14, 23]);
- determinarea de noi IT cu relevanţă în studiul structurilor moleculare;
- determinarea grafurilor extremale pentru un IT dat;
- explorarea conexiunilor dintre IT şi anumite noţiuni matematice sau de teoria grafurilor. Un exemplu interesant în acest sens este legătura dintre indicele Harary şi hamiltoneitate: s-a demonstrat ca un graf bipartit conex cu n noduri şi partiţii de cardinale egale este hamiltonian atunci când indicele său Harary este mai mare sau egal decât $\frac{3}{2}n^2 - n + \frac{1}{2}$ ([25]). Un alt exemplu este faptul că indicele Merrifield-Simons pe lanţuri are valori egale cu numerele lui Fibonacci ([21]).

Obiectivul acestei teze este de a analiza grafurile extremale pentru diferite clase de grafuri în raport cu anumiţi indici topologici bazaţi pe grade.

Mai întai, **Capitolul 2** prezină principala metodă folosită pentru detectarea grafurilor extremale, şi anume folosirea unor transformări potrivite pentru a creşte/descreşte valoarea IT investigat. Apoi sunt prezentate principalele clase de grafuri pe care IT sunt de obicei analizaţi.

Următoarele două capitole prezintă contribuţii originale: rezultate publicate în articole de specialitate sau prezentate în conferinţe. Astfel, în **Capitolul 3** sunt analizaţi diferiţi *indici topologici bazaţi pe noduri*, precum *indicele Randić general de ordin zero*, *primul indice Zagreb*, *indicii Zagreb multiplicativi* şi *indicele Narumi-Katayama* cu varianta sa modificată. Rezultatele din acest capitol au fost publicate în [19, 18]. Sunt detectate grafurile extremale pentru arbori, grafuri biciclice şi grafurile cactuşi având număr fixat de noduri pendante şi/sau grosime dată. Notăm ca un fapt interesant că o anumită familie de grafuri extremale coincide pentru mai mulţi IT.

Capitolul 4 conţine rezultate asupra *indicelui suma conectivitate generalizat* χ_α pentru $\alpha > 1$, ce face parte din categoria *indicilor topologici bazaţi pe muchii*. În **secţiunea 4.1** detectăm grafurile biciclice maximale (rezultat obţinut în [16]), grafurile biciclice minimale ([17]) şi grafurile biciclice maximale având un număr fixat de noduri pendante sau grosime dată ([19]), pentru acest indice. **Secţiunea 4.2** prezintă grafurile cacti extremale. În **secţiunea 4.2.1** obţinem grafurile cactuşi minimale cu număr fix de noduri pendante, apoi determinăm grafurile maximale în familia generală a grafurilor cacti şi în subfamilia grafurilor cacti cu grosime fixată şi/sau număr dat de noduri pendante.

Sintetizând, rezultatele de mai sus au fost publicate în:

- [16] în *MATCH Commun. Math. Comput. Chem* (**jurnal ISI de categorie B** şi **factor de impact 3.858**). Potrivit Google Scholar, acest articol a fost **citat de 8 ori**:
  - M.F. Nadeem, S. Zafar, Z. Zahid, On certain topological indices of the line graph of subdivision graphs, pp. 790–794, Applied Mathematics and Computation, Elsevier, 2015 - **categorie B**;
  - M.F. Nadeem, S. Zafar, Z. Zahid, On topological properties of the line graphs of subdivision graphs of certain nanostructures, Applied Mathematics and Computation, Elsevier, 2016 - **categorie B**;
  - Z. Zhu, H. Lu, On the general sum-connectivity index of tricyclic graph, Journal of Applied Mathematics and Computing, pp 177-188, Springer, 2016 - **categorie B**;
  - L. Yan, W. Gao, J. Li, General harmonic index and general sum connectivity index of polyomino chains and nanotubes, Journal of Computational and Theoretical Nanoscience, pp. 3940-3944(5), 2015 – **categorie B**;
  - K.C. Das, S. Das, B. Zhou, Sum-connectivity index of a grap, Frontiers of Mathematics in China, pp 47-54, Springer, 2016 - **categorie C**;
  - I. Tomescu, Extremal results concerning the general sum-connectivity index in some classes of connected graphs, ROMAI J., pp 45–51, 2014 - **categorie D**;
  - N. Akhter, I. Tomescu, Bicyclic graphs with minimum general sum-connectivity index for $-1 \leq a < 0$, Proceedings of the Romanian Academy, Series A, pp. 484–489, 2015;
  - W. Gao, Second Geometric-Arithmetic Index and General Sum Connectivity Index of Molecule Graphs with Special Structure, International Journal of Contemporary Mathematical Sciences, 2015.

- [19] în *MATCH Commun. Math. Comput. Chem* (**jurnal ISI de categorie B** şi **factor de impact 3.858**) - **o citare**;
- [20] în *IEEE Proc. SYNASC 2015* (conferinţă ISI de **categorie C**);
- [17] în *Proceedings of DACS* (workshop asociat ICTAC 2014, conferiţă ISI de **categorie B**);
- [18] în *Proceedings of DACS* (workshop asociat CiE 2015, conferiţă ISI de **categorie C**);

În afara acestor articole, unele rezultate au fost incluse în prezentări pe bază de abstract în următoarele conferinţe:

- MACOS - International Conference on Mathematics and Computer Science, 26-28 iunie 2014, Braşov;
- The Eight Congress of Romanian Mathematicians, 26 iunie - 1 iulie 2015, Iaşi;
- ICTAMI - International Conference on Theory and Applications in Mathematics and Informatics, 17-20 septembrie 2015, Alba Iulia;
- Diaspora în Cercetarea Ştiinţifică şi Învăţământul Superior din România - Diaspora şi prietenii săi, 25-28 aprilie 2016, Timişoara.

Rezumând, principalele contribuţii ale acestei teze sunt:

- analiza anumitor IT pe unele clase de grafuri neabordate anterior în literatura de specialitate (grafuri biciclice şi catuşi) în [15–17];
- definirea unor noi transformări de grafuri ce ajută la detectarea anumitor clase de grafuri extremale: transformări care aduc mai multe muchii în acelaşi nod ([15, 16, 19, 20]) şi transformări folosite pentru a "împrăştia" muchiile unui graf ([15]);
- obţinerea într-un mod simplificat - pe calea transformărilor de grafuri - a unor rezultate ce generalizează rezultate existente în literatura de specialitate ([19]).

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Contributions to the Theory of Topological Indices
- Summary -

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Chapter 1

Introduction

Molecular descriptors are numerical values that characterize different properties of molecules. They are used mainly in the construction of Quantitative Structure-Activity Relationship (QSAR) or Quantitative Structure-Property Relationship (QSPR) models to generate predictions about the biological activity or physico-chemical properties of new substances ([4, 29, 40]).

A special family of molecular descriptors is represented by the topological indices (TIs), invariants that characterize the topology of a graph, indicating its ramification. TIs are mainly studied in connection with chemical graphs, which are undirected, connected graphs that model organic compounds by considering only the carbon-carbon and carbon-hydrogen type atomic bonds. Analyzed in this context, the TIs appeared from the desire of studying structural properties of chemical compounds. Since the structures of substances, even modeled as graphs, cannot be readily investigated as such, numerical quantities associated with these structures have to be considered for successful studies in this area.

The extremal graph theory with regard to topological indices entered in a new phase following the leading article of Bollobás and Erdös ([6]). Since then, for every known or newly introduced topological index a growing segment of research has been dedicated to finding extremal graphs (both maximal and minimal) for various classes, such as chemical graphs (fullerenes, nanotubes, hexagonal systems or chains, phenylenes, etc.) or general trees, uni/bi/tricyclic or cacti graphs. Monographs partly or entirely dedicated to this subject have been writen for the most useful TIs ([33, 36]). A considerable part of this research is dedicated to finding extremal graphs for TIs with some suplementary graph theoretic conditions, such as fixed minimum/maximum degree, matching number, diameter, number of pendants, girth or number of cycles.

Due to a proliferation of these indices, a classification scheme has been attempted in the literature. The main two categories of this classification are degree-based TIs and distance-based TIs. In this thesis we are interested in the extremal study of various degree-based TIs. More exactly, the extremal bicyclic and cacti graphs with given number of pendants, girth and/or number of cycles were detected for *the general sum-connectivity index with* $\alpha > 1$, *the general zeroth-order Randić index*, *the first Zagreb index*, *the multiplicative Zagreb indices* and *the (modified) Narumi-Katayama index*.

Since then more and more topological indices are being considered, in the attempt to offer as good as possible instruments for QSAR, QSPR modeling or to solve certain problems, such as distinguishing between the isomers of a given substance or predicting the toxicity of certain substances. A good example in this regard is the building of models to predict the effects of different medicines on some species of viruses known for their aggressivity like Hepatitis B and C, Papillomavirus, Cytomegalovirus or HIV-1. Such models have an accuracy of up to 90%, and their importance is amplified by the fact that certain serious diseases like HIV or some types of cancer are generated by viruses ([29]).

Another example is the construction of a QSAR model which used 27 molecular descriptors, 13 of which were TIs (one of them being Alexandru T. Balaban's J-index) to obtain a new immunosuppressive drug. Thus, from a data base of 250000 chemical compounds, only 25 peptides were selected based on predictions made with this model. Five of them were synthesized and clinically tested, the best of which was proved to be 100 times more active than the best known immunosuppressive ([3]).

Chapter 2

The aim and structure of the thesis

One of the most investigated categories of topological indices used in mathematical chemistry is that of the so-called *degree-based topological indices*, which are defined in terms of the degrees of the vertices of a graph. Thus, we can write the definition of such a topological index in the form given in [31] as

$$TI(G) = \sum_{uv \in E(G)} F(d(u), d(v)), \tag{2.1}$$

where $G = (V(G), E(G))$ is a simple, undirected, connected graph, $d(u)$ denotes the degree of the vertex u and F is a real function.

In what follows, we shall split the above mentioned degree-based topological indices in two categories. The first category is made out of those indices in whose definition we have a sum or a product after the graph's vertices, whereas the second is formed by those indices for which the sum or the product in their definition is taken after the graph's edges. In this paper, we shall call the first category *topological indices based on vertices* and the second *topological indices based on edges*.

We outline below the main directions of research in the field of chemical graph theory and exemplify each of them in the case of some important and intensive studied TIs:

- finding mathematical relations between different TIs (e.g. between the Szeged and the Wiener indices [8], the Wiener and the Zagreb indices [63]);

- finding Nordhaus-Gaddum type inequalities - in which sums or products of a TI for a graph and it's complement are considered (for the general sum-connectivity index [2], for the Wiener polarity index [65], for the Zagreb indices [13]);

- the inverse problem: checking if a given number can represent the value of a certain TI ([37]);
- finding upper and lower bounds for TIs in terms of graph theoretic numerical concepts like minimum/maximum degree, girth, chromatic number, radius, diameter or average distance (for Randić index: [6, 12, 15, 23, 38, 39, 64]);
- finding new TIs with relevance to the study of molecular structures;
- finding the extremal graphs for a given TI;
- exploring connections between TIs and different graph theoretical notions or mathematical concepts. An interesting example in this regard is the connection between the Harary index and hamiltoneity: it was shown in [66] that a bipartite connected graph with n vertices and partitions of equal cardinality is hamiltonian if its Harary index is greater or equal to $\frac{3}{2}n^2 - n + \frac{1}{2}$. Another example is that for paths the Merrifield-Simmons index are Fibonacci numbers (see [60]).

The objective of this thesis is to analyze extremal graphs for different classes of graphs and with respect to certain degree-based topological indices.

First, **Chapter 2** presents the main method used in finding extremal graphs, namely using appropriate graph transformations to increase/decrease the value of a fixed TI. Then it presents the main classes of graphs on which TIs are usualy analyzed.

The next two chapters present original contributions: results published in research articles or presented in conferences. Thus, in **Chapter 3** different *topological indices based on vertices* are analyzed, like *the general zeroth-order Randić index*, *the first Zagreb index*, *the multiplicative Zagreb indices*, *the Narumi-Katayama index* and its modified version. Results from this chapter were published in [49, 48]. Extremal graphs are determined for trees, bicyclic and cacti graphs having fixed number of pendants and/or given girth. We note as an interesting fact that a certain family of extremal graphs coincides for several TIs.

Chapter 4 contains results regarding the general sum-connectivity index χ_α for $\alpha > 1$, which is part of the category of *topological indices based on edges*. In **section 4.1** we determine the bicyclic maximal graphs (result obtained in [46]), the bicyclic minimal graphs ([47]) and the bicyclic maximal graphs having a fixed number of pendants or a given girth ([49]) with respect to this index. **Section 4.2** presents the extremal cacti graphs. First we obtain the minimal cacti graphs with fixed number of pendants in section 4.2.1, then we determine the maximal graphs in the general family of cacti graphs, and in the subfamily of cacti graphs with fixed girth and/or number of pendants.

Synthesising, the above results have been published in:

- [46] in *MATCH Commun. Math. Comput. Chem* (**ISI journal, category B, impact factor 3.858**). According to Google Scholar, this article has been **cited 8 times**:
  - M.F. Nadeem, S. Zafar, Z. Zahid, On certain topological indices of the line graph of subdivision graphs, pp. 790–794, Applied Mathematics and Computation, Elsevier, 2015 - **category B**;
  - M.F. Nadeem, S. Zafar, Z. Zahid, On topological properties of the line graphs of subdivision graphs of certain nanostructures, Applied Mathematics and Computation, Elsevier, 2016 - **category B**;
  - Z. Zhu, H. Lu, On the general sum-connectivity index of tricyclic graph, Journal of Applied Mathematics and Computing, pp 177-188, Springer, 2016 – **category B**;
  - L. Yan, W. Gao, J. Li, General harmonic index and general sum connectivity index of polyomino chains and nanotubes, Journal of Computational and Theoretical Nanoscience, pp. 3940-3944(5), 2015 – **category B**;
  - K.C. Das, S. Das, B. Zhou, Sum-connectivity index of a graph, Frontiers of Mathematics in China, pp 47-54, Springer, 2016 – **category C**;
  - I. Tomescu, Extremal results concerning the general sum-connectivity index in some classes of connected graphs, ROMAI J., pp 45–51, 2014 – **category D**;
  - N. Akhter, I. Tomescu, Bicyclic graphs with minimum general sum-connectivity index for $-1 \leq a < 0$, Proceedings of the Romanian Academy, Series A, pp. 484–489, 2015;
  - W. Gao, Second Geometric-Arithmetic Index and General Sum Connectivity Index of Molecule Graphs with Special Structure, International Journal of Contemporary Mathematical Sciences, 2015.
- [49] in *MATCH Commun. Math. Comput. Chem* (**ISI journal, category B, impact factor 3.858**) - **cited once**;
- [50] *IEEE Proc. SYNASC 2015* (**ISI conference, category C**);
- [47] in *Proceedings of DACS* (workshop associated with ICTAC 2014, ISI conference, **category B**);

- [48] in *Proceedings of DACS* (workshop associated with CiE 2015, ISI conference, **category C**);

Besides the above articles, some results were included in presentations based on abstracts in the following conferences:

- MACOS - International Conference on Mathematics and Computer Science, 26-28 June 2014, Braşov;
- The Eight Congress of Romanian Mathematicians, 26 June - 1 July 2015, Iaşi;
- ICTAMI - International Conference on Theory and Applications in Mathematics and Informatics, 17-20 September 2015, Alba Iulia;
- Diaspora în Cercetarea Ştiinţifică şi Învăţământul Superior din România - Diaspora şi prietenii săi, 25-28 April 2016, Timişoara.

Summarising, the main contributions of this thesis are:

- analysis of some classes of graphs for certain TIs that had not been addressed in the literature before (bicyclic and cacti graphs) in [45–47];
- definitions of new graph transformations that help in finding some classes of extremal graphs: transformations that bring together several edges into one vertex ([45, 46, 49, 50]) and transformations used for "spreading" the edges of a graph ([45]);
- obtaining in a simplified manner, by way of graph transformations, results that generalize already existing results in the literature ([49]).

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