SOME DISTANCE AND DEGREE GRAPH INVARIANTS AND FULLERENE STRUCTURES

Doctoral thesis

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NEKAJ RAZDALJNIH IN STOPENJSKIH GRAFOVSKIH INVARIANT TER FULERENSKE STRUKTURE

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Abstract

In the thesis we concentrate to the part of graph theory that can be applied in chemistry. One of the aims is applying graph-theoretical methods to predict the properties of a chemical compound based on its molecule structure. Molecular descriptors or topological indices is one way of predicting some properties. We dedicate our attention to Zagreb indices, a modification of Randić index called $R'$ index, and Gutman index.

For a simple graph $G$ with $n$ vertices and $m$ edges, the inequality $M_1(G)/n \leq M_2(G)/m$, where $M_1(G)$ and $M_2(G)$ are the first and the second Zagreb indices of $G$, is known as Zagreb indices inequality. We characterize the intervals of vertex degrees that satisfy this inequality, and find an infinite family of connected graphs dissatisfying this inequality. We also present an algorithm that decides if an arbitrary set of vertex degrees satisfies the inequality and consider variable Zagreb index inequality.

We also determine the graphs with extremal values for Gutman and $R'$ indices, and find a triangle-free graph on $n$ vertices with minimum $R'(G)$ index.

Fullerene molecules are carbon cage molecules arranged only in pentagons and hexagons. These molecules are of high importance for the contemporary science because of the wide spectra of properties they have depending on the number of atoms and the shape of the molecule. Fullerene graphs are 3-connected 3-regular planar graphs with only pentagonal and hexagonal faces. We have established new lower and upper bounds on the diameter of fullerene graphs and combined it with recently established upper bounds on the bipartite edge frustration to derive improved bounds on the independence number, the smallest eigenvalue, and the saturation number of fullerene graphs. We also determine the diameter of a special class of graphs with full icosahedral symmetry, and state a conjecture on the diameter of any fullerene graph.

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Povzetek

V doktorskem delu se bomo osredotočili na del teorije grafov, ki se uporablja v kemiji. Eden izmed problemov tega področja je z uporabo metod teorije grafov napovedati lastnosti kemijskih spojin glede na strukturo molekule. Molekulski deskriptorji oz. topološki indeksi predstavljajo enega izmed načinov napovedovanja nekaterih lastnosti. V delu pozornost posvetimo Zagrebskim indeksom, varianti Randićevega indeksa, imenovani $R'$ indeks, ter Gutmanovemu indeksu.

Za enostaven graf $G$ z $n$ točkami in $m$ povezavami velja neenakost $M_1(G)/n \leq M_2(G)/m$, kjer sta $M_1(G)$ in $M_2(G)$ prvi in drugi Zagrebski indeks grafa $G$, znana kot neenakost Zagrebskih indeksov. Karakterizirali smo intervale stopenj vozlišč, ki zadoščajo tej neenakosti, ter dobili neskončno družino povezanih grafov, za katero neenakost ne velja. Nadalje predstavimo algoritem, ki odloči ali dana množica stopenj vozlišč izpolnjuje neenakost, in analiziramo neenakost za Zagrebski indeks z spremenljivko.

V drugem delu določimo grafe z ekstremalnimi vrednostmi Gutmanovega in $R'$ indeksa. To so grafi brez trikotnikov z $n$ vozlišči in minimalnim $R'$ indeksom.

Fuleren je molekula sestavljena iz ogljikovih atomov, ki tvorijo petkotniške in šestkotniške. Fulerenske molekule imajo v sodobni znanosti izjemen pomen zaradi širokega spektra lastnosti, odvisnega od števila atomov in oblike molekule. Fulerenski grafi so 3-povezani 3-regularni ravninski grafi, ki imajo le lica velikosti 5 in 6. V doktorskem delu določimo nove spodnje in zgornje meje premera fulerenskih grafov, s pomočjo nove meje o nedvodelnosti grafa izboljšamo neodvisnostno število, vrednost najmanjše lastne vrednosti, in naščenostnega števila fulerenskih grafov. Prav tako določimo premer posebnega razreda grafov s popolno ikozaedersko simetrijo in navedemo domnevo o premeru splošnih fulerenskih grafov

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Kljucne besede: Topološki indeksi, Zagrebski indeksi, Gutmanov indeks, $R'$ indeks, fulerenski graf, premer, ikozaedrični fulereni.
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Preface

This thesis is a result of the work done in the past three years together with my advisors and our collaborators. It considers problems in graph theory that are applicable in chemistry.

The thesis is organized in four chapters. First chapter gives a short overview of possible applications of graph theory, especially its applications in chemistry. We also present two main areas of interest in the thesis, topological indices or molecular descriptors, and fullerene graphs. Second chapter contains all the basic graph theory definitions, properties and theorems needed later in the text.

Next two chapters are the core of the thesis. Chapter 3 is dedicated to the topological indices as one of the two areas of interest. Among the vast number of topological indices, we concentrate our attention to the first and the second Zagreb index and their variable form, the Gutman index (in literature also known as Schultz index of the second kind) and recently introduced modification of Randić index called $R'$ index. This chapter is a sublimate of the papers [3, 4, 5, 6, 8, 9, 10]. Chapter 4 treats the second area of interest, the fullerenes, and graph invariants related to their stability, with a special accent to the diameter of fullerene graphs. The work from fourth chapter is published in papers [7, 10].
Chapter 1

Introduction

Graph theory is an important part of mathematics. The very beginnings date back to 1735, when Leonard Euler reformulated the problem of *Seven Bridges of Königsberg* in a new and inventive way. At that moment he introduced *graphs*.

Later in 1852, Francis Guthrie, a former student at University College London came to an interesting observation that every map can be colored with precisely four colors in a way that no two neighboring countries have the same color. His brother Frederick at that time was a student of De Morgan, so he asked him about it. De Morgan was unable to give an answer so he wrote to Hamilton:

*A student of mine asked me today to give him a reason for a fact which I did not know was a fact - and do not yet. He says that if a figure be anyhow divided and the compartments differently colored so that figures with any portion of common boundary line are differently colored - four colors may be wanted, but not more - the following is the case in which four colors are wanted. Query cannot a necessity for five or more be invented. ... If you retort with some very simple case which makes me out a stupid animal, I think I must do as the Sphynx did...*

Hamilton response was:

*I am not likely to attempt your quaternion of colors very soon.*

De Morgan kept asking for a solution to Guthrie’s problem, and motivated several mathematicians to work on it. Guthrie’s problem was for a long time known as The Four Color Conjecture. In 1976 this conjecture became the Four Color Theorem. It was proven by Appel and Haken, basing their methods on reducibility using Kempe chains.

Later, the concept of graph was independently introduced by Kirchhoff while he was working on electrical circuits and Cayley who at that time was working on enumeration of organic isomers.
Since the first beginnings, graph theory developed rapidly and found its application in very different fields like in other parts of mathematics, computer science, physics, linguistics, sociology, biology, anthropology, communications, etc. Nowadays, graphs are one of the most common models of natural and human-made structures. In computer science, graphs are used to represent networks of communication, the flow of computation, data organization, computational devices, etc. In statistical physics, graphs can represent local connections between particular parts of a system and the dynamics of a physical process on such systems. Graphs found their application in different parts of mathematics as well, and there is a very close relation between algebraic graph theory and theory of groups.

The methods of graph theory are very useful in linguistics and social sciences. Syntax and compositional semantics in natural languages usually follow tree-based structures modeled in a hierarchical graph. Sociologists use graphs in order to model social networks or to represent the interaction between people in a specific group. In the same way graphs can be used in biology, in drug target identification, determining a protein’s or gene’s function, designing effective strategies for treating various diseases or providing early diagnosis of disorders, as well for describing different biological networks: protein-protein interaction networks, biochemical networks, transcriptional regulation networks, etc.

The beauty of graphs is that this structure can be extended for the needs of the given practical problem and a given structure. When needed, weight can be assigned to edges of graph, multiple edges can be allowed, or every edge can get a direction. Weighted graphs are used to represent structures in which the connections between two objects have some numerical values, like the number of joint papers between two researchers, or the length (price) of a flight between two cities; if two or more different companies are flying between two cities, we can represent that situation by multiple edges.

In this thesis we concentrate to the part of graph theory that is applied in chemistry. Since the XVII-th century it is known that the molecules have a specific structure. During the history, the molecule structure was represented in many different ways. One of the many molecule representations is by graphs. In this representation each atom is presented as a vertex, and the bonds between them are the edges in the graph. It is obvious that here we are not interested in the types of atoms used to build the molecule, but only in their valences i.e., the connections between them. In this sense, graph theory is used to mathematically model molecules in order to gain insight into some physical property or activity of the molecules.
1.1 Topological indices

Some physical properties such as the boiling point are correlated with the molecule structure. This is especially true for a group of substances called the alkanes, organic compounds comprised only by carbon and hydrogen atoms. Since each carbon atom is four valent and hydrogen atoms have only one bond, the same information from the structure of the molecule will be obtained if in the graph representation the hydrogen atoms are suppressed.

In this sense chemists wanted to relate different properties to the molecule structure. On one side they had the structure of the molecule, and on the other some physical quantity. A problem was assigning a numerical value to a different structure that will closely correlate with the physical quantities. Topological indices, or also known as molecular descriptors are invariants that are calculated from the topological information contained in the structure of the graph of a molecule [100]. Topological indices are numerical parameters of a graph which describe its structure and are usually graph invariants. Topological information of a molecule comprises the position and sometimes the type of the atoms defined in relation to the bonds that connect them. Such topological descriptors correlate with certain compound properties and activities.

1.1.1 QSAR and QSPR

In chemical graph theory QSAR and QSPR are often used terms derived from Quantitative Structure Property Relations and Quantitative Structure Activity Relations. QSAR and QSPR are regression models that relate a set of “predictor” variables to the power of the response variable. In QSAR modeling, the predictors consist of physico-chemical properties or theoretical molecular descriptors of chemicals, while the QSAR response-variable could be a biological, pharmacological, medical, ecological, ... activity of the chemicals. Both QSAR and QSPR are showing the tendency of contemporary theoretical and mathematical chemistry, to predict the properties of a compound based on its molecule structure. The research in this field are mainly done by combining graph molecular descriptors and experimental results.

The importance of QSAR and QSPR is clear; predicting the properties or the activities of a compound can save money and time finding the right medicine or a compound with desired physico-chemical properties.

In the 70’s very few molecular descriptors were known. Since then their number has grown, so now several hundreds descriptors are known; some more studied than others.
Todeschini and Consonni [99] defined molecular descriptors as:

A molecular descriptor is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment.

By examining the boiling point of the normal alkanes, chemists established that it is related to the molecule size, but when they considered the isomers of hexane, they realized that the boiling point is also related to the structure of the molecule. The question was how to measure or quantify a structure. Usually, when organic compounds are considered, structure of a molecule often refers to the degree of branching.

Harry Wiener, back in 1947, “measured” the structure of the molecule by polarity number, count of all paths of length three, and the path number [107]. The path number sums the distances between all pairs of vertices in the graph, and now is called the Wiener index, the first topological index introduced. Based on the success of Wiener index, many new molecular descriptors have been developed afterwards. This index has been studied in pure mathematics under different names, and has found application in sociometry and the theory of social networks. Wiener index is closely related to the closeness centrality of a vertex in a graph, and hence to closeness and farness, an important concepts in social networks. The farness of a vertex is defined as the sum of its distances to all other vertices, and its closeness is the inverse of the farness. Thus, the most central vertex has the lowest total distance to all other vertices. These quantities can be regarded as a measure of how fast an information will spread in a given network (graph) when started at a specific vertex.

The first molecular descriptor recognized by the chemical graph theory, also known as Z index, is Hosoya index. Haruo Hosoya defined it back in 1971 [75] in order to report a good correlation between the boiling point and the Z index of alkane isomers based on its unpublished work from 1957. Hosoya index of a graph $G$ is the total number of matchings in $G$. These days is used for investigation of chemical compounds.

Later a list of molecular descriptors was introduced, among them are: the first and the second Zagreb index, Wiener index, Randić index, Estrada index, etc.

The first and the second Zagreb indices are among the oldest topological indices [13, 34, 65, 81, 99], defined in 1971 by Gutman and Trinajstić [67], and are given different names in the literature, such as Zagreb group indices, Zagreb group parameters and most often, Zagreb indices. Since then, they have been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. Overall, Zagreb indices exhibit a potential applicability for deriving multi-linear regression models.

Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. Zagreb
indices are defined as
\[ M_1(G) = \sum_{v \in V} d(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E} d(u)d(v). \]

For the sake of simplicity, we often use \( M_1 \) and \( M_2 \) instead of \( M_1(G) \) and \( M_2(G) \), respectively.

In 2003, an article \[92\] repopularized Zagreb indices, and since then a lot of work was done on this topic. For more results concerning Zagreb indices see \[89, 104\].

The concept of the variable molecular descriptors was proposed as an alternative way of characterizing heteroatoms in molecules, but also to assess the structural differences, such as, for example, the relative role of carbon atoms of acyclic and cyclic parts in cycloalkanes. The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for the studied property is as small as possible. Several molecular descriptors have already been generalized in their variable forms, but here we will only pay attention to Zagreb indices.

Similarly, the first and the second variable Zagreb indices are defined by
\[ ^\lambda M_1(G) = \sum_{v \in V} d(v)^{2\lambda} \quad \text{and} \quad ^\lambda M_2(G) = \sum_{uv \in E} d^\lambda(u)d^\lambda(v), \]
where \( \lambda \) is a real number. For the sake of simplicity, we use \( ^\lambda M_1 \) and \( ^\lambda M_2 \) instead of \( ^\lambda M_1(G) \) and \( ^\lambda M_2(G) \), respectively.

In 1975 Randić \[94\] introduced the topological connectivity index \( R(G) \) of a graph \( G \) defined as the sum of weights \( (d(u)d(v))^{-\frac{1}{2}} \) over all edges \( uv \) of \( G \), i.e.,
\[ R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}, \]
where \( d(v) \) is the degree of the vertex \( v \) in \( G \). Originally this index was named “branching index” or “molecular connectivity index” and it has been proved to be suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Nowadays this parameter is known as the Randić index. Later, in 1998 Bollobás and Erdős \[16\] generalized this index by replacing the exponent \(-\frac{1}{2}\) with an arbitrary real number \( \alpha \) to obtain the general Randić index \( R_\alpha \). Thus,
\[ R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha}. \]

Notice that second variable Zagreb index \( ^\lambda M_2 \) and general Randić index \( R_\alpha \) for a given graph overlap.
Randić has shown that there exists a correlation of the Randić index with several physico-chemical properties of alkanes such as boiling point, chromatographic retention time, enthalpy of formation, parameters in the Antoine equation for vapor pressure, Kovats constant, calculated surface area and others [82, 94]. According to Caprossi and Hansen [22], Randić index together with its generalization is certainly the molecular-graph-based structure-descriptor that found many applications in organic chemistry, medicinal chemistry, and pharmacology, and therefore is an interesting topic in graph theory. For more results concerning Randić index see [86].

In the past years, several conjectures were proposed [12, 49] concerning Randić index. From mathematical perspective, Randić index is difficult to follow during graph transformations. In order to attack some open problems on Randić index, Dvořák et al. [44] introduced a modification of this index called $R'$ index. The newly introduced index is degree based and it is defined as

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d(u), d(v)\}}.$$

In 1989 Schultz [95] lead by the idea of characterizing the alkanes defined a new index that is degree and distance based. This index now is known as Schultz index (of first kind), and it is defined by

$$S(G) = \sum_{u,v \in V(G)} (d(u) + d(v)) d(u, v).$$

Inspired by the Schultz index, Ivan Gutman [64] back in 1994 introduced a new index,

$$\text{Gut}(G) = \sum_{u,v \in V(G)} d(u)d(v)d(u, v),$$

and named it Schultz index of second kind. Nowadays this index is also known as Gutman index.

All of the above mention topological indices are degree and distance based molecular descriptors. The index introduced by Ernesto Estrada in 2000 includes the eigenvalues of the adjacency matrix of the graph $G$. It is defined by:

$$\text{EE}(G) = \sum_{i=1}^{n} e^{\lambda_i},$$

where $\lambda_i$, $i = 1, \ldots, n$, are the eigenvalues of the adjacency matrix of the graph $G$. Although this index is relatively new, it found a numerous applications in chemistry, physics and complex networks. The original aim was to measure the degree of folding of long-chain molecules, especially proteins, and later was used to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks.
1.2 Introduction to fullerenes

For a long period of time chemists believed that the only carbon allotropes were: graphite, diamond and amorphous carbon. In 1970, Japanese chemist, Eiji Osawa predicted the existence of a highly symmetric carbon molecule where the atoms are arranged in pentagons and hexagons. Fifteen years latter, Sir Harry Kroto together with Robert Curl and Richard Smalley made a success and finally synthesize a fullerene $C_{60}$ [84], and later in 1996 they got the Nobel Prize in chemistry for “their discovery of fullerenes”. In 1991, the buckminsterfullerene $C_{60}$ was pronounced the “Molecule of the year” by the Science magazine.

The structure of this molecule, in the shape of a soccer ball, was already seen in the drawings of the great artist, Leonardo da Vinci. He produced drawings for Luca Pacioli’s book “About perfection of the world”, published at the beginning of XVI century. He drew the perfect polyhedron on 60 vertices which represents the truncated icosahedron.

The name of the molecule $C_{60}$, buckminsterfullerene, was a homage to Richard Buckminster Fuller, whose geodetic dome it resembles. Although $C_{60}$ was produced in laboratories 25 years ago, it has just recently been detected in nature, as expected: in space as a component in certain meteorites. The observations on the planetary nebula showed presence of $C_{60}$ and $C_{70}$. On Earth, fullerenes can be found in soot and in some types of rocks.

Fullerenes can also be seen as graphs, vertices represent atoms and edges represent bonds between atoms.

From the very beginning, fullerenes have been attracting attention of diverse research communities. They are most studied in the fields of nanotechnology, hydrogen storage, superconductive materials, and in nanomedicine as magnetic or nuclear probes. The experimental work was paralleled by theoretical investigations, applying the methods of graph theory to the mathematical models of fullerene molecules called fullerene graphs. One of the main driving forces behind that work has been a desire to identify structural properties characteristic for stable fullerenes, i.e., for fullerene isomers verified in macroscopic quantities. A number of graph-theoretical invariants were examined as potential stability predictors with various degrees of success [1, 50, 38, 32, 70, 96]. As a result, we have achieved a fairly thorough understanding of fullerene graphs and their properties. For more results and questions on fullerenes see [39, 55, 56, 91]. However, some problems and questions still remain open [33, 91, 56]. Special place among them have several interesting conjectures made by Graffiti, a conjecture making software [48]. The main goal of the second part of this thesis is to consider several of those open questions starting from our
results on the fullerene diameters and a recent result on the bipartite edge frustration [43].
Chapter 2

Concepts in graph theory

Many different real situations can be graphically presented in the following manner: an object is presented as a node (vertex), and if there is a specific relation between two objects, corresponding nodes will be connected by an edge. This idea can be applied to a number of different every day situations, for example the nodes can be people and the edges will join pairs of friends. If applied in chemistry, every molecule can be represented in this fashion; the atoms are nodes, and edges represent the bonds in the molecule.

2.1 Basics of graph theory

A graph $G$ is an ordered pair $(V(G), E(G))$ consisting of a set of vertices $V(G)$ and set of edges $E(G)$ such that each edge connects a pair of vertices. If there is no possibility of confusion we write $V$ and $E$ for the set of vertices and the set of edges respectively. The number of vertices and edges of $G$ are called order and size of $G$ and are denoted as $n = |V(G)|$ and $m = |E(G)|$. A graph is simple if it has no loops or multiple (parallel) edges. The vertices $u$ and $v$ are adjacent if there is an edge that joins them. If $u$ and $v$ are adjacent we write $u \sim v$. Two different adjacent vertices are called neighbors. The set of neighbors to the vertex $v$ in the graph $G$ is denoted by $N_G(v)$. Two edges are adjacent if they have a vertex in common. The ends of an edge are incident with the edge. The two incident vertices to an edge $e$ are called end-vertices.

For $v \in V$, the number of edges adjacent to $v$ is called degree of $v$ and it is denoted by $d_G(v)$ (if there is no possibility of confusion we will simply use $d(v)$). A vertex of degree 0 is isolated vertex. By $\delta(G)$ and $\Delta(G)$ we denote the minimal and maximal degrees of the vertices in $G$. A graph $G$ is $k$-regular if every vertex has degree $k$. A 3-regular graph is also called a cubic graph.
Let \( G_1 = (V_1, E_1) \) and \( G_2 = (V_2, E_2) \) be two graphs. We call \( G_1 \) and \( G_2 \) isomorphic, \( G_1 \cong G_2 \), if there is a bijection \( \varphi : V_1 \to V_2 \) such that \( u \sim_{G_1} v \) if and only if \( \varphi(u) \sim_{G_2} \varphi(v) \).

Graph invariants are some properties of the graph that are invariant under isomorphism. Such properties are: number of vertices, number of edges, “bipartitiness”, number of triangles (or cycles with length \( k \)), number of components, etc.

If \( V_1 \subset V_2 \) and \( E_1 \subset E_2 \), then \( G_1 = (V_1, E_1) \) is a subgraph of \( G_2 = (V_2, E_2) \); \( G_2 \) is a supergraph of \( G_1 \). If \( G_1 \) is a subgraph of \( G_2 \) and all the edges of \( G_2 \) with end-vertices in \( V_1 \) are also edges of \( G_1 \), then \( G_1 \) is called an induced subgraph of \( G_2 \).

### 2.2 Some families of graphs

A **path** is a simple graph with vertices \( \{v_1, v_2, \ldots, v_n\} \) and edges \( \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n\} \). A **k-path** \( P_k \) is the path of length \( k \). By inserting an edge between the two vertices of degree one in a path, we obtain a **cycle**. A cycle with \( k \) edges, \( C_k \), is called a \( k \)-cycle.

A **complete** graph on \( n \) vertices \( K_n \) is a simple graph in which any two vertices are adjacent. A **clique** of a graph is a set of mutually adjacent vertices. A graph is **bipartite**, if its vertex set can be presented as a disjoint union of two subsets \( X \) and \( Y \) such that each edge has one end in \( X \) and the other one in \( Y \). If every vertex in \( X \) is joined with every vertex in \( Y \), then \( G \) is a **complete** bipartite graph. We denote by \( K_{a,b} \) the complete bipartite graph with \( a \) vertices in one class and \( b \) vertices in the other one.

**Proposition 2.2.1.** A graph is bipartite if and only if it contains no odd cycle.

A **star** is a complete bipartite graph with \( a = 1 \) or \( b = 1 \). A **k-star** \( S_k \) is a star with \( k \) edges (and \( k + 1 \) vertices).

### 2.3 Adjacency and Laplacian matrices

Let \( G \) be a graph of order \( n \) and a set of vertices \( V = \{v_1, \ldots, v_n\} \). The **adjacency** matrix of \( G \) is the \( n \times n \) matrix \( A_G = [a_{ij}] \), where \( a_{ij} \) is the number of edges joining vertices \( v_i \) and \( v_j \). If the graph \( G \) is simple graph

\[
    a_{ij} = \begin{cases} 
      1, & v_i \sim v_j \\
      0, & v_i \not\sim v_j.
    \end{cases}
\]
The Laplacian matrix of a simple graph $G$ is the $n \times n$ matrix $L_G = [l_{ij}]$, where
\[
l_{ij} = \begin{cases} 
  d(v_i), & i = j \\
  -1, & i \neq j \text{ and } v_i \sim v_j \\
  0, & \text{otherwise}.
\end{cases}
\]

The spectrum of a graph $G$ is the set of numbers corresponding to the eigenvalues of the adjacency matrix of $G$ together with their multiplicities. Similarly is defined the Laplacian spectrum of the graph $G$.

**Theorem 2.3.1.** Let $A_G$ be the adjacency matrix of a graph $G$. Then the Laplacian matrix $L_G$ satisfies
\[
L_G = \Delta - A_G,
\]
where $\Delta$ is the diagonal matrix whose $i$-th diagonal element is the degree of the vertex $v_i$, $1 \leq i \leq n$.

Directly from the previous theorem we find the following.

**Corollary 2.3.2.** Let $G$ be a $k$-regular graph. If the adjacency matrix $A_G$ has eigenvalues $\lambda_1, \ldots, \lambda_n$, then the Laplacian matrix $L_G$ has eigenvalues $k - \lambda_1, \ldots, k - \lambda_n$.

### 2.4 Connectivity

Two vertices are called connected in a graph $G$ if $G$ contains a path between those two vertices. A graph $G$ is connected if every pair of vertices in $G$ is connected.

The distance between two vertices $u, v \in V(G)$ in a connected graph $G$ is the length of any shortest path between these vertices, and it is denoted by $d_G(u, v)$ (or simply $d(u, v)$ if there is no possibility of confusion). A diameter of connected graph $G$, diam($G$), is the maximum distance between two vertices of $G$, i.e.,
\[
\text{diam}(G) = \max \{d(u, v) \mid u, v \in V(G)\}.
\]
The vertices $u, v \in V(G)$ are diametral vertices if $d(u, v) = \text{diam}(G)$, and any shortest path between them is called a diametral path. Radius of a graph rad($G$) is
\[
\text{rad}(G) = \min_{u \in V(G)} \max_{v \in V(G)} d(u, v).
\]

A central vertex in a graph $G$ is the vertex that achieves the radius.

**Proposition 2.4.1.** If $G$ is a connected graph, then
\[
\text{rad}(G) \leq \text{diam}(G) \leq 2 \text{rad}(G).
\]
A graph is said to be \(k\)-(vertex) connected if \(G\) has at least \(k+1\) vertices, and there is no subset of \(k-1\) vertices whose removal disconnects the graph. An edge-cut of a connected graph \(G\) is a set of edges \(C \subseteq E(G)\) such that \(G - C\) is disconnected. A graph \(G\) is \(k\)-edge-connected if \(G\) cannot be separated into two components by removing less than \(k\) edges. An edge-cut \(C\) of \(G\) is cyclic if each component of \(G - C\) contains a cycle. A graph is cyclically \(k\)-edge-connected if at least \(k\) edges must be removed to disconnect it into two components such that each contains a cycle.

### 2.5 Trees

An acyclic graph, a graph that contains no cycles, is called a forest. A connected acyclic graph is called a tree, the vertices of degree one are called leaves.

**Theorem 2.5.1.** In a tree, any two vertices are connected by exactly one path.

The relation between the number of vertices and the number of edges is given by the next theorem.

**Theorem 2.5.2.** If \(T\) is a tree, then \(|E(T)| = |V(T)| - 1\).

A rooted tree \(T(x)\) is a tree \(T\) with a specified vertex \(x\), called the root of \(T\). In a rooted tree, the parent of a vertex is the vertex connected to it on the path to the root; every vertex except the root has a unique parent. If \(w\) is the parent of \(u\), then we call \(u\) a child of \(w\). A tree \(T\) is complete \(k\)-regular if every vertex has degree 1 or \(k\). A rooted tree where all leaves are on the same distance to the root is called a balanced tree.

### 2.6 Cyclomatic number

For a graph \(G\), the cyclomatic number is \(\nu(G) = m - n + 1\). Thus, every tree has cyclomatic number 0. The unicyclic graphs are the graphs with cyclomatic number 1. Note that such a graph has precisely one cycle. The bicyclic graphs are those which have cyclomatic number 2. Such a graph has two or three cycles.

In chemistry trees, unicyclic graphs, bicyclic graphs, and so on, are important graphs since they represent classes of molecules. Trees are graph representation of acyclic molecules like alkanes (also known as paraffins). Cycloalkanes are types of alkanes which have one or more rings of carbon atoms in the chemical structure of their molecules, so their graph structures are unicyclic graphs, bicyclic graphs, etc.
Chapter 2. Concepts in graph theory

2.7 Planar graphs

A graph $G$ is planar or embedded in a plane, if it can be drawn in the plane so that its edges intersect only in their end-vertices.

**Theorem 2.7.1.** A graph $G$ is embeddable in the plane if and only if it is embeddable in the sphere.

A planar graph with a given plane embedding is called a plane graph. Every plane graph partitions the plane into several connected regions, called faces. The set of all faces is denoted by $F(G)$. Each plane graph has precisely one unbounded face called the outer face. The boundary of a face is the subgraph induced by the edges on the faces frontier. The face is incident to the vertices (or edges) in its boundary. Two faces are adjacent if they have a common edge. The length of a face is the length of a facial walk. Sometimes the length of a face can be longer then the number of incident edges.

The distance between the faces $F_1$ and $F_2$ is the minimal distance between the vertices from $F_1$ and $F_2$ or $d(F_1, F_2) = \min\{d(u, v) \mid u \in V(F_1), v \in V(F_2)\}$.

**Theorem 2.7.2.** In a plane 2-connected graphs, every face is bounded by a cycle.

The numbers of vertices, edges and faces in a planar graph are closely related. The relation is given by Euler’s formula.

**Theorem 2.7.3** (Euler’s Formula). If $G$ is a connected planar graph then the number of faces in every plane embedding of $G$ satisfies

$$|V(G)| - |E(G)| + |F(G)| = 2.$$ 

**Theorem 2.7.4.** Every simple 3-connected graph has a unique planar embedding.

2.8 Matchings and independent sets

A matching in $G$ is a collection $M$ of edges of $G$ such that no two edges from $M$ have a common vertex. If a matching $M$ covers all vertices of $G$ we say that $M$ is a perfect matching. Every perfect matching is also a maximum matching, i.e., a matching of maximum cardinality. The number of edges in a maximum matching of a graph $G$ is called the matching number of $G$ and denoted by $\alpha'(G)$. A matching $M$ is maximal if it cannot be extended to a larger matching of $G$. Recall that no graph of odd order can have a perfect matching, because every matching clearly covers an even number of vertices.
A set $I \subseteq V(G)$ is independent if no two vertices from $I$ are adjacent in $G$. The cardinality of a largest independent set in $G$ is called the independence number of $G$ and is denoted by $\alpha(G)$.

A graph $G$ is called $k$-extendable if for any set $M$ of $k$ independent edges, there exists a perfect matching in $G$ containing all the edges of $M$. 
Chapter 3

Topological indices

Among the vast number of degree and distance based topological indices we pay our attention to only few: Zagreb indices and their variable modification, Schultz index of the second kind (also called Gutman index) and a modification of Randić index.

Zagreb indices and their variable form are mainly connected to a computer generated conjecture \[^{21}\]. Soon after, it turned out that this conjecture known as Zagreb indices inequality (defined later) does not hold in general. In the thesis we are considering classes of graphs that (dis)satisfy this conjecture.

As chemists established long ago, isomers of a same compound have different properties. Since the components of the molecules are the same, the reason for different properties or activities lies in the molecule structure. The main idea with topological indices is to describe the structure of a molecule with a number. To every molecule is assigned a unique real number that gives a specific information (depending on the topological index that is used).

Let consider molecules with same composition (isomers). Each topological index will make its own ordering of the molecules, and that ordering will tell how strong a property or activity is compared to the other isomers of a compound. From that perspective is important to know the graphs with extreme value for each topological index among all graphs on \( n \) vertices.

In the thesis we determine the graphs with extremal values for Gutman index and \( R' \) index, and find a triangle-free graph on \( n \) vertices with minimum \( R'(G) \) index.
3.1 Zagreb Index

Let \( G = (V, E) \) be a simple graph with \( n = |V| \) vertices and \( m = |E| \) edges. First and second Zagreb index are defined as

\[
M_1(G) = \sum_{v \in V} d(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E} d(u)d(v).
\]

For the sake of simplicity, we will often use \( M_1 \) and \( M_2 \) instead of \( M_1(G) \) and \( M_2(G) \), respectively. See [31, 32, 88, 71, 109, 110, 111] for more work done on these indices.

In spite of the fact that these two indices were introduced simultaneously and examined almost always together, relations between them became interesting recently. Comparing the values of these indices on the same graph was one very natural aim, which gave, and still gives, very interesting results. The following observation suggests that it is more reasonable to compare \( \frac{M_1}{n} \) with \( \frac{M_2}{m} \), instead of comparing \( M_1 \) with \( M_2 \). Namely, for general graphs, \( m \) is bounded from above by \( n^2 \), and thus, the orders of magnitude of \( M_1 \) and \( M_2 \) are \( O(n^3) \) and \( O(n^4) \) respectively. The following computer generated conjecture was proposed in [22]:

**Conjecture 3.1.1 (Zagreb indices inequality).** If \( G \) is a simple graph, then

\[
\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m},
\]

and the bound is tight for complete graphs.

If the graph is regular then this bound is tight, but it is also tight if \( G \) is a star. The Zagreb indices inequality holds for trees [103], graphs of maximum degree four, also called chemical graphs [72], and unicyclic graphs [24], but does not hold in general. See [72, 103, 24, 98] for various examples of graphs dissatisfying the Zagreb indices inequality (3.1).

A graph \( G \) is called *good* if the Zagreb indices the inequality (3.1) holds.

Since, we will discuss conditions when the Zagreb indices inequality holds, for the sake of simplicity, we will introduce \( m_{i,j} \) to be the number of edges that connect vertices of degrees \( i \) and \( j \) in the graph \( G \). Then as shown in [72]:

\[
\frac{M_2}{m} - \frac{M_1}{n} = \sum_{i \leq j, k \leq \ell \atop (i,j),(k,\ell) \in \mathbb{N}^2} \left[ \left( i j \left( \frac{1}{k} + \frac{1}{\ell} \right) + k \ell \left( \frac{1}{i} + \frac{1}{j} \right) - i - j - k - \ell \right) m_{i,j} m_{k,\ell} \right].
\]

(3.2)

In order to examine whether the Zagreb indices inequality holds, one can consider whether \( \frac{M_2}{m} - \frac{M_1}{n} \) is nonnegative. The difference that we are considering is given by
In order to simplify (3.2), we define a function \( f \), and study some of its properties. Namely, for integers \( i, j, k, \ell \), let

\[
f(i, j, k, \ell) = ij \left( \frac{1}{k} + \frac{1}{\ell} \right) + k\ell \left( \frac{1}{i} + \frac{1}{j} \right) - i - j - k - \ell.
\]

Now, (3.2) can be restated as

\[
\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i \leq j \leq k \leq \ell \leq \infty \atop (i, j, k, \ell) \in \mathbb{N}^2}} f(i, j, k, \ell)m_{i,j}m_{k,\ell}.
\]

Notice that \( f \) can be represented in the following way

\[
f(i, j, k, \ell) = (ij - k\ell) \left( \frac{1}{k} + \frac{1}{\ell} - \frac{1}{i} - \frac{1}{j} \right),
\]

and that it has some symmetry properties. For example, for every \( i, j, k \) and \( \ell \) where:

\[
f(i, j, k, \ell) = f(j, i, k, \ell) \quad \text{and} \quad f(i, j, k, \ell) = f(k, \ell, i, j).
\]

Since it makes sense to consider only positive values of the integers \( i, j, k, \ell \), in the rest of the section, the term integers will be used for positive integers.

Let \( D(G) \) be the set of the degrees of vertices in \( G \), i.e., \( D(G) = \{d(v) \mid v \in V\} \). A set \( S \) of integers is good if for every graph \( G \) with \( D(G) \subseteq \mathbb{S} \) the Zagreb indices inequality holds. Otherwise, \( S \) is a bad set.

First, we present an alternative proofs concerning the Zagreb indices inequality for trees and unicyclic graphs. We also show that every graph with cyclomatic number at most 2 is a subgraph of a good bicyclic graph. Then we present some other classes of graphs with prescribed degrees for which Zagreb indices inequality holds, and more generally conditions on the distribution of degrees in a graph \( G \) implying the relation (3.1). We also show that there are arbitrarily long intervals \([a, b]\) such that a graph with minimal degree at least \( a \) and maximum degree at most \( b \) satisfies the same relation. We prove that for any \( \Delta \geq 5 \), there is an infinite family of connected graphs of maximum degree \( \Delta \) such that the inequality is false, and give an algorithm for deciding if a given set of integers \( S \) of cardinality \( s \) is good, which requires \( O(s^2 \log s) \) time and \( O(s) \) space.

### 3.1.1 Sign of function \( f \)

Determining the sign of the function \( f \) will help us to see whether the difference \( M_2/m - M_1/n \) is nonnegative, and to determine when the Zagreb indices inequality holds. By the decomposition (3.3) of \( f \), the next lemma follows immediately [5].
Lemma 3.1.1. For any integers $i, j, k, \ell$, the value $f(i, j, k, \ell) < 0$ if and only if

(a) $ij > k\ell$ and $\frac{1}{k} + \frac{1}{\ell} < \frac{1}{i} + \frac{1}{j}$, or

(b) $ij < k\ell$ and $\frac{1}{k} + \frac{1}{\ell} > \frac{1}{i} + \frac{1}{j}$.

Proof. This result follows immediately by the decomposition of $f$. Namely

$$f(i, j, k, \ell) = \frac{ij}{k\ell}(k + \ell) - (k + \ell) + \frac{k\ell}{ij}(i + j) - (i + j)$$

$$= (k + \ell) \left[ \frac{ij - k\ell}{k\ell} \right] + (i + j) \left[ \frac{k\ell - ij}{ij} \right]$$

$$= (ij - k\ell) \left( \frac{1}{k} + \frac{1}{\ell} - \frac{1}{i} - \frac{1}{j} \right).$$

□

Lemma 3.1.2. If $f(i, j, k, \ell) < 0$ for some integers $i \leq j$ and $k \leq \ell$, then

$$i < k \leq \ell < j \quad \text{or} \quad k < i \leq j < \ell.$$

Proof. Suppose first that $i \leq k$. There are only three possible orderings:

- $i \leq j \leq k \leq \ell$;
- $i \leq k \leq j \leq \ell$;
- $i \leq k \leq \ell \leq j$.

If $i \leq j \leq k \leq \ell$, then $ij \leq k\ell$, but $\frac{1}{k} + \frac{1}{\ell} < \frac{1}{i} + \frac{1}{j}$, so this is impossible by Lemma 3.1.1 (a). If $i \leq k \leq j \leq \ell$, then $ij \leq k\ell$ and $\frac{1}{k} + \frac{1}{\ell} < \frac{1}{i} + \frac{1}{j}$. This ordering is also impossible by Lemma 3.1.1 (a). So, the only possible ordering for $f(i, j, k, \ell)$ to be negative is $i \leq k \leq \ell \leq j$.

Now, if $i = k (i = k \leq \ell \leq j)$, then $ij \geq k\ell$ and $\frac{1}{i} + \frac{1}{j} > \frac{1}{k} + \frac{1}{\ell}$, which contradicts Lemma 3.1.1 (a). So we conclude that $i < k$. Similarly, one can show that $\ell \neq j$. Thus, we obtain the first ordering $i < k \leq \ell < j$ given in the lemma.

Suppose now that $k \leq i$. Applying a similar argument as above, one obtains that $k < i \leq j < \ell$ is the only possible ordering. □

The following simple lemma will be used in the proof of Lemma 3.1.4.

Lemma 3.1.3. Let $i \leq k \leq \ell \leq j$ and $k + \ell \geq i + j$ for some four integers $i, j, k, \ell$. Then, $k\ell \geq ij$. 

 Lemma 3.1.4.
Proof. Since \( k - i \geq j - \ell \) and \( j \) is the largest, we infer \( k\ell - ij = (k - i)j - (j - \ell)k \geq (j - \ell)(j - k) \geq 0 \). Hence, \( k\ell \geq ij \). \( \Box \)

Now, we will present a condition on integers \( i, j, k, \ell \), for which \( f(i, j, k, \ell) \) is nonnegative.

Lemma 3.1.4. Let \( k + \ell \geq i + j \) and \( i < k \leq \ell < j \) for some four integers \( i, j, k, \ell \). Then, \( f(i, j, k, \ell) \geq 0 \).

Proof. Since \( k - i \geq j - \ell \) by Lemma 3.1.3, we have \( k\ell \geq ij \), and so

\[
\frac{1}{i} + \frac{1}{j} - \frac{1}{k} - \frac{1}{\ell} = \frac{k - i}{ki} + \frac{\ell - j}{j\ell} \geq (j - \ell) \left( \frac{1}{ki} - \frac{1}{j\ell} \right) \geq 0.
\]

Now the proof is straightforward by Lemma 3.1.1. \( \Box \)

The following proposition gives an equivalence between the sign of \( f(i, j, k, \ell) \) and a relation of the integers \( i, j, k, \ell \).

Proposition 3.1.5. Let \( i, j, k, \ell \) be integers satisfying \( i < k \leq \ell < j \). Then, \( f(i, j, k, \ell) < 0 \) if and only if \( \frac{k + \ell}{i + j} < \frac{k\ell}{ij} < 1 \).

Proof. First, suppose that \( \frac{k + \ell}{i + j} < \frac{k\ell}{ij} < 1 \). Left inequality implies that \( \frac{1}{k} + \frac{1}{\ell} < \frac{1}{i} + \frac{1}{j} \), and from the right inequality, it follows that \( ij > k\ell \). Thus, by Lemma 3.1.1, we have \( f(i, j, k, \ell) < 0 \).

Suppose now that \( f(i, j, k, \ell) < 0 \). By Lemma 3.1.4, we have that \( k + \ell < i + j \). If \( ij \leq k\ell \) then

\[
\frac{1}{k} + \frac{1}{\ell} - \frac{1}{i} - \frac{1}{j} = \frac{k + \ell}{k\ell} - \frac{i + j}{ij} < 0,
\]

and by Lemma 3.1.1, we have \( f(i, j, k, \ell) \geq 0 \), which is a contradiction to the assumption. Thus, we may assume that \( ij > k\ell \), i.e., \( \frac{k\ell}{ij} < 1 \). Since \( f(i, j, k, \ell) \) is negative, by Lemma 3.1.1(a) where \( \frac{1}{k} + \frac{1}{\ell} < \frac{1}{i} + \frac{1}{j} \), and hence \( \frac{k + \ell}{i + j} < \frac{k\ell}{ij} \). This concludes the proof. \( \Box \)

3.1.2 An alternative proof for trees and unicyclic graphs

As we said before, trees and unicyclic graphs satisfy \( M_1/n \leq M_2/m \), in other words these graphs are good. Here, the same results are proven in a shorter way [5].

Let \( p_3(G) \) be the number of 3-paths in \( G \), \( p_2(G) \) the number of 2-paths, and \( c_3(G) \) is the number of 3-cycles. Fix an edge \( uv \). There are \((d(u) - 1)(d(v) - 1)\) ways to extend
uv to a sequence of three consecutive adjacent edges, uv being in the middle. Via this extension we either obtain a 3-path, or a 3-cycle if the neighbors of u and v coincide. Now, we have

\[ p_3(G) + 3c_3(G) = \sum_{uv \in E} (d(v) - 1)(d(u) - 1). \] (3.5)

**Theorem 3.1.6.** If \( G \neq K_1 \) is a tree, then \( \frac{M_1}{n} \leq \frac{M_2}{m} \). Moreover, equality holds if and only if \( G \) is a star.

**Proof.** If \( G \) is a k-star, then \( M_1 = kn \) and \( M_2 = km \), by which we have equality in (3.1). So assume now that \( G \) has at least two internal adjacent vertices \( u \) and \( v \) and that \( v \) is the only internal neighbor of \( u \). Observe that \( M_1 = \sum_{v \in V} d(v)^2 = 2(p_2(G) + m) \). We have

\[ M_2 = \sum_{uv \in E} \left[ (d(v) - 1)(d(u) - 1) + (d(u) + d(v)) - 1 \right] = p_3(G) + M_1 - m. \] (3.6)

Now, since \( m = n - 1 \), we obtain

\[
(n - 1)M_1 < nM_2 \\
(n - 1)M_1 < n[p_3(G) + M_1 - (n - 1)] \\
0 < p_3(G) + \frac{2}{n}(p_2(G) + (n - 1)) - (n - 1).
\]

Since \( G \) is not a star, \( p_2(G) \geq 2 \). We will prove now that \( p_3(G) \geq n - 3 \), and this will establish the theorem. Let \( \ell_1, \ldots, \ell_k \) be the leaves adjacent to \( u \), and let \( w \neq u \) be a neighbor of \( v \). To any vertex \( x \) at distance at least 2 from \( u \) we associate the 3-path built from the first three edges of the shortest path from \( x \) to \( \ell_1 \). To any leaf \( \ell_i, (i \neq 1) \), we associate the path from \( w \) to \( \ell_i \). These 3-paths being all different, we associated a 3-path to any vertex except three, namely \( \ell_1, u, v \), which ensures that \( p_3(G) \geq n - 3 \). \( \square \)

**Theorem 3.1.7.** If \( G \) is an arbitrary unicyclic graph, then \( \frac{M_1}{n} \leq \frac{M_2}{m} \). Moreover, equality holds if and only if \( G \) is a cycle.

**Proof.** Since \( G \) is an unicyclic graph, \( m = n \). If \( G \) is a k-cycle then \( M_1 = 4k \) and \( M_2 = 4k \), so we have equality in (3.1). Now, let \( C = x_1x_2 \ldots x_kx_1 \) be the unique cycle of \( G \) and suppose that \( x_1 \) has a neighbor \( y \notin V(C) \). Such a vertex exists as \( G \neq C \). From (3.5) and the left equality of (3.6), we have

\[ M_2 = p_3(G) + 3c_3(G) + M_1 - m. \]
Now, we will show that $M_1 + 1 \leq M_2$ which is equivalent to $M_1 \leq p_3(G) + 3C_3(G) + M_1 - n - 1$, which is in term equivalent to

$$n + 1 \leq p_3(G) + 3C_3(G). \quad (3.7)$$

Now, remove the edge $x_1x_2$ from the cycle. Then $G - \{x_1x_2\}$ is a tree and $p_3(G - \{x_1x_2\}) \geq n - 3$. Including $yx_1x_2x_3$ we have at least $n - 2$ different 3-paths.

If $C$ is a 3-cycle, then it is obvious that (3.7) holds. Now, assume $\ell \geq 4$. Observe that $x_1x_2x_3x_4, x_{\ell}x_1x_2x_3, x_{\ell-1}x_{\ell}x_1x_2$ are 3-paths all distinct from the 3-paths described. Hence, $p_3(G) \geq n + 1$.

### 3.1.3 Good bicyclic graphs

In this section we will show that every graph with cyclomatic number at most 2 is a subgraph of a good bicyclic graph. The proof of the next proposition also gives a way to construct a good bicyclic graph starting form any graph with cyclomatic number at most 2.

**Proposition 3.1.8.** Let $G$ be graph of order $n$ with cyclomatic number at most 2. Then $G$ is subgraph of a good bicyclic graph.

**Proof.** If $G$ is not bicyclic, we can safely add edges or vertices to change it. Let us then choose some large integer value for $d$, and add leaves to the $n_1$ vertices of the 1-core (maximum subgraph of minimum degree 2) of $G$ until each of them is adjacent to $d$ leaves: we call this new graph $G_d$. Let us compute asymptotic estimates for $M_1$ and $M_2$ according to $d$

$$M_1(G_d) = \sum_{v \in V(G_d)} d(v)^2 = n_1d + n_1(d + 2)^2 + O(d) = n_1d^2 + O(d),$$

$$M_2(G_d) = \sum_{uv \in E(G_d)} d(v)d(u) \geq n_1d(d + 2) + (n_1 + 1)(d + 2)^2 = (n_1 + 2)d^2.$$

Hence, as there are $n_1d + O(1)$ edges and vertices:

$$m M_1(G_d) = (n_1d + O(1))(n_1d^2 + O(d)) = n_1^2d^3 + O(d^2)$$

$$< (n_1^2 + 2n_1)d^3 + O(d^2) = (n_1d + O(1))(n_1 + 2)d^2$$

$$\leq n M_2(G_d).$$

\[ \square \]
3.1.4 Zagreb indices inequality of graphs with prescribed vertex degree

At first let make some observations, when a set of size two, three, or four is a good set.

Small good sets

It is easy to see that if $G$ is a $k$-regular graph, then (3.1) is valid, since

$$\frac{M_1}{n} = k^2 = \frac{M_2}{m}.$$ 

As Conjecture 3.1.1 is false in general, but true for $k$-regular graphs, one may wonder if it also holds for “almost regular” graphs, i.e., graphs with only a few different vertex degrees. Now, we verify that this holds for graphs with only two vertex degrees. We give a direct short proof avoiding using the properties of the function $f$.

**Proposition 3.1.9.** Let $x, y \in \mathbb{N}$, and let $G$ be a graph with $n$ vertices, $m$ edges, and $d(v) \in \{x, y\}$ for every vertex $v$ of $G$. Then, the Zagreb indices inequality holds for $G$.

**Proof.** Since $d(v) = x$ or $y$ for every vertex $v \in V$, we conclude that if $i, j \notin \{x, y\}$, then $m_{i,j} = 0$. By (3.2), we infer

$$\frac{M_2}{m} - \frac{M_1}{n} = 2 \left[ \frac{x^3(x-y)^2}{x^3y}m_{x,x}m_{x,y} + \frac{2xy(x-y)^2(x+y)}{x^2y^2}m_{x,x}m_{y,y} ight]
+ \frac{y^3(x-y)^2}{xy^3}m_{x,y}m_{y,y}
= 2(x-y)^2 \left[ \frac{1}{y}m_{x,x}m_{x,y} + 2 \left( \frac{1}{x} \right) m_{x,x}m_{y,y} + \frac{1}{x}m_{x,y}m_{y,y} \right]
\geq 0$$

which establishes the claim. \qed

In Proposition 3.1.9 we have shown that for a graph $G$ with $|D(G)| = 2$, the Zagreb index inequality holds. Sun and Chen [97] showed that any graph $G$ with $\Delta(G) - \delta(G) \leq 2$ satisfies Zagreb index inequality. Thus, any interval of length three is good. One can generalize this result for arithmetic sequences with three terms.

**Proposition 3.1.10.** Let $s, x \in \mathbb{N}$. If $G$ is a graph with $n$ vertices, $m$ edges, and $D(G) \subseteq \{x - s, x, x + s\}$, the Zagreb indices inequality holds.
Proof. The Zagreb indices inequality holds if \( M_2/m - M_1/n \) is non-negative. The difference (3.10) is non-negative if for any integers \( i, j, k, \ell \), the function \( f(i, j, k, \ell) \) is non-negative. So we are interested whether \( f(i, j, k, \ell) \) can be negative for some integers \( i, j, k, \ell \). By Lemma 3.1.2, we may assume, up to symmetry, that the ordering of \( i, j, k, \ell \) is \( i < k \leq \ell < j \). Since \( i, j, k, \ell \in \{x - s, x, x + s\} \), we have that \( f(i, j, k, \ell) \) can be negative only if \( i = x - s, k = \ell = x \) and \( j = x + s \). But \( f(x - s, x + s, x, x) = \frac{1}{x - s} - \frac{2}{x} + \frac{1}{x + s} > 0 \). Hence, we conclude that \( \frac{M_2}{m} - \frac{M_1}{n} = \sum_{i,j,k,\ell \in \{x-s, x, x+s\}} f(i,j,k,\ell) m_{i,j} m_{k,\ell} > 0 \). \( \square \)

Notice that the above result cannot be extended to an arbitrary interval of length 4 as Sun and Chen [97] gave a non-connected counterexample. For a connected counterexample, consider the graph \( G(\ell, k, s) \) with \( \ell = 4 \) from Figure 3.3. It is obvious that \( D(G(4, k, s)) \) is a subset of the interval \([2, 5]\), but this graph for appropriate values of \( k \) and \( s \) does not satisfy the inequality (3.1), see Theorem 3.1.16. Both graphs contain vertices of degree 2. It is interesting that Sun and Chen [97] proved that every graph \( G \) with \( \Delta(G) - \delta(G) \leq 3 \) and \( \delta(G) \neq 2 \) satisfies (3.1). Thus, every interval \([x, x + 3]\) is good with only exception of \([2, 5]\).

The proof of Proposition 3.1.10 motivates a more general conclusion.

**Proposition 3.1.11.** The set of integers \( \{a, b, c\} \), where \( a < b < c \), is good if and only if

(a) \( b^2 \geq ac \) and \( b(a + c) \geq 2ac \), or

(b) \( b^2 \leq ac \) and \( b(a + c) \leq 2ac \).

**Proof.** Since \( a < b < c \), by Lemma 3.1.2 the function \( f \) can be negative in \( f(i, j, k, \ell) \) only if either \( i = a, k = \ell = b \), and \( j = c \), or \( k = a, i = j = b \), and \( \ell = c \), i.e., only \( f(a, c, b, b) = f(b, b, a, c) = (ac - b^2) \left( \frac{2}{b} - \frac{1}{a} - \frac{1}{c} \right) \) can be negative. If (a) or (b) holds, then it is obvious that \( f(i, j, k, \ell) \geq 0 \) for any integers \( i, j, k, \ell \in \{a, b, c\} \), and the inequality (3.1) is valid for every graph \( G \) such that \( D(G) = \{a, b, c\} \).

For the other direction, suppose that neither (a) nor (b) holds. In this case \( f(a, c, b, b) < 0 \). We construct a graph \( G_{x,y} \) with \( D(G_{x,y}) = \{a, b, c\} \), \( m_{a,a} = m_{c,c} = 0 \) and \( m_{a,b} = m_{b,c} = 1 \) (see Figure 3.1). The graph \( G_{x,y} \) can be created in the following way:

(A) Make a sequence of \( x \) copies of \( K_{a,c} \) and then continue that sequence with \( y \) copies of \( K_{b,b} \).
Figure 3.1: A connected graph $G$ with $D(G) = \{a, b, c\}$. The edges that should be removed are drawn with dashed lines.

(B) Choose an edge from the first $K_{a,c}$ graph and an edge from the second $K_{a,c}$ graph. Let denote these edges by $v_1^a v_1^c$ and $v_2^a v_2^c$, respectively. Replace $v_1^a v_1^c$ and $v_2^a v_2^c$ by edges $v_1^a v_2^c$ and $v_2^a v_1^c$. Continue this kind of replacement between all consecutive copies of $K_{a,c}$. Notice that these replacements do not change the degrees of the vertices.

(C) Next, choose an edge from the last $K_{a,c}$ graph and an edge from the first $K_{b,b}$ graph. Let denote these edges by $v_x^a v_x^c$ and $v_1^b v_1^b$, respectively. Replace $v_x^a v_x^c$ and $v_1^b v_1^b$ by edges $v_x^a v_1^b$ and $v_1^b v_x^c$.

(D) Apply the same procedure between all consecutive graphs $K_{b,b}$ in the sequence. This completes the construction of $G_{x,y}$.

We emphasize that this binding procedure is done only once between $K_{a,c}$ and $K_{b,b}$ graphs. Now,

$$\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i,j,k,\ell \leq \ell \leq \ell \in \{a,b,c\}}} f(i, j, k; \ell) m_{i,j} m_{k,\ell}$$

$$= 2 \left[ f(a, c, b, b) m_{a,c} m_{b,b} + \left[ f(a, c, a, b) + f(a, c, b, c) \right] m_{a,c} \right.$$ 

$$+ \left[ f(a, b, b, b) + f(c, b, b, b) \right] m_{b,b} + f(a, b, b, c) \right].$$

If we increase the number of $K_{a,c}$ and $K_{b,b}$ graphs, i.e., $x$ and $y$, in the graph $G_{x,y}$, shown on Figure 3.1, then $m_{a,c}$ and $m_{b,b}$ will increase as well. For $m_{a,c}$ and $m_{b,b}$ big enough, the difference $M_2/m - M_1/n$ will be negative.

**Long good intervals**

Our next goal is to determine long good intervals. The next Theorem provides a construction of good intervals of any length. Notice that the following result holds for $c \leq 9$ by
the results of Sun and Chen [97] mentioned in the previous section, as in these cases the considered interval is of size at most 4.

At first we showed the following theorem [4].

**Theorem 3.1.12.** For every integer \( c \), the interval \([c, c + \lceil \sqrt{c} \rceil]\) is good.

**Corollary 3.1.13.** If \( G \) is a graph with \( \Delta(G) - \delta(G) \leq \lceil \sqrt{c} \rceil \) and \( \delta(G) \geq c \) for some integer \( c \), then \( G \) satisfies the inequality (3.1).

![Figure 3.2: A connected graph \( G_{x,y} \) with \( D(G_{x,y}) = \{i, j, k, \ell\} \) constructed from \( x \) copies of \( K_{i,j} \) and \( y \) copies of \( K_{k,\ell} \). The dashed edges are those that are removed from the corresponding complete bipartite graphs.](image)

**Proposition 3.1.14.** The interval \([a, b]\) is bad if and only if \( f(i, j, k, \ell) < 0 \) for some positive integers \( i, j, k, \ell \in [a, b] \).

**Proof.** If the interval \([a, b]\) is bad then for some graph \( G \) such that \( D(G) \subseteq [a, b] \) holds

\[
\frac{M_2(G)}{m} - \frac{M_1(G)}{n} = \sum_{i, j, k, \ell \in D(G)} f(i, j, k, \ell)m_{i,j}m_{k,\ell} < 0.
\]

Since \( m_{i,j} \geq 0 \) for all \( i, j \in D(G) \), there is quadruple \( (i, j, k, \ell) \), \( i, j, k, \ell \in D(G) \subseteq [a, b] \) such that \( f(i, j, k, \ell) < 0 \).

Now, let prove the opposite direction. Let \( a > 1 \). We postpone the case \( a = 1 \) until the end of this proof.

Whenever \( f(i, j, k, \ell) < 0 \) and \( i, j, k, \ell \in [a, b] \), we can construct a connected graph \( G_{x,y} \), with \( D(G_{x,y}) = \{i, j, k, \ell\} \), that does not satisfies (3.1). An illustration of \( G_{x,y} \) is given in Figure 3.2. The construction of \( G_{x,y} \) is adapted from the proof of Proposition 3.1.11 and it goes as follows:
(A’) Make a sequence of $x$ copies of $K_{i,j}$ and then continue that sequence with $y$ copies of $K_{k,\ell}$.

(B’) Connect the copies of $K_{i,j}$ and the copies of $K_{k,\ell}$ as in (B).

(C’) Next, choose an edge from the last $K_{i,j}$ graph and an edge from the first $K_{k,\ell}$ graph.

Let denote these edges by $v_i^x v_j^x$ and $v_k^x v_\ell^x$, respectively. Replace $v_i^x v_j^x$ and $v_k^x v_\ell^x$ by edges $v_i^x v_i^x$ and $v_k^x v_\ell^x$.

From the construction, it follows that $m_{i,j} = x \cdot i \cdot j - 1$, $m_{k,\ell} = y \cdot k \cdot \ell - 1$, $m_{i,\ell} = m_{j,k} = 1$, and $m_{i,i} = m_{i,k} = m_{j,j} = m_{j,\ell} = m_{k,k} = m_{\ell,\ell} = 0$. Thus,

$$
\frac{M_2}{m} - \frac{M_1}{n} = \sum_{q,r,s,t \in (i,j,k,\ell)} f(q,r,s,t) m_{q,r} m_{s,t} \\
= 2 \left( f(i,j,k,\ell) m_{i,j} + \left( f(i,\ell, i, \ell) + f(i, j, j, k) \right) m_{i,j} \right) \\
+ \left( f(k,\ell, i, \ell) + f(k, j, j, k) \right) m_{k,\ell} + f(i, j, j, k) \left( m_{i,j} \right) \\
= m_{i,j} \left[ f(i,j,k,\ell) m_{i,j} + 2 f(i,\ell, i, \ell) + 2 f(i, j, j, k) + \frac{f(i, j, j, k)}{m_{i,j}} \right] \\
+ m_{k,\ell} \left[ f(i,j,k,\ell) m_{i,j} + 2 f(k,\ell, i, \ell) + 2 f(k, j, j, k) + \frac{f(i, j, j, k)}{m_{k,\ell}} \right] \\
= m_{i,j} \left[ f(i,j,k,\ell) (y \cdot k \cdot \ell - 1) + 2 f(i,\ell, i, \ell) + 2 f(i, j, j, k) + \frac{f(i, j, j, k)}{(x \cdot i \cdot j - 1)} \right] \\
+ m_{k,\ell} \left[ f(i,j,k,\ell) (x \cdot i \cdot j - 1) + 2 f(k,\ell, i, \ell) + 2 f(k, j, j, k) + \frac{f(i, j, j, k)}{(y \cdot k \cdot \ell - 1)} \right].
$$

Since $f(i,j,k,\ell) < 0$, there exist $x$ and $y$ sufficiently large, so that

$$
\left[ f(i,j,k,\ell) (y \cdot k \cdot \ell - 1) + 2 f(i,\ell, i, \ell) + 2 f(i, j, j, k) + \frac{f(i, j, j, k)}{(x \cdot i \cdot j - 1)} \right] < 0,
$$

and

$$
\left[ f(i,j,k,\ell) (x \cdot i \cdot j - 1) + 2 f(k,\ell, i, \ell) + 2 f(k, j, j, k) + \frac{f(i, j, j, k)}{(y \cdot k \cdot \ell - 1)} \right] < 0.
$$

Thus, for such chosen $x$ and $y$, that correspond to the number of $K_{i,j}$ and $K_{k,\ell}$ subgraphs shown in Figure 3.2, the difference $M_2/m - M_1/n$ of $G_{x,y}$ is also negative.

If $a = 1$ and $\min(i,j,k,\ell) = 1$, then $G_{x,y}$ is disconnected. Thus, we consider the intervals $[1, b]$, $b \geq 1$, separately. For $1 \leq b \leq 4$, these intervals are good. The function $f(2,5,3,3)$ is negative, and by the above construction interval $[1, b]$, is bad for every $b \geq 5$.

This establishes the proposition. \(\square\)
From [3] we have:

**Theorem 3.1.15.** For every positive integer \( n \), the interval \([a, a+n]\) is good if and only if \( a \geq \frac{n(n-1)}{2} \) or \([a, a+n] = [1,4]\).

**Proof.** As \([1,4]\) is good interval, in order to prove “if” direction of the theorem, it suffices to show that \( f(i,j,k,\ell) \geq 0 \) whenever \( i, j, k, \ell \in [a,a+n] \) and \( a \geq \frac{n(n-1)}{2} \). Suppose in contrary that there is a quadruple \((i,j,k,\ell)\), \( i, j, k, \ell \in [a,a+n] \) such that \( f(i,j,k,\ell) < 0 \). By Lemma 3.1.2 and (3.4), we can assume that \( a \leq i < k \leq \ell < j \leq a+n \). Let \( k = i + s, \ell = i + t, j = i + q \), where \( 0 < s \leq t < q \leq n \). Now,

\[
\frac{1}{k} + \frac{1}{\ell} = \frac{2i + s + t}{(i+s)(i+t)} \quad \text{and} \quad \frac{1}{i} + \frac{1}{j} = \frac{2i + q}{i(i+q)}.
\]

Since \( f(i,j,k,\ell) < 0 \), Proposition 3.1.5, implies that \( kl < ij \) and \( k + \ell < i + j \). Thus, we obtain \( s + t < q \). As \( st \leq \frac{(s+t)^2}{4} \), we obtain \( st \leq \frac{(q-1)^2}{4} \leq \frac{(n-1)^2}{4} \). By Lemma 3.1.1, it follows that \( f(i,j,k,\ell) < 0 \) if \( \frac{1}{k} + \frac{1}{\ell} < \frac{1}{i} + \frac{1}{j} \). Hence,

\[
\frac{2i + s + t}{(i+s)(i+t)} < \frac{2i + q}{i(i+q)}
\]

\[
(2i + s + t)(i^2 + iq) < (2i + q)(i^2 + (s+t)i + st)
\]

\[
2i^3 + (s+t+2q)i^2 + (s+t)iq < 2i^3 + (2s + 2t + q)i^2 + 2sti + (s+t)iq + stq
\]

\[
q i^2 < (s+t)i^2 + 2sti + stq
\]

\[
q i^2 < (q-1)i^2 + 2sti + stq,
\]

from here

\[
i^2 < 2sti + stq
\]

\[
\leq 2 \left( \frac{n-1}{2} \right)^2 i + \left( \frac{n-1}{2} \right)^2 n
\]

\[
\leq 2 \left( \frac{n-1}{2} \right)^2 i + \frac{n-1}{2} i
\]

\[
= \frac{i}{2} \frac{n(n-1)}{2},
\]

which is clearly impossible.

Thus, we have shown that \( f(i,j,k,\ell) \geq 0 \) for arbitrary \( i, j, k, \ell \) from an interval \([a,a+n]\) with \( a \geq \frac{n(n-1)}{2} \). Therefore, such an interval is a good one.
Now, we prove the opposite direction. For \( n = 0, 1, 2 \) and an arbitrary integer \( a \), all intervals \([a, a + n]\) are good, see [97], and they satisfy the inequality \( a \geq \frac{n(n-1)}{2} \). For \( n = 3 \), \([1, 4]\) is the only good interval that does not satisfy \( a \geq \frac{n(n-1)}{2} \).

For \( n \geq 4 \), we proceed as follows. By Proposition 3.1.14, it suffices to show that \( f(i, j, k, \ell) < 0 \) for some integers \( i, j, k, \ell \in [a, a + n] \), and \( a \in A_n = \left\{ 1, 2, 3, \ldots, \binom{n}{2} - 1 \right\} \).

We show this by induction on \( n \). For the base of the induction, \( n = 4 \), we have \( a < 6 \), and the intervals of interest are \([1, 5]\), \([2, 6]\), \([3, 7]\), \([4, 8]\), and \([5, 9]\). Functions \( f(2, 5, 3, 3) \), \( f(3, 7, 4, 5) \), \( f(4, 8, 5, 6) \), and \( f(5, 9, 6, 7) \) are negative, and each corresponds to at least one of the above intervals.

By induction hypothesis we can assume that, for \( n - 1 \geq 4 \) and \( a \in A_{n-1} \), the interval \([a, a + n - 1]\) is bad.

Now we show that for an integer \( n \) and \( a \in A_n \) the interval \([a, a + n]\) is bad. First, notice that \( A_{n-1} \subset A_n \). Suppose first that \( a \in A_{n-1} \). Since \([a, a + n - 1]\) is a subinterval of \([a, a + n]\), and by induction hypothesis \([a, a + n - 1]\) is a bad interval, it follows that also \([a, a + n]\) is bad.

It remains to show that \([a, a + n]\) is a bad interval for \( a \in A_n \setminus A_{n-1} \), i.e., for \( a \in \left( \frac{(n-1)(n-2)}{2}, \frac{n(n-1)}{2} \right) \). We consider two cases regarding the parity of \( n \):

- \( n = 2s + 1 \): Then, \( s \geq 2 \) and \( 2s^2 - s \leq a < 2s^2 + s \). Now, it can be easily verified that
  \[
  f(a, a + 2s + 1, a + s, a + s) = \frac{(a - s - 2s^2)(a - s^2)}{a(a + s)(a + 2s + 1)} < 0.
  \]

- \( n = 2s \): Then, \( s \geq 3 \) and \((s - 1)(2s - 1) \leq a < s(2s - 1)\). Now we show that
  \[
  f(a, a + 2s, a + s - 1, a + s) = \frac{(a - s^2 + s)(a^2 + 2as + 2s^2 - 2as^2 - 2s^3)}{a(a + 2s)(a + s - 1)(a + s)}
  \]
  is negative. Observe that \( a - s^2 + s \geq (s - 1)^2 \geq 4 \) and
  \[
  a^2 + 2as + 2s^2 - 2as^2 - 2s^3 = (a + s)^2 - 2s^2(a + s) + s^2 \\
  \leq (a + s)(2s^2 - s - 1 + s - 2s^2) + s^2 \\
  = -a - s + s^2 < -s^2 + 2s - 1 \\
  = -(s - 1)^2 \leq -4.
  \]

Thus, the proof is completed. \(\square\)
3.1.5 Graphs of maximum degree at least 5

As we already mentioned, the inequality (3.1) holds for chemical graphs, but not in general. In [72, 103, 24, 69, 98, 97] examples of connected simple graph $G$ are given such that $M_1/n > M_2/m$. What strikes the eye in these counterexamples is that either the maximum degree of a vertex is at least 10 or the graph is disconnected. We now produce for each $\Delta \geq 5$ an infinite family of connected planar counterexamples to (3.1) of maximum degree $\Delta$ [4].

**Theorem 3.1.16.** There exists infinitely many graphs $G$ of maximum degree $\geq 5$ for which $\frac{M_1}{n} > \frac{M_2}{m}$.

**Proof.** Let $G$ be the graph shown on Figure 3.3. This graph has $2k$ vertices of degree 5, $2s + 2$ of degree 3, $5k + \ell$ vertices of degree 2, and two vertices of degree $\ell + 1$. Also $m_{5,2} = 10k - 2$, $m_{3,3} = 3s + 2$, $m_{3,5} = 2$ and $m_{\ell+1,2} = 2(\ell + 1)$. Then $n = 7k + 2s + \ell + 4$, $m = 10k + 3s + 2\ell + 4$, $M_1 = 2(35k + 9s + \ell^2 + 4\ell + 10)$, $M_2 = 100k + 27s + 4\ell^2 + 8\ell + 32$. From here one can obtained that

$$mM_1 - nM_2 = -2\ell^2 s + k(-144 + 64\ell - 8\ell^2 + s) - 8(6 + 5s) + \ell(8 + 17s).$$

For every $\ell$, we can find $k$ and $s$ big enough such that $mM_1 - nM_2 > 0$. Obviously, we can find infinitely many such pairs $(k, s)$.

Observe that the right side of the graph $G(\ell, k, s)$ is the cubic graph $K_2 \square C_s$ with one edge subdivided twice. This graph can be substituted with any other cubic graph of appropriate size. The graph $G(4,9,33)$ is the smallest graph for which the inequality of Theorem 3.1.16 holds, and it has 137 vertices.
3.1.6 Decision algorithm

In this section, we consider the problem whether deciding if a given set of positive integers $S$ of cardinality $s$ is a good one.

A straightforward algorithm that solves the above problem is to check if $f(i, j, k, \ell) < 0$ for all 4-tuples $(i, j, k, \ell)$ from $S$, where the 4-tuples $(i, j, k, \ell)$ are variations with repetitions. This checking that suffices to determine whether $S$ is good, since by Proposition 3.1.14, if $f(i, j, k, \ell) < 0$, we can construct a graph that does not satisfy (3.1). Verifying if $f(i, j, k, \ell) < 0$ can be done in constant time by Lemma 3.1.1. Thus, the time complexity of this approach is $O(s^4)$.

We now show that, using simple algorithmic tricks, one can obtain an $O(s^2 \log s)$ algorithm.

**Lemma 3.1.17.** There exists an algorithm that checks whether a given set $S$ of $s$ positive integers is good in $O(s^2 \log s)$ time and $O(s^2)$ space.

**Proof.** Let $P_1(i, j) = ij$ and $P_2(i, j) = \frac{i}{j} + \frac{j}{i}$. From (3.3) we obtain that $f(i, j, k, \ell) < 0$ if and only if $P_1(i, j) < P_1(k, \ell)$ and $P_2(i, j) < P_2(k, \ell)$ or $P_1(i, j) > P_1(k, \ell)$ and $P_2(i, j) > P_2(k, \ell)$. Using the symmetry of the function $f$, the set $S$ is good if and only if there are no pairs $(k, \ell)$ and $(i, j)$ from $S \times S$ such that $P_1(i, j) < P_1(k, \ell)$ and $P_2(i, j) < P_2(k, \ell)$.

Let us assign $P(i, j) = (P_1(i, j), -P_2(i, j))$ and compare values $P(i, j)$ lexicographically (that is, $P(i, j) < P(k, \ell)$ if $P_1(i, j) < P_1(k, \ell)$, or $P_1(i, j) = P_1(k, \ell)$ and $-P_2(i, j) < -P_2(k, \ell)$, i.e., $P_2(i, j) > P_2(k, \ell)$). Note that now the set $S$ is good if and only if for each two pairs $(i, j), (k, \ell) \in S \times S$ if $P(i, j) < P(k, \ell)$ then $P_2(i, j) \geq P_2(k, \ell)$.

The algorithm, sketched in Pseudocode 3.1.1, simply checks the above condition. We sort all pairs $(i, j) \in S \times S$ increasingly according to the value of $P(i, j)$ and then iterate over the sorted array $T$ and check if there exist consecutive pairs $(k', \ell')$ and $(k, \ell)$ such that $P_2(k', \ell') < P_2(k, \ell)$. If we find such pairs, we have $P_1(k', \ell') \leq P_1(k, \ell)$ since $P(k', \ell') \leq P(k, \ell)$, and so, the set $S$ is not good. Otherwise, we find that the array is sorted non-increasingly according to $P_2$ and, thus, for any $(i, j), (k, \ell) \in S \times S$ we have if $P_1(i, j) < P_1(k, \ell)$ then $P(i, j) < P(k, \ell)$ and $P_2(i, j) \geq P_2(k, \ell)$, and so, the set $S$ is good.

Note that in Pseudocode 3.1.1 we do not keep the indices $(k', \ell')$ of the previously considered pair, but we only store the value $P_2(k', \ell')$ in the variable $p_2$.

Let us now analyze consumed time and space. Sorting of array $T$ according to the value of $P$ consumes $O(s^2 \log s)$ time if we use Merge Sort or Heap Sort. We use $O(s^2)$ space to store the sorted pairs in the array $T$. □

The space complexity can be further improved to $O(s)$. The algorithm from Lemma
Algorithm 3.1.1  An $O(s^2 \log s)$ algorithm that checks whether $S$ is a good set.

1:  procedure CheckGoodSet($S$)
2:      $T \leftarrow$ the set of all pairs $(k, \ell) \in S \times S$
3:      sort $T$ in the increasing order of $P(k, \ell) = (P_1(k, \ell), -P_2(k, \ell))$
4:      $p_2 \leftarrow \infty$
5:      for each pair $(k, \ell) \in T$ in the increasing order of $P(k, \ell)$ do
6:          if $p_2 < P_2(k, \ell)$ then
7:              return NO
8:          $p_2 \leftarrow P_2(k, \ell)$
9:      return YES

3.1.17 uses superlinear space only to store the array $T$. The array $T$ is first sorted in the increasing order of $P(k, \ell) = (P_1(k, \ell), -P_2(k, \ell))$, and then the algorithm once iterates over its elements in Line 5. Thus, we do not need to store the whole array $T$ — it is sufficient to generate all pairs $(k, \ell)$ in the appropriate order. The following technical lemma shows that such iterator exists and uses only $O(s)$ space. The proof of this lemma is postponed to the end of this section.

**Lemma 3.1.18.** There exists an algorithm that, given a set $S$ of $s$ positive integers, generates a sequence of pairs $(k, \ell) \in S \times S$ in the increasing order of

$$P(k, \ell) = (P_1(k, \ell), -P_2(k, \ell)).$$

The algorithm consists of the initialization procedure `initializeIterator` that uses $O(s \log s)$ time and the generating procedure `nextStep`. Each call to `nextStep` returns a subsequent pair $(k, \ell) \in S \times S$ in the increasing order of $P(k, \ell)$ and uses $O(s \log s)$ time. The algorithm uses $O(s)$ additional space.

Combining Lemma 3.1.17 and Lemma 3.1.18 we obtain the final theorem [3].

**Theorem 3.1.19.** There exists an algorithm that checks whether a given set of positive integers $S$ is good and requires $O(s^2 \log s)$ time and $O(s)$ space.

**Proof.** We use the algorithm of Lemma 3.1.17, but instead of the array $T$ we use iterator described in Lemma 3.1.18. Thus, instead of lines 2–3 of Pseudocode 3.1.1 we call the procedure `initializeIterator` and in Line 5 we repeatedly call the procedure `nextPair` instead of iterating over the array $T$.

The iterator uses $O(s)$ space. The `initializeIterator` call uses $O(s \log s)$ time and each of $s^2$ calls to `nextPair` uses $O(\log s)$ time. Thus, the total running time of this algorithm is $O(s^2 \log s)$. \hfill \qed
We are left with the technical proof of Lemma 3.1.18.

Algorithm 3.1.2 An iterator of pairs \((k, \ell) \in S\) in the increasing order of \(P(k, \ell)\).

```
1: procedure InitializeIterator(S)
2:     S[1 \ldots s] \leftarrow \text{sorted set } S
3:     H \leftarrow \text{an empty binary heap, storing pairs of integers } (a, b), \text{ and sorting according}
4:         \text{to key } P(S[a], S[b]), \text{ with the smallest key on the top}
5:     for a := 1 to s do
6:         H \leftarrow H \cup (a, 1)
7: procedure NextPair
8:     (a, b) \leftarrow \text{minimum element of } H
9:     remove the minimum element of H
10:    if b < s then
11:        H \leftarrow H \cup (a, b + 1)
12:    return (S[a], S[b])
```

Proof of Lemma 3.1.18. First observe that for each \(k \in S\), if \(\ell < \ell'\), the algorithm should first provide the pair \((k, \ell)\) before the pair \((k, \ell')\). Thus, for a fixed \(k\), the pairs \((k, \ell)\) should be generated in the increasing order of \(\ell\).

We make use of this observation in our algorithm. The idea is to store, for each \(k \in S\), the element \(\ell(k) \in S\) such that from all pairs with \(k\) in the first coordinate the pair \((k, \ell(k))\) should be generated next. At each call to NextPair we choose the pair \((k, \ell(k))\) with the smallest value of \(P(k, \ell(k))\). We use standard binary heap to extract this pair in \(O(\log s)\) time. The space complexity is \(O(s)\), since for each \(k \in S\) we store only one pair \((k, \ell(k))\) in the heap.

Let us now analyze this algorithm, described in Pseudocode 3.1.2, in greater details. In the initialization part we first sort the set \(S\) and store it in an array \(S[1 \ldots s]\). The algorithm uses a standard binary heap that stores pairs of indices \((a, b) \in \{1, 2, \ldots, s\} \times \{1, 2, \ldots, s\}\) and sorts them according to the key \(P(S[a], S[b])\). A pair \((a, b)\) in the heap means that the algorithm has not yet generated pair \((S[a], S[b])\), but has already generated all pairs \((S[a], S[b'])\) for \(1 \leq b' < b\). Thus, for each \(a\), the heap contains the pair \((a, b)\) that corresponds to the pair \((S[a], S[b])\) that should be the first generated pair with \(S[a]\) on the first coordinate. At each step of the iterator (i.e., at each call to the NextPair procedure) we simply return the minimum element of the heap \(H\) and update the heap.

The initialization costs \(O(s \log s)\) time and uses \(O(s)\) space for the array \(S[1 \ldots s]\). At every time there is at most one pair \((a, b)\) for each \(1 \leq a \leq s\) stored in the heap \(H\), so the
heap $H$ uses $O(s)$ space. Each call to \texttt{NextPair} results in a few operations on the heap $H$, thus each call needs $O(\log s)$ time. In total, we consumed $O(s^2 \log s)$ time to generate all pairs.

3.1.7 Zagreb indices equality

In spite of an extensive research on inequality (3.1), little attention was paid on the equality case, i.e., on the characterization of graphs for which

$$M_1/n = M_2/m.$$  \hfill (3.8)

We say that a graph $G$ is \textit{biregular} if its vertex degrees assume exactly two distinct values, say $d_a$ and $d_b$, \((d_a \neq d_b). \) Let the number of vertices of degree $d_a$ and $d_b$ be $a$ and $b$, respectively. By definition, $a > 0$, $b > 0$, and we may assume that $a \leq b$. We distinguish between two types of biregular graphs: \textit{Biregular graphs of class 1} have the property that no two vertices of the same degree are adjacent. A \textit{biregular graph of class 2} contains at least one edge connecting vertices of equal degree. Biregular graphs of class 1 are necessarily bipartite. The complete bipartite graphs $K_{a,b}$ belong to class 1. Recall that for all biregular graphs Zagreb indices inequality holds.

In [106] we prove the following two theorems.

**Theorem 3.1.20.** Every biregular graph of class one satisfies Zagreb indices equality, no biregular graph of class 2 satisfies Zagreb indices equality

Let $a$, $b$ and $c$ be three positive integers, $1 \leq a < b < c \leq n - 1$. The graph $G$ is said to be \textit{triregular} if for $1, 2, \ldots, n$, either $d_i = a$ or $d_i = b$ or $d_i = c$, and $G$ is neither regular or biregular.

If so, then $G$ is a triregular graph of degrees $a$, $b$ and $c$, or for brevity, an $(a,b,c)$-triregular graph. Similarly, as in the case of biregular graphs, we distinguish two types of triregular graphs: \textit{Triregular graphs of class 1} have the property that no two vertices of the same degree are adjacent. In \textit{triregular graphs of class 2} at least one edge connects vertices of equal degree.

**Theorem 3.1.21.** No connected $(a,b,c)$-triregular graph $G$ of class 1 satisfies the Zagreb indices equality. Moreover, every connected $(a,b,c)$-triregular graph $G$ of class 1 satisfies the strict Zagreb indices inequality.
3.1.8 Variable Zagreb indices

The Zagreb indices are generally related to the inequality $M_1(G)/n \leq M_2(G)/m$ and the question: When does this inequality hold? Similarly to this, many mathematicians analyzed the inequality

$$\frac{\lambda M_1(G)}{n} \leq \frac{\lambda M_2(G)}{m}$$

(3.9)

when $\lambda \in [0, 1]$, and showed that it is true for the following cases: all chemical graphs [101], all trees [102], all unicyclic graphs [74]. For more results on this topic see [77, 89, 90, 108].

Vukičević [101] also analyzed the inequality (3.9) and showed that it does not hold for $\lambda \in \left[\frac{\sqrt{2}}{2}, 1\right]$. The case when $\lambda \in \left[\frac{1}{2}, \frac{\sqrt{2}}{2}\right]$ is still an open problem. In the same paper an incomplete proof of the following theorem is given:

**Theorem 3.1.22.** Let $G$ be a arbitrary graph and $\lambda \in [0, \frac{1}{2}]$. Then, $\lambda M_1/n \leq \lambda M_2/m$.

The case when $\lambda \in \left[\frac{1}{2}, \frac{\sqrt{2}}{2}\right]$ was later considered by Bogoev [15].

Since we discuss sufficient conditions for (3.9) to hold, for the sake of simplicity we denote by $m_{i,j}$ the number of edges that connect vertices of degrees $i$ and $j$ in the graph $G$. Then, as shown in [101]:

$$\lambda M_1/n - \lambda M_2/m = \sum_{i \leq j, i, j \in \mathbb{N}} f(i, j)m_{i,j}^2 + \sum_{i \leq j, k \leq \ell \neq (k, \ell)} g(i, j, k, \ell)m_{ij}m_{k\ell},$$

(3.10)

where the functions $f$ and $g$ are defined in the following way:

$$f(i, j) = i^\lambda j^\lambda \left(\frac{1}{i} + \frac{1}{j}\right) - i^{2\lambda-1} - j^{2\lambda-1},$$

(3.11)

and

$$g(i, j, k, \ell) = i^\lambda j^\lambda \left(\frac{1}{k} + \frac{1}{\ell}\right) + k^\lambda \ell^\lambda \left(\frac{1}{i} + \frac{1}{j}\right) - i^{2\lambda-1} - j^{2\lambda-1} - k^{2\lambda-1} - \ell^{2\lambda-1}.$$

(3.12)

In order to examine whether the inequality (3.9) holds, one can consider whether $\lambda M_2/m - \lambda M_1/n$ is non-negative. If $f(i, j) < 0$ or $g(i, j, k, \ell) < 0$ for some integers $i, j, k, \ell$, then there is a graph $G$ such that the inequality (3.9) does not hold. The construction of such graph can be done in the same way as the one for Zagreb indices in [101].

The proof of the Theorem 3.1.22 we present in [9] is based on the following two lemmas:

**Lemma 3.1.23.** Let $i$ and $j$ be different natural numbers and let $f(i, j)$ be as in (3.11). Then, $f(i, j) \geq 0$ for $\lambda \in [0, 1]$ and $f(i, j) < 0$ for $\lambda \in \mathbb{R}\setminus[0, 1]$. 
Lemma 3.1.24. Let $i, j, k$ and $\ell$ be different natural numbers and let $\lambda \in [0, \frac{1}{2}]$. Then the function $g(i, j, k, \ell)$ defined by (3.12) in non-negative.

Without loss of generality, we may assume that $i = \max\{j, k, \ell\}$ and that $k \geq \ell$. Now, there are three possible orderings:

\[(a)\ i \geq j \geq k \geq \ell, \quad (b)\ i \geq k \geq j \geq \ell, \quad (c)\ i \geq k \geq \ell \geq j.\]

The cases (a) and (b) are proven in [101]. Even more, for these orderings we have $g(i, j, k, \ell) \geq 0$ for all $\lambda \in [0, 1]$.

The incompleteness in the proof of Lemma 3.1.24 is for the third ordering. Namely, $\frac{\partial g(i, j, k, \ell)}{\partial i}$ is not non-negative [101] in the case (c).

By the above discussion, one can easily see that the main problem here is determining the sign of $g$ for $\lambda \in [0, \frac{1}{2}]$. In order to do that, we will use some already known results [78].

Lemma 3.1.25 (Karamata’s inequality). Let $U \subseteq \mathbb{R}$ be an open interval and $f : U \to U$ be a convex function. Let $a_1 \geq a_2 \geq \cdots \geq a_n$ and $b_1 \geq b_2 \geq \cdots \geq b_n$ be elements of $U$ such that $a_1 + a_2 + \cdots + a_i \geq b_1 + b_2 + \cdots + b_i$ for every $i \in \{1, 2, \ldots, n\}$ with equality for $i = n$. Then $f(a_1) + f(a_2) + \cdots + f(a_n) \geq f(b_1) + f(b_2) + \cdots + f(b_n)$.

Since monotonicity of the $a_i$’s only strengthens the majorizing conditions $a_1 + a_2 + \cdots + a_i \geq b_1 + b_2 + \cdots + b_i$ for every $i \in \{1, 2, \ldots, n\}$ with equality for $i = n$, we have that the same inequality holds without any restrictions on order on the $a_i$’s.

If in addition $U = \mathbb{R}$ and the function $f$ is non-decreasing on $U$, then the majorizing conditions can be further relaxed from "with equality for $i = n". Namely if $a_1 + a_2 + \cdots + a_n > b_1 + b_2 + \cdots + b_n$, then we take $a'_n = b_1 + b_2 + \cdots + b_n - a_1 - a_2 - \cdots - a_{n-1}$. Replacing $a_n$ with $a'_n$ the conditions of Kramata’s are satisfied and also $f(a_n) \geq f(a'_n)$, which goes on our hand.

These comments explain how the following is derived from Lemma 3.1.25.

Lemma 3.1.26 (Majorizing inequality). Let $f : \mathbb{R} \to \mathbb{R}$ be a non-decreasing convex function. Let $a_1, a_2, \ldots, a_n$ and $b_1 \geq b_2 \geq \cdots \geq b_n$ be reals such that $a_1 + a_2 + \cdots + a_i \geq b_1 + b_2 + \cdots + b_i$ for every $i \in \{1, 2, \ldots, n\}$. Then $f(a_1) + f(a_2) + \cdots + f(a_n) \geq f(b_1) + f(b_2) + \cdots + f(b_n)$.

A Lemma 3.1.26 will be are use to prove the following result.

Theorem 3.1.27. Let $a, b, c, d \in \mathbb{R}^+$ and $x \in [0, \frac{1}{2}]$. Then

$$a^x b^x \left(\frac{1}{c} + \frac{1}{d}\right) + c^x d^x \left(\frac{1}{a} + \frac{1}{b}\right) \geq a^{2x-1} + b^{2x-1} + c^{2x-1} + d^{2x-1}.$$
Proof. Put \( A = -\log_t a, B = -\log_t b, C = -\log_t c, D = -\log_t d \), for a fixed real \( t > 1 \). Then this inequality takes on the form

\[
t^A - (C+D)x + t^B - (C+D)x + t^C - (A+B)x + t^D - (A+B)x \geq t^{(1-2x)A} + t^{(1-2x)B} + t^{(1-2x)C} + t^{(1-2x)D}.
\]

Put \( a_1 = A - (C+D)x, a_2 = B - (C+D)x, a_3 = C - (A+B)x, a_4 = D - (A+B)x \) and \( b_1 = (1-2x)A, b_2 = (1-2x)B, b_3 = (1-2x)C, b_4 = (1-2x)D \).

Without loss of generality we can take that \( A \geq B, C, D \) and \( C \geq D \). There are three cases to be considered regarding how \( B \) is positioned to \( C, D \):

1. If \( B \geq C \), then \( A \geq B \geq C \geq D \). Since \( x \in [0, 1/2] \) \((x \geq 0 \text{ and } 1-2x \geq 0)\), it is obvious that \( b_1 \geq b_2 \geq b_3 \geq b_4 \) and \( \sum_{i=1}^{j} a_i \geq \sum_{i=1}^{j} b_i \), for \( j = 1, 2, 3, 4 \). So now the sequences \( a_1, a_2, a_3, a_4 \) and \( b_1, b_2, b_3, b_4 \) satisfy the conditions for the majorizing inequality.

Similarly to case (1) the orderings of \( a \)'s and \( b \)'s for the other two cases are:

2. if \( C \geq B \geq D \), then \( A \geq C \geq B \geq D \), and \( a_1, a_3, a_2, a_4 \) and \( b_1, b_3, b_2, b_4 \);

3. if \( D \geq B \), then \( A \geq C \geq D \geq B \), and \( a_1, a_3, a_4, a_2 \) and \( b_1, b_3, b_4, b_2 \);

and they satisfy the conditions for the majorizing inequality. \( \square \)

Proof of Theorem 3.1.22. By Theorem 3.1.25 we have that the function \( g(i, j, k, \ell) \) is non-negative for any positive integers \( i, j, k, \ell \) and every \( \lambda \in [0, 1/2] \). By Lemma 3.1.23, the function \( f(i, j) \) is also non-negative for \( \lambda \in [0, 1/2] \subset [0, 1] \). Since \( f \) and \( g \) are non-negative for \( \lambda \in [0, 1/2] \) we have \( \lambda M_2/m - \lambda M_1/n \geq 0 \) i.e., \( \lambda M_1/n \leq \lambda M_2/m \). This completes the proof. \( \square \)
3.2 $R'$ index

One of the most used indices is Randić index, and it is defined as follows:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) \cdot d_G(v)}}.$$  

There are several conjectures connecting Randić index to other graph parameters, like radius and diameter. Fajtlowicz in [48] proposed the following problem:

**Conjecture 3.2.1.** For every connected graph $G$, it holds $R(G) \geq \text{rad}(G) - 1$.

Regarding the diameter, Aouchiche at al. [12] conjectured the following:

**Conjecture 3.2.2.** Any connected graph $G$ of order $n \geq 3$ satisfies

$$R(G) - \text{diam}(G) \geq \sqrt{2} - \frac{n + 1}{2} \quad \text{and} \quad \frac{R(G)}{\text{diam}(G)} \geq \frac{n - 3 + 2\sqrt{2}}{2n - 2}.$$  

Instead of working with Randić index Dvořák et al. [44] introduced a one modification and worked with it. They introduced a new index $R'(G)$ defined as:

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_G(u), d_G(v)\}}.$$  

Note that $R(G) \geq R'(G)$ for every graph $G$, with the equality achieved only if every connected component of $G$ is regular. Using this index they have shown that $R'(G) \geq \text{diam}(G)/2$, and since $\text{diam}(G) \geq \text{rad}(G)$, immediately follows that $R(G) \geq \text{rad}(G)/2$, where $\text{rad}(G)$ is the radius of $G$.

Although no application of the index $R'$ in chemistry is known so far, still this index turns out to be very useful, especially from mathematical point of view, since it is much easier to follow during graph modifications than Randić index. Using $R'$ index, Cygan et al. [29] proved that for any connected graph $G$ of maximum degree at most four with the exception of a path with even number of vertices, $R(G) \geq \text{rad}(G)$. As a consequence, they resolve the conjecture $R(G) \geq \text{rad}(G) - 1$ given by Fajtlowicz [49] in 1988 for the case when $G$ is a chemical graph. They actually showed that for all connected chemical graphs $G$ the inequality $R'(G) \geq \text{rad}(G) - \frac{1}{2}$ holds.

Let $v$ be a vertex of a graph $G$. The graph $G - v$ is obtained from $G$ when $v$ and all edges incident to $v$ are removed. By $G^+$ we denote a graph obtained from $G$ by adding one edge joining two vertices of degree 1. If $G$ is a tree then $G^+$ is a unicyclic graph. Observe that $G^+$ is not determined uniquely. A subdivision of an edge is a replacement of this edge by a path of positive length. Of course, all internal vertices of this new path have degrees 2. A graph $H$ is a subdivision of $G$ if $H$ arises by subdivision of some edges of $G$. 
3.2.1 Basic properties of $R'$

Here we present some basic properties of $R'$. From the definition of $R'$, it is obvious that if $G$ is not connected, then $R'(G)$ is the sum of the $R'$ indices of its components. Therefore, in what follows we consider only connected graphs. We start with upper and lower bounds for $R'$ in general graphs.

**Proposition 3.2.1.** Let $G$ be a graph on $n \geq 2$ vertices. Then, $R'(G) \leq R(G) \leq \frac{n}{2}$. Moreover, $R'(G) = \frac{n}{2}$ if and only if $G$ is a regular graph.

**Proof.** From the definitions of $R$ and $R'$ it is obvious that $R(G) \geq R'(G)$. It is known that among all connected graphs of order $n$, regular graphs attain the maximum Randić index [20], and in that case $R'(G) = R(G) = \frac{n}{2}$. Now, let $R'(G) = \frac{n}{2}$. Then $R(G) = \frac{n}{2}$ as well, and using the result in [20] we obtain the statement. \qed

To obtain a lower bound for $R'$ we need the following lemma. Recall that all our graphs are connected.

**Lemma 3.2.2.** Let $G$ be a graph on at least 2 vertices. Further, let $S$ be an independent set of vertices of $G$, such that for every $u, v \in V(G)$, where $v \in S$ and $uv \in E(G)$, we have $d_G(u) \leq d_G(v)$. Denote by $E_S$ those edges $xy$ of $G$ for which neither $x$ nor $y$ is in $S$. Then

$$R'(G) = |S| + \sum_{uv \in E_S} \frac{1}{\max\{d_G(u), d_G(v)\}}.$$

**Proof.** Let $v \in S$. Denote by $E_v$ the edges of $G$ incident to $v$. Then $\{E_v : v \in S\} \cup \{E_S\}$ is a partition of $E(G)$. Since every edge of $E_v$ contributes to $R'(G)$ precisely $1/d_G(v)$ and since there are $d_G(v)$ edges in $E_v$, we have

$$R'(G) = \sum_{v \in S} \left( \sum_{uv \in E_v} \frac{1}{\max\{d_G(u), d_G(v)\}} \right) + \sum_{uv \in E_S} \frac{1}{\max\{d_G(u), d_G(v)\}}$$

$$= |S| + \sum_{uv \in E_S} \frac{1}{\max\{d_G(u), d_G(v)\}}.$$

\qed

Since the contribution of every edge to $R'$ is positive, Lemma 3.2.2 can be used to bound $R'$.

**Corollary 3.2.3.** Let $G$ be a graph on at least 2 vertices. Further, let $S$ be an independent set of vertices of $G$, such that for every $u, v \in V(G)$, where $v \in S$ and $uv \in E(G)$, we have $d_G(u) \leq d_G(v)$. Then $R'(G) \geq |S|$.
We can now obtain the following consequence of Corollary 3.2.3 and Lemma 3.2.2.

**Corollary 3.2.4.** For every graph $G$ on at least 2 vertices we have $R'(G) \geq 1$. Moreover, $R'(G) = 1$ if and only if $G$ is the star $S_n$.

**Proof.** Let $S$ consist of a single vertex $v$ of maximum degree in $G$. Then $d_G(u) \leq d_G(v)$ for every $uv \in E(G)$, so that $R'(G) \geq 1$ for every graph $G$ on at least 2 vertices by Corollary 3.2.3.

On the other hand, if $R'(G) = 1$ then all the edges of $G$ must be incident to $v$, by Lemma 3.2.2. Hence, if $R'(G) = 1$ then $G$ is a star. □

By using different methods, Bollobás and Erdős [16], and Pavlović and Gutman [93] independently showed that among all graphs of order $n$ without isolated vertices, the star $S_n$ attains the minimum Randić index as well, and $R(S_n) = \sqrt{n - 1}$.

Lemma 3.2.2 gives an interesting bound for trees with small diameter.

**Corollary 3.2.5.** Let $T$ be a tree of order $n$, $n \geq 3$, and let $v$ be an internal vertex of $T$ with minimal degree. Denote $k = d_T(v)$ and denote by $l$ the number of leaves adjacent to $v$. Then, $R'(G) \geq k - l + \frac{l}{k}$.

**Proof.** Denote $T_0 = T - v$. Then $T_0$ is a disconnected graph and $k - l$ components of $T_0$ have at least one edge. Denote these components by $T_1, T_2, \ldots, T_{k-l}$. Since $v$ is an internal vertex with minimal degree, each $T_i$, $1 \leq i \leq k - l$, contains a vertex $u_i$ such that $d_T(u_i) \geq d_T(x)$ for every vertex $x$ such that $xu_i \in E(T)$. As $u_iu_j \notin E(T)$ for $1 \leq i < j \leq k - l$, the set $S = \{u_1, u_2, \ldots, u_{k-l}\}$ satisfies the assumptions of Lemma 3.2.2. Since the pendant edges incident with $v$ contain none of $u_1, u_2, \ldots, u_{k-l}$, we have $R'(T) \geq (k - l) + \frac{l}{k}$ by Lemma 3.2.2. □

As we show in Table 1, the bound of Corollary 3.2.5 is tight. Next lemma shows that removing a vertex of degree 1 does not increase the value of $R'$.

**Lemma 3.2.6.** Let $G_1$ be a connected graph on at least 3 vertices and let $v \in V(G_1)$ such that $d_{G_1}(v) = 1$. Denote $G_2 = G_1 - v$. Let $u$ be the unique neighbor of $v$. Denote $a = d_{G_1}(u)$ and denote by $l$ the number of neighbors of $u$ whose degree is at least $a$. Then

$$R'(G_1) - R'(G_2) = \frac{l}{a(a - 1)}.$$ 

**Proof.** When $v$ is removed, the degree of $u$ decreases by 1 while the vertices of $V(G_1) \setminus \{u, v\}$ have the same degree in $G_2$ as in $G_1$. Hence, only edges incident with $u$ affect the difference
Let \( x_1, x_2, \ldots, x_l \) be neighbors of \( u \) such that \( d_{G_1}(x_i) \geq d_{G_1}(u) \) for \( i = 1, 2, \ldots, l \). Then

\[
R'(G_1) - R'(G_2) = \frac{a - l}{a - 1} - \frac{1}{a - 1} + \left( \frac{1}{d_{G_1}(x_1)} + \frac{1}{d_{G_1}(x_2)} + \cdots + \frac{1}{d_{G_1}(x_l)} \right) - \left( \frac{a - l - 1}{a - 1} + \left( \frac{1}{d_{G_2}(x_1)} + \frac{1}{d_{G_2}(x_2)} + \cdots + \frac{1}{d_{G_2}(x_l)} \right) \right) = \frac{a - l}{a - 1} - \frac{1}{a - 1} + l \frac{1}{a(a - 1)},
\]

which completes the proof.

Using the previous result we describe a situation when a leaf is removed from his position and it is attached to another leaf. Next lemma shows that in this case the value of \( R' \) is not decreasing.

**Lemma 3.2.7.** Let a connected graph \( G_1 \) have at least four vertices, let \( v \) be a vertex of degree 1 in \( G_1 \) and let \( u \) be its neighbor. Denote \( a = d_{G_1}(u) \) and denote by \( l \) the number of neighbors of \( u \) whose degree is at least \( a \). Denote \( G_2 = G_1 - v \). Let \( w \) be a vertex of degree 1 in \( G_2 \) and let \( G_3 \) be a graph obtained by attaching a pendant edge to \( w \). Then

\[
R'(G_3) - R'(G_1) = \frac{1}{2} - \frac{l}{a(a - 1)} \geq 0.
\]

**Proof.** By Lemma 3.2.6, \( R'(G_1) - R'(G_2) = \frac{l}{a(a - 1)} \). Now we calculate \( R'(G_3) - R'(G_2) \). Since \( G_2 \) has at least 3 vertices, there is a unique neighbor of \( w \) whose degree is at least 2 in \( G_3 \). Since the degree of \( w \) is 2 in \( G_3 \), by Lemma 3.2.6 we have \( R'(G_3) - R'(G_2) = \frac{1}{2} \). Hence,

\[
R'(G_3) - R'(G_1) = \left( R'(G_3) - R'(G_2) \right) - \left( R'(G_1) - R'(G_2) \right) = \frac{1}{2} - \frac{l}{a(a - 1)} \geq \frac{1}{2} - \frac{1}{a} \geq 0,
\]

as \( a > l \geq 0 \) and \( a \geq 2 \). \( \square \)

### 3.2.2 Unicyclic graphs and trees

Here we determine trees and unicyclic graphs attaining the smallest (the greatest) values of \( R' \). We start with their definition.

By \( D_{k,n} \) we denote a double star on \( n \) vertices, i.e., a tree having one vertex of degree \( k \), one vertex of degree \( n - k \) and \( n - 2 \) leaves. By \( S_{k,n} \) we denote a tree of order \( n \) which is a subdivision of the star \( S_k \). Hence, \( S_{k,n} \) has one vertex of degree \( k - 1 \), every other vertex
has degree either 1 or 2. Observe that the graph of double star $D_{3,6}$ resembles the letter H. Therefore by $H_{k,n}$ we denote a subdivision of $D_{3,6}$ on $n$ vertices in which the vertices of degree 3 are joined by a path of length $k$.

By $B_{k,n}^S$ we denote the unicyclic graph obtained from a triangle by identifying centers of two stars, $S_k$ and $S_{n-k-1}$, with two different vertices of the triangle. Observe that $B_{k,n}^S$ has one vertex of degree $k+1$, one vertex of degree $n-k$, one vertex of degree 2 and $n-3$ vertices of degree 1. Note that $B_{k,n}^S = B_{l,n}^S$ for $l = n-k-1$. Analogously, by $B_{n}^P$ (and $D_{n}^P$) we denote the unicyclic graph on $n$ vertices obtained from a triangle (a quadrangle) by identifying end-vertices of two paths with two different vertices of the triangle (with two nonadjacent vertices of the quadrangle). Then both $B_{n}^P$ and $D_{n}^P$ have two vertices of degree 3, 2 vertices of degree 1 and $n-4$ vertices of degree 2. Finally, by $Y_{n}^P$ we denote the unicyclic graph on $n$ vertices obtained from a triangle by identifying end-vertices of three distinct paths with three distinct vertices of the triangle. Then $Y_{n}^P$ has three vertices of degree 3, three vertices of degree 1 and $n-6$ vertices of degree 2.

First we discuss trees on $n$ vertices, $n \geq 2$, with smallest value of $R'$.

**Proposition 3.2.8.** Let $T$ be a tree on at least 2 vertices. Then, $R'(T) \geq 2$ if and only if $\text{diam}(T) > 3$. Moreover, if $\text{diam}(T) = 3$ then $R'(T) = 2 - \frac{1}{a}$, where $a$ is the smallest degree in $T$ which is greater than 1.

**Proof.** We distinguish three cases. Suppose first that $\text{diam}(T) \leq 2$. Since $T$ has at least 2 vertices, $T$ is a star $S_n$ and $R'(S_n) = 1$ by Corollary 3.2.4.

Suppose now that $\text{diam}(T) = 3$. Then $T$ has exactly 2 vertices, say $u$ and $v$, whose degree is greater than 1, and moreover, these two vertices are adjacent. All the other vertices have degree 1. Hence, $T$ is a double star. Assume that $d_T(u) \geq d_T(v)$. Then

$$ R'(T) = \sum_{ux \in E(T)} \frac{1}{d_T(u)} + \sum_{vy \in E(T) \setminus \{vu\}} \frac{1}{d_T(v)} = 2 - \frac{1}{d_T(v)}. $$

Finally, suppose that $\text{diam}(T) \geq 4$. Then there are vertices $x$ and $y$ such that $d_G(x, y) = 4$. Therefore, there is a path $P : xv_1v_2v_3y$ of length 4 in $T$. Applying Lemma 3.2.6, we can remove vertices from $T$, one by one, until we obtain the path $P$. By Lemma 3.2.6, $R'(T) \geq R'(P)$. Since for $S = \{v_1, v_3\}$ we get $R'(P) = 2$ by Lemma 3.2.2, we have $R'(T) \geq 2$. \qed

By Proposition 3.2.8, if $T$ is not a star and $R'(T) < 2$, then $\text{diam}(T) = 3$. Hence, the trees with smallest values of $R'$ and the corresponding values of $R'$ are given in Table 1,
where $k = \lfloor n/2 \rfloor$. We remark that the next value of $R'(T)$ is 2 but there are more types of trees attaining this value.

<table>
<thead>
<tr>
<th>$G$</th>
<th>$S_n$</th>
<th>$S_{n-1,n}$</th>
<th>$D_{3,n}$</th>
<th>$D_{4,n}$</th>
<th>$D_{5,n}$</th>
<th>$\ldots$</th>
<th>$D_{k,n}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R'(G)$</td>
<td>1</td>
<td>$3/2$</td>
<td>$5/3$</td>
<td>$7/4$</td>
<td>$9/5$</td>
<td>$\ldots$</td>
<td>$(2k - 1)/k$</td>
</tr>
</tbody>
</table>

Table 1. Trees with smallest values of $R'$.

As mentioned above, $S_n$ attains minimum Randić index among all trees on $n$ vertices and $R(S_n) = \sqrt{n - 1}$.

For unicyclic graphs we use the following proposition.

Proposition 3.2.9. Let $C$ be the unique cycle in a connected unicyclic graph $G$. If the length of $C$ is at least 4, or if $G$ has a vertex at distance at least 2 to $C$, or if the length of $C$ is 3 and all the vertices of $C$ have degrees at least 3 in $G$, then $R'(G) \geq 2$. On the other hand, $R'(S_n^+) = \frac{3}{2}$ and $R'(B_{k,n}^S) = \frac{2k + 1}{k + 1}$, where $2 \leq k \leq n - k - 1$.

Proof. Denote $G_0 = G$. Remove a vertex of degree 1 from $G_0$ and denote the resulting graph by $G_1$. Repeat removing of vertices of degree 1 to obtain $G_2, G_3, \ldots$ until we get a graph $G_r = C$. By Lemma 3.2.6, we have $R'(G_0) \geq R'(G_1) \geq \cdots \geq R'(G_r)$. By Proposition 4.2.8, if $C$ has length $c$ then $R'(G_r) = R'(C) = \frac{c}{2}$. Hence, if $c \geq 4$ then $R'(G_r) \geq 2$ and consequently $R'(G) \geq 2$. In what follows suppose that $C$ has length 3. Then $R'(G_r) = R'(C) = \frac{3}{2}$.

If $G = S_n^+$ then all vertices of degree 1 are adjacent to one vertex, say $u$, of $C$. Since there is a unique edge which is not incident with $u$ in $G$ and both endvertices of this edge have degrees 2, we have $R'(S_n^+) = \frac{3}{2}$ by Lemma 3.2.2.

If there is a vertex at distance at least 2 from $C$, then there exists $G_t, 0 \leq t < r$, such that to obtain $G_{t+1}$ we remove a vertex adjacent to a vertex of degree 2. Then $R'(G_t) - R'(G_{t+1}) = \frac{1}{2}$, by Lemma 3.2.6, and hence $R'(G) \geq 2$. Thus, in the following we may assume that all vertices of $V(G) - V(C)$ have degree 1 and are adjacent to a vertex of $C$.

Suppose that there are exactly two vertices of $C$, say $u$ and $v$, whose degrees are greater than 2. Assume that $d_G(u) \geq d_G(v)$. Then all the edges of $G$ are incident to $u$ or $v$, so that

$$R'(G) = \sum_{ux \in E(T)} \frac{1}{d_T(u)} + \sum_{vy \in E(T) \setminus \{uv\}} \frac{1}{d_T(v)} = 2 - \frac{1}{d_T(v)},$$

i.e., $R'(B_{k,n}^S) = \frac{2k + 1}{k + 1}$ with $2 \leq k \leq n - k - 1$. Observe that in any case $R'(G) \geq 2 - \frac{1}{3}$. 


Finally, suppose that all the vertices of \( C \) have degree at least 3 in \( G \). Then there is a smallest \( t \) such that \( G_{t+1} = B^S_{k,n} \) for some \( k \). By Lemma 3.2.6 we have \( R'(G_t) - R'(G_{t+1}) = \frac{1}{3} \). As \( R'(G_{t+1}) \geq 2 - \frac{1}{3} \), we have \( R'(G) \geq 2 \). \( \square \)

Table 2 contains unicyclic graphs with greatest values of \( R' \) and the corresponding values of \( R' \) according to Proposition 3.2.9. We remark that the next value of \( R' \) in a unicyclic graph is 2, but as it can be seen from the proof of Proposition 3.2.9, there are more types of unicyclic graphs \( G \) for which \( R'(G) = 2 \).

Gao and Lu [58] show that among all unicyclic graphs, \( S^\pm_n \) also attains minimum for Randić index, \( R(S^\pm_n) = \frac{n-3+\sqrt{7}}{\sqrt{n-1}} + \frac{1}{2} \).

<table>
<thead>
<tr>
<th>( G )</th>
<th>( S^\pm_n )</th>
<th>( B^S_{2,n} )</th>
<th>( B^S_{3,n} )</th>
<th>( B^S_{4,n} )</th>
<th>( \ldots )</th>
<th>( B^S_{k,n} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R'(G) )</td>
<td>3/2</td>
<td>5/3</td>
<td>7/4</td>
<td>9/5</td>
<td>( \ldots )</td>
<td>( (2k+1)/(k+1) )</td>
</tr>
</tbody>
</table>

Table 2. Unicyclic graphs with smallest values of \( R' \). In the last column \( k = \lfloor (n-1)/2 \rfloor \).

Now we turn our attention to trees with greatest values of \( R' \). Caporossi et al. [20] have shown that among all trees on \( n \) vertices, the path \( P_n \) attains the maximum value of Randić index. In the same paper they prove that \( S_{4,n} \) attains the second maximum value of Randić index, \( R(P_n) = \frac{n-1}{2} + \sqrt{2} - 1 \).

Next proposition shows that the same holds for \( R' \) as well.

<table>
<thead>
<tr>
<th>( G )</th>
<th>( P_n )</th>
<th>( S_{4,n} )</th>
<th>( H_{1,n} )</th>
<th>( H_{k,n}, S_{5,n} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R'(G) )</td>
<td>( (n-1)/2 )</td>
<td>( (n-2)/2 )</td>
<td>( (n-2)/2 - 1/3 )</td>
<td>( (n-3)/2 )</td>
</tr>
</tbody>
</table>

Table 3. Trees with greatest values of \( R' \).

**Proposition 3.2.10.** The trees listed in Table 3, where \( k \geq 2 \), attain the greatest values of \( R' \). All the remaining trees on \( n \) vertices have \( R' \) strictly smaller than \( (n-3)/2 \).

**Proof.** Let \( T = T_0 \) be any tree on \( n \) vertices different from the trees present in Table 3, and let \( P^0 \) be a longest path in \( T_0 \). Take a leaf \( u_0 \) which is not on \( P^0 \), remove it from \( T_0 \), join it by an edge to an endvertex of \( P^0 \) and denote the resulting graph by \( T_1 \). Repeating this process we get a sequence of trees \( T_0, T_1, \ldots, T_r \), such that \( T_r = P_n \). By Lemma 3.2.7, we have \( R'(T_0) \leq R'(T_1) \leq \cdots \leq R'(T_r) \). Moreover, by Lemma 3.2.7 again, if \( u_i \) is adjacent to a vertex of degree 2 in \( T_i \), \( 0 \leq i < r \), then \( R'(T_i) = R'(T_{i+1}) \), otherwise \( R'(T_i) < R'(T_{i+1}) \). Since \( u_{r-1} \) is adjacent to a vertex of degree 3 in \( T_{r-1} \), the path \( P_n = T_r \) is the unique tree
on \( n \) vertices achieving the maximum value of \( R' \). As \( \Delta(P_n) = 2 \) and every edge of \( P_n \) is incident to a vertex of degree 2, we have \( R'(P_n) = \frac{n-1}{2} \).

From the discussion above it is obvious that the tree with the second greatest value of \( R' \) is \( T_{r-1} \). By Lemma 3.2.7 if a leaf incident to a vertex of degree 2 is removed and joined to another leaf, then the value of the \( R' \) index is not changing. Hence, all trees with one vertex of degree 3, and all others of degree 2 and 1 attain the second greatest value of \( R' \). Let \( s \) be the greatest value, \( 0 \leq s < r - 1 \), such that \( u_s \) is adjacent to a vertex of degree at least 3. Then \( T_{s+1}, T_{s+2}, \ldots, T_{r-1} \) all are subdivisions of \( S_4 \). Since \( R'(S_{4,n}) = \frac{n-2}{2} \), we have \( R'(T_{s+1}) = R'(T_{s+2}) = \cdots = R'(T_{r-1}) = \frac{n-2}{2} \) and \( R'(T_s) < R'(T_{s+1}) \).

Now, we are going backwards in the sequence of trees \( T_s, T_{s-1}, \ldots, T_0 \). Since \( S_{4,n} \), a subdivision of the star \( S_4 \), attains the second greatest value of \( R' \), it is clear that the third greatest value will be attained for a tree with two vertices, \( v_1 \) and \( v_2 \), of degree 3, or one vertex of degree 4 and all others of degree 2 and 1. So, candidates for graph attaining the third greatest value of \( R' \) are \( H_{1,n} \), if \( v_1 \) and \( v_2 \) are adjacent, \( H_{k,n} \) where \( k \geq 2 \), if \( v_1 \) and \( v_2 \) are nonadjacent, and \( S_{5,n} \).

Let \( t \) be the greatest value, \( 0 \leq t < s \), such that \( u_t \) is adjacent to a vertex of degree at least 3. Denote by \( v_t \) the unique neighbor of \( u_t \) in \( T_t \). As \( R'(H_{1,n}) = \frac{n-2}{2} - \frac{1}{3} \) and \( R'(H_{k,n}) = R'(S_{5,n}) = \frac{n-3}{2} \) if \( k \geq 2 \), to finish the proof it suffices to show that \( R'(T_t) < \frac{n-3}{2} \).

Since \( R'(T_t) < R'(T_s) \), we can assume that \( T_s = H_{1,n} \). If the degree of \( v_t \) is 4, then \( R'(T_s) - R'(T_t) = R'(T_{t+1}) - R'(T_t) = \frac{1}{2} \), by Lemma 3.2.7, as no neighbor of \( v_t \) has degree at least 4 in \( T_t \). Thus, \( R'(T_t) = \left(\frac{n-2}{2} - \frac{1}{3}\right) - \frac{1}{2} < \frac{n-3}{2} \). On the other hand if the degree of \( v_t \) is 3, then \( R'(T_s) - R'(T_t) \geq \frac{1}{2} - \frac{1}{6} \), by Lemma 3.2.7, as at most one neighbor of \( v_t \) has degree at least 3 in \( T_t \). Thus, \( R'(T_t) \leq \left(\frac{n-2}{2} - \frac{1}{3}\right) - \frac{1}{2} + \frac{1}{6} < \frac{n-3}{2} \).

Finally, we consider unicyclic graphs with the greatest values of \( R' \). Caporossi et al. [20] also considered the maximum values of Randić index in the class of unicyclic graphs. They have shown that among all unicyclic graphs of order \( n \) the cycle \( C_n \) attains the maximum value, \( \frac{n}{2} \). We show that the same holds for \( R' \).

<table>
<thead>
<tr>
<th>( G )</th>
<th>( C_n )</th>
<th>( S_{4,n}^+ )</th>
<th>( H_{1,n}^+, B_n^p )</th>
<th>( H_{k,n}^+, S_{5,n}^+, D_n^p, Y_n^p )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R'(G) )</td>
<td>( n/2 )</td>
<td>( (n-1)/2 )</td>
<td>( (n-1)/2 - 1/3 )</td>
<td>( (n-2)/2 )</td>
</tr>
</tbody>
</table>

Table 4. Unicyclic graphs with greatest values of \( R' \).

**Proposition 3.2.11.** The unicyclic graphs listed in Table 4, where \( k \geq 2 \), attain the greatest values of \( R' \). All the remaining connected unicyclic graphs on \( n \) vertices have \( R' \) strictly smaller than \( (n-2)/2 \).
Proof. First observe that if \( R'(G) = \ell \) then \( R'(G^+) = \ell + \frac{1}{2} \). Therefore \( R'(C_n) = R'(P_n^+) = \frac{n}{2} \), \( R'(S_{4,n}^+) = \frac{n-1}{2} \), \( R'(H_{1,n}^+) = \frac{n}{2} - \frac{1}{3} \) and \( R'(H_{k,n}^+) = R'(S_{5,n}^+) = \frac{n-2}{2} \) if \( k \geq 2 \). Since \( B_n^P \) has 5 edges incident to vertices of degree 3 while every other vertex is incident to a vertex of degree 2, we have \( R'(B_n^P) = \frac{5}{3} + \frac{n-5}{2} \). Finally, as both \( D_n^P \) and \( Y_n^P \) have 6 edges incident to vertices of degree 3 while every other vertex is incident to a vertex of degree 2, we have \( R'(D_n^P) = R'(Y_n^P) = \frac{6}{3} + \frac{n-6}{2} \).

Let \( G \) be a unicyclic graph with the unique cycle \( C \). If the length of \( C \) is \( n \) then \( G = C_n \). Hence, suppose that the length of \( C \) is smaller than \( n \). Denote \( G_0 = G \) and denote by \( P_0 \) a longest path in \( G_0 \). Then at least one vertex of \( P_0 \) has degree 1 and denote the resulting graph by \( G_1 \). Repeating this process we get a sequence of unicyclic graphs \( G_0, G_1, \ldots, G_r \) with \( R'(G_0) \leq R'(G_1) \leq \cdots \leq R'(G_r) \), by Lemma 3.2.7. Observe that \( G_r \) consists of the cycle \( C \) with a path, attached to \( C \) by an endvertex. Analogously as in the proof of Proposition 3.2.10 we get \( R'(G_{r-1}) < R'(G_r) \). As \( G_r = S_{4,n}^+ \), the graph \( S_{4,n}^+ \) has the greatest value of \( R' \) among unicyclic graphs with cycles of length strictly smaller than \( n \).

Now consider \( G_{r-1} \) and denote by \( v_{r-1} \) the unique vertex adjacent to \( u_{r-1} \). If \( d_{G_{r-1}}(v_{r-1}) \) is 4, then \( G_{r-1} = S_{5,n}^+ \). Now suppose that \( d_{G_{r-1}}(v_{r-1}) = 3 \). Denote by \( w \) the other vertex of degree 3 in \( G_{r-1} \). We distinguish six cases:

- \( v_{r-1} \in V(C) \), \( d_{G_{r-1}}(w, v_{r-1}) = 1 \) and \( C = C_3 \): Then \( G_{r-1} = B_n^P \).
- \( v_{r-1} \in V(C) \), \( d_{G_{r-1}}(w, v_{r-1}) = 1 \) and \( C \neq C_3 \): Then \( G_{r-1} = H_{1,n}^+ \).
- \( v_{r-1} \in V(C) \), \( d_{G_{r-1}}(w, v_{r-1}) = 2 \) and \( C = C_4 \): Then \( G_{r-1} = D_n^P \).
- \( v_{r-1} \in V(C) \) and either \( d_{G_{r-1}}(w, v_{r-1}) > 2 \) or \( d_{G_{r-1}}(w, v_{r-1}) = 2 \) and \( C \neq C_4 \): Then \( G_{r-1} = H_{k,n}^+ \) for \( k \geq 2 \).
- \( v_{r-1} \notin V(C) \) and \( d_{G_{r-1}}(w, v_{r-1}) = 1 \): Then \( G_{r-1} = H_{1,n}^+ \).
- \( v_{r-1} \notin V(C) \) and \( d_{G_{r-1}}(w, v_{r-1}) > 1 \): Then \( G_{r-1} = H_{k,n}^+ \) for \( k \geq 2 \).

Observe that in every case \( G_{r-1} \) is a graph presented in Table 4.

Let \( t \) be the greatest value, \( 0 \leq t < r - 1 \), such that \( u_t \) is adjacent to a vertex, say \( v_t \), of degree at least 3. Then \( R'(G_{t+1}) = R'(G_{t+2}) = \cdots = R'(G_{r-1}) \) and \( R'(G_t) < R'(G_{t+1}) \) by Lemma 3.2.7. To finish the proof we have to find all \( G_t \) with \( R'(G_t) \geq \frac{n-2}{2} \) in the case when \( G_{r-1} = H_{1,n}^+ \) or \( G_{r-1} = B_n^P \), see Table 4. If \( d_{G_t}(u_t) = 4 \) then \( R'(G_{r-1}) - R'(G_t) = R'(G_{t+1}) - R'(G_t) = \frac{1}{2} \) because there is no vertex in \( G_t - v_t \) of degree at least 4. Hence let
us assume that \( d_{G_i}(v_t) = 3 \). Observe that \( R'(G_{t+1}) = \frac{n-1}{2} - \frac{1}{3} \) and so \( \frac{n-2}{2} - R'(G_{t+1}) = \frac{1}{6} \). Hence, if \( R'(G_t) \geq \frac{n-2}{2} \), then \( \frac{1}{2} - \frac{l}{a(a-1)} \leq \frac{1}{6} \) by Lemma 3.2.7, where \( a = d_{G_i}(v_t) \) and \( l \) is the number of neighbors of \( v_t \) whose degree is at least 3. This gives \( l = 2 \) and \( R'(G_{t+1}) - R'(G_t) = \frac{1}{6} \). Therefore \( G_{t+1} = B_n^P \) and \( v_t \) is a vertex of \( C = C_3 \). Consequently, \( G_t = Y_n^P \), which finishes the proof.

### 3.2.3 Triangle-free graphs

Favaron et al. [52], showed that for any triangle-free graph \( G \) with \( m \) edges, we have \( R(G) \geq \sqrt{m} \). Later Li and Liu [85] proved the following: For any triangle-free graph \( G \) of order \( n \) and minimum degree \( \delta(G) = k \geq 1 \), we have \( R(G) \geq \sqrt{k(n-k)} \). Equality holds if and only if \( G = K_{k,n-k} \).

In this section we show that if a graph \( G \) on \( n \) vertices has maximum degree at most \( n - \delta(G) \), then \( R'(G) \geq \delta(G) \). Consequently, this gives a lower bound for triangle-free graphs, and this bound is attained by \( K_{k,n-k} \) [8].

**Theorem 3.2.12.** Let \( G \) be a simple graph on \( n \) vertices with \( \delta(G) = k \), \( k \geq 1 \), \( \Delta(G) \leq n - k \), \( n > 2k \), and such that when satisfying all these conditions, \( R'(G) \) is as small as possible. Then \( R'(G) = k \) and \( G = K_{k,n-k} \).

In order to prove Theorem 3.2.12, we extend it to graphs with multiple edges. Hence, suppose that \( G \) is a graph on \( n \) vertices, possibly with multiple edges, with \( \delta(G) = k \), \( k \geq 1 \), \( \Delta(G) \leq n - k \), \( n > 2k \), not necessarily connected, and such that when satisfying all these conditions, the parameter \( R'(G) \) is as small as possible. In the following two lemmas we prove that \( G \) is a bipartite graph with bipartition \( (V_{n-k}(G), V_k(G)) \). Observe that since \( R'(K_{k,n-k}) = k \), we already have \( R'(G) \leq k \).

In the following two Lemmas, we consider graphs that satisfy the conditions of Theorem 3.2.12.

**Lemma 3.2.13.** If \(|V(G)| \leq |V_{n-k}(G)| + |V_k(G)| + 1\), then \(|V(G)| = |V_{n-k}(G)| + |V_k(G)|\) and \( G \) is a bipartite graph with bipartition \( (V_{n-k}(G), V_k(G)) \).

**Proof.** First assume that \(|V(G)| = |V_{n-k}(G)| + |V_k(G)| + 1\). Let \( v \) be the vertex such that \( k < d_G(v) < n - k \). Then \( v \) has neighbors only in \( V_k(G) \) and \( V_{n-k}(G) \). Let \( l = d_G(v) \) and \( \alpha = |N_G(v) \cap V_k(G)| \). Then \(|N_G(v) \cap V_{n-k}(G)| = l - \alpha \). Further, let \( a = |V_k(G)| \) and \( b = |V_{n-k}(G)| \). Finally, assume that there are \( s \) and \( t \) edges whose both endvertices are in \( V_{n-k}(G) \) and \( V_k(G) \), respectively. Counting the number of edges in two ways, namely through their endvertices of “higher”, respectively “smaller” degree gives

\[ |E(G)| = b(n - k) - s + \alpha + t = ak - t + (l - \alpha) + s. \]
Since \(a + b = n - 1\), after dividing by \(n\) we obtain
\[
b = k - \frac{2\alpha}{n} + \frac{l - k}{n} + \frac{2s}{n} - \frac{2t}{n}.
\]
Now we evaluate \(R'(G)\). There are \(b(n - k) - s\) edges with an endvertex in \(V_{n-k}(G)\), \(\alpha\) edges connecting \(v\) with a vertex of \(V_k(G)\) and \(t\) edges connecting two vertices of \(V_k(G)\). Hence,
\[
R'(G) = \frac{b(n - k) - s}{n - k} + \frac{\alpha}{l} + \frac{t}{k},
\]
and after substituting for \(b\) the previous expression we obtain
\[
R'(G) = k + \frac{\alpha}{n} - \frac{2l}{nl} + \frac{l - k}{n} + \frac{s}{n(n - k)} + \frac{t}{nk}.
\]
Since \(n - 2k > 0\), we have \(s\frac{n - 2k}{n(n - k)} + t\frac{n - 2k}{nk} \geq 0\), and as \(l > k\), we have \(\frac{l - k}{n} > 0\). Consider two cases.

- \(n \geq 2l\): Then \(\alpha \frac{n - 2l}{nl} \geq 0\), so that \(R'(G) \geq k + \frac{l - k}{n} > k\).
- \(n < 2l\): Since \(\alpha \leq l\), we have \(\alpha \frac{n - 2l}{nl} \leq \frac{l - 2l}{nl} = 0\). As \(l < n - k\), we have \(R'(G) \geq k + \frac{n - 2l}{n} + \frac{l - k}{n} = k + \frac{n - k - l}{n} > k\).

In both cases we have a contradiction as \(R'(G) \leq k\).

Now consider the case \(|V(G)| = |V_{n-k}(G)| + |V_k(G)|\). Using the notation as above we get
\[
|E(G)| = b(n - k) - s + t = ak - t + s.
\]
Since \(a + b = n\), after dividing by \(n\) we obtain
\[
b = k + \frac{2s}{n} - \frac{2t}{n}.
\]
For \(R'(G)\) we get
\[
R'(G) = \frac{b(n - k) - s}{n - k} + \frac{t}{k},
\]
and after substituting for \(b\) the previous expression we obtain
\[
R'(G) = k + \frac{s}{n} - \frac{2k}{n(n - k)} + \frac{t}{nk}.
\]
Obviously, \(R'(G) \geq k\) with equality only if \(s = t = 0\). Hence, \(G\) is a bipartite graph with bipartition \((V_{n-k}(G), V_k(G))\), as required. \(\square\)
We remark that, although \( G \) is bipartite if the assumptions of Lemma 3.2.13 are satisfied, \( G \) can possibly have multiple edges and does not need to be connected. This assumption is important as in the proof of the next lemma we possibly create multiple edges and we may disconnect the graph.

**Lemma 3.2.14.** We have \(|V(G)| = |V_{n-k}(G)| + |V_k(G)|\).

**Proof.** By Lemma 3.2.13, we cannot have \(|V(G)| = |V_{n-k}(G)| + |V_k(G)| + 1\). Thus, by way of contradiction, suppose that there are \( u, v \in V(G) \), such that \( k < d_G(u) \leq d_G(v) < n-k \). Moreover, assume that among the vertices of \( V(G) \setminus (V_k(G) \cup V_{n-k}(G)) \), the vertex \( u \) has the smallest degree and \( v \) has the greatest degree. Denote \( A(u) = \{wu \in E(G); d_G(w) < d_G(u)\} \) and \( A(v) = \{vz \in E(G); d_G(v) < d_G(z)\} \). Let \( a = \min\{|A(u)|, |A(v)|\} \). Remove \( a \) edges \( uw \in A(u) \) and replace them by \( a \) edges \( uv \); remove \( a \) edges \( vz \in A(v) \) and replace them by \( a \) edges \( uz \); and denote the resulting graph by \( G_0 \). Then \( d_G(x) = d_{G_0}(x) \) for every \( x \in V(G) \). Since \( d_G(u) \leq d_G(v) \), we have \( R'(G_0) \leq R'(G) \).

Denote \( A_0(u) = \{wu \in E(G_0); d_{G_0}(w) < d_{G_0}(u)\} \) and \( A_0(v) = \{vz \in E(G_0); d_{G_0}(v) < d_{G_0}(z)\} \). Then either \( A_0(u) = \emptyset \) or \( A_0(v) = \emptyset \). Consider three cases. Notice that in all three cases the degree of the vertex \( u \) decreases.

- \( A_0(u) \neq \emptyset \): Choose \( uw \in A_0(u) \), remove this edge from \( G_0 \), replace it by \( uv \) and denote the resulting graph by \( G_1 \). Now \( d_{G_1}(u) = d_{G_0}(u) - 1 \) and \( d_{G_1}(v) = d_{G_0}(v) + 1 \). Since \( A_0(u) \neq \emptyset \), we have \( A_0(v) = \emptyset \), and as \( v \) has the maximum degree among the vertices of \( V(G) \setminus (V_k(G) \cup V_{n-k}(G)) \), edges incident with \( v \) in \( G_0 \) contribute by 1 to \( R'(G_0) \), and analogously edges incident with \( v \) in \( G_1 \) contribute by 1 to \( R'(G_1) \). Therefore, to count \( R'(G_0) - R'(G_1) \) it suffices to consider the edges incident with \( u \). Let \( l = |A_0(u)| \) and \( d = d_{G_0}(u) \). As \( u \) has the minimum degree among the vertices of \( V(G) \setminus (V_k(G) \cup V_{n-k}(G)) \), we have \( R'(G_1) = R'(G_0) - \frac{l}{d} + \frac{l-1}{d-1} \). Since \( -\frac{l}{d} + \frac{l-1}{d-1} = \frac{d-ld}{d(d-1)} \leq 0 \), we have \( R'(G_1) \leq R'(G_0) \) with equality only if \( d = l \).

- \( A_0(u) = \emptyset \) and there is an edge \( uv \in E(G_0) \) such that \( uv \neq uw \): Remove the edge \( uv \) from \( G_0 \) and add the edge \( uw \). Denote the resulting graph by \( G_1 \). Analogously as in the previous case, \( d_{G_1}(u) = d_{G_0}(u) - 1 \) and \( d_{G_1}(v) = d_{G_0}(v) + 1 \). Since \( A_0(u) = \emptyset \) and \( u \) has the minimum degree among the vertices of \( V(G) \setminus (V_k(G) \cup V_{n-k}(G)) \), the edges incident with \( u \) contribute to \( R' \) by the same value in \( G_0 \) as in \( G_1 \), with the possible exception of the edge \( uw \), which is now replaced by \( vw \), and its contribution to \( R'(G_1) \) is not greater as its contribution to \( R'(G_0) \). Let \( l = |\{vz \in E(G_0); d_{G_0}(z) \leq d_{G_0}(v)\}| \) and \( d = d_{G_0}(v) \). Then \( R'(G_1) \leq R'(G_0) - \frac{l}{d} + \frac{l-1}{d+1} \leq R'(G_0) \) with equality only if \( l = 0 \) (and \( d_{G_0}(w) > d_{G_0}(v) \)).
\( A_0(u) = \emptyset \) and the only neighbor of \( u \) is the vertex \( v \): Then there are at least \( k+1 \geq 2 \) parallel edges \( uv \) in \( G_0 \). Remove one of the edges \( uv \) from \( G_0 \) and denote the resulting graph by \( G_1 \). Then \( d_{G_1}(u) = d_{G_0}(u) - 1 \), \( d_{G_1}(v) = d_{G_0}(v) - 1 \) and the degrees of the other vertices are unchanged. Now, if \( d_{G_0}(u) = d_{G_0}(v) \) then also \( u \) is the unique neighbor of \( v \), and hence \( R'(G_1) = R'(G_0) \). On the other hand, if \( d_{G_0}(u) < d_{G_0}(v) \) then the deletion of the edge \( uv \) influences only the contribution of the edges \( vx \) such that \( d_{G_0}(x) < d_{G_0}(v) \). Let \( l = |\{ vz \in E(G_0); d_{G_0}(z) < d_{G_0}(v)\}| \) and \( d = d_{G_0}(v) \). Then \( R'(G_1) = R'(G_0) - \frac{1}{d} + \frac{k}{d+1} \leq R'(G_0) \) with equality only if \( d = l \).

Now define \( A_1(u) \) and \( A_1(v) \) analogously as \( A_0(u) \) and \( A_0(v) \). Observe that if \( A_0(u) \neq \emptyset \) then \( A_1(v) = \emptyset \) and if \( A_0(u) = \emptyset \) then \( A_1(u) = \emptyset \). Hence, repeat the process described in the previous cases to obtain \( G_2, G_3, \ldots \) until we get a graph \( G_r \) such that either \( d_{G_r}(u) = k \) or \( d_{G_r}(v) = n - k \). In this way we have decreased the number of vertices \( x \) whose degree is in the open interval \((k, n-k)\).

Now repeat the process with other pair of vertices whose degree is in the interval \((k, n-k)\) and yet another and so on. At the end we have either a single vertex of degree in \((k, n-k)\), which contradicts Lemma 3.2.13, or exactly two such vertices. Thus, we can assume that \( G \) has exactly two vertices, say \( u \) and \( v \), with \( k < d(u) \leq d(v) < n - k \). By Lemma 3.2.13 and the process described above, we have either \( u \in V_k(G_r) \) and \( v \in V_{n-k}(G_r) \) or \( u, v \in V_k(G_r) \) and \( v \in V_{n-k}(G_r) \). However, in the later case we have an edge \( uv \) in \( G_r \), which contradicts Lemma 3.2.13. Thus, \( u \in V_k(G_r) \) and \( v \in V_{n-k}(G_r) \). If \( R'(G_r) < R'(G_{r-1}) \), that finishes the proof of the lemma. So, we may assume that \( R'(G_{r-1}) = R'(G_r) \) and \( G_r \) was obtained from \( G_{r-1} \) by the first or by the second of the tree cases discussed above. Consider each of these two cases separately:

\( A_{r-1}(u) \neq \emptyset \): Then \( A_{r-1}(v) = \emptyset \) and \( d_{G_{r-1}}(u) = d = l \), see the analogous case above, so that both \( u \) and \( v \) have neighbors only in \( V_k(G_{r-1}) \). This means that also in \( G_r \) the vertex \( u \) has neighbors only in \( V_k(G_r) \). Hence, \( V_k(G_r) \) is not an independent set, which contradicts Lemma 3.2.13.

\( A_{r-1}(u) = \emptyset \) and there is an edge \( uv \in E(G_{r-1}) \) such that \( uv \neq uv \): Then \( l = 0 \), see the analogous case above, so that \( uv \notin E(G_{r-1}) \) and both \( u \) and \( v \) have neighbors only in \( V_{n-k}(G_{r-1}) \). This means that in \( G_r \) the vertex \( v \) has neighbors only in \( V_{n-k}(G_r) \). Hence, \( V_{n-k}(G_r) \) is not an independent set, which contradicts Lemma 3.2.13.

\( \square \)
Observe that in the final contradiction of the previous proof we use the fact that Lemma 3.2.13 is stated for graphs which may be disconnected and which may have multiple edges.

Proof of Theorem 3.2.12. By Lemmas 3.2.13 and 3.2.14, $G$ is a bipartite graph with bipartition $(V_{n-k}(G), V_k(G))$, possibly with multiple edges.

Denote $a = |V_k(G)|$ and $b = |V_{n-k}(G)|$. Then $|E(G)| = ak = b(n - k)$, so that $(a + b)k = bn$. As $a + b = n$, we get $b = k$ and consequently $a = n - k$. Hence, $R'(G) = \frac{b(n-k)}{n-k} = b = k$. Since there is a unique simple graph satisfying $|V_k(G)| = n - k$ and $|V_{n-k}(G)| = k$, namely $K_{k,n-k}$, the theorem is proved.

Corollary 3.2.15. Let $G$ be a triangle-free graph on $n$ vertices with $\delta(G) = k$, $k \geq 1$. Then $R'(G) \geq k$ with equality if and only if $G = K_{k,n-k}$.

Proof. Suppose that there is a vertex $v$ in $G$ such that $d_G(v) > n - k$. Let $u$ be a neighbor of $v$. Since $G$ is triangle-free, $N_G(u) \cap N_G(v) = \emptyset$, so that $N_G(u) \subseteq V(G) \setminus N_G(v)$. Hence, $d_G(u) < k$, a contradiction. Thus, $\Delta(G) \leq n - k$. As $\delta(G) \leq \Delta(G)$, we have $k \leq n - k$, so that $n \geq 2k$. Now, consider two cases:

- $n > 2k$: By Theorem 3.2.12 we have $R'(G) \geq k$ with equality if and only if $G = K_{k,n-k}$.

- $n = 2k$: As $n - k = k$, $G$ is a regular graph. Since $|E(G)| = \frac{kn}{2}$, we have $R'(G) = \frac{kn}{2k} = k$. Choose two vertices, say $u$ and $v$, such that $uv \in E(G)$. Since both $N_G(u)$ and $N_G(v)$ are disjoint independent sets of $k$ vertices each, we have $G = K_{k,k}$.
3.3 Gutman index

Let $v$ be a vertex of a graph $G$. The graph $G - v$ is obtained from $G$ by removing both $v$ and all edges incident to $v$ are removed. By $G^+$ we denote a graph obtained from $G$ by adding one edge joining two vertices of degree 1.

Wiener index, $W(G)$, of a connected graph is defined as

$$W(G) = \sum_{u,v \in V(G)} d(u, v).$$

It is a frequently studied graph invariant in both mathematical and chemical literature; for details see the reviews [18, 37, 45, 64, 66, 68]. In this paper we are concerned with a variant of the Wiener index called Gutman index [99]. Some authors use alternative name Schultz index of second [64] instead of Gutman index. Throughout this paper, the latter name is used. Another variant of Wiener index is the edge-Wiener index, $W_e(G)$, defined as the sum of the distances between all pairs of edges of a connected graph $G$:

$$W_e(G) = \sum_{e,f \in E(G)} d(e, f);$$

where the distance between two edges is the distance between the corresponding vertices in the line graph of $G$.

The Gutman index of a connected graph $G$ is defined as

$$\text{Gut}(G) = \sum_{u,v \in V(G)} d(u)d(v)d(u, v).$$

The Gutman index of graphs and its application in chemistry has just recently attracted. Dankelmann et al. [30] presented an asymptotic upper bound for the Gutman index and also established the relation between the edge-Wiener index and Gutman index of graphs. Chen and Liu studied the maximal and minimal Gutman index of unicyclic graphs [26], and they also determined the minimal Gutman index of bicyclic graphs [27]. Gutman [64] gave the following relation between the Gutman and the Wiener index for a tree $T$ on $n$ vertices,

$$\text{Gut}(T) = 4W(T) - (2n - 1)(n - 1). \quad (3.13)$$

In [46] lower and upper bounds for the Wiener index for a graph $G$ on $n$ vertices were given. Namely, there it was shown that

$$\binom{n}{2} = W(K_n) \leq W(G) \leq W(P_n) = \binom{n + 1}{3}, \quad (3.14)$$

where $K_n$ and $P_n$ are the complete graph and path, respectively, on $n$ vertices.
3.3.1 Graph with minimal Gutman index

First, we show a general lower bound on Gutman index [6].

**Theorem 3.3.1.** If $G$ is a connected graph on $n$ vertices, then
\[(2n - 3)(n - 1) = \text{Gut}(S_n) \leq \text{Gut}(G).\]

The equality holds if and only if $G$ is star $S_n$.

**Proof.** First, consider the case when $G$ has no leaves, i.e., $\delta(G) \geq 2$. Then,
\[
\text{Gut}(G) = \sum_{u,v \in V(G)} d(u)d(v)d(u,v) \geq 4 \sum_{u,v \in V(G)} d(u,v) \\
\geq 4\left(\frac{n}{2}\right) = 2n(n - 1) > (2n - 3)(n - 1) = \text{Gut}(S_n).
\]

We bear the case $\delta(G) = 1$ by induction on the number of vertices. For $n = 1$ the claim of the proposition is obvious. Assume that the theorem holds for a graph $G$ on $n$ vertices. We construct a graph $G'$ on $n + 1$ vertices from $G$ by adding a leaf $x$ incident to $a \in V(G)$. We show that by adding $x$, Gutman index increases by at least $4n - 3 = \text{Gut}(S_{n+1}) - \text{Gut}(S_n)$.

To simplify the exposition of the proof, let $D_G(u,v) = d_G(u)d_G(v)d_G(u,v)$, and similarly $D_{G'}(u,v) = d_{G'}(u)d_{G'}(v)d_{G'}(u,v)$.

\[
\text{Gut}(G') - \text{Gut}(G) = \sum_{v \in V(G) \setminus \{a\}} [D_{G'}(a,v) - D_G(a,v)] + \sum_{v \in V(G)} D_{G'}(x,v) \\
+ \sum_{u,v \in V(G) \setminus \{a\}} [D_{G'}(u,v) - D_G(u,v)].
\]

From the construction of the graph $G'$, it is obvious that $d_{G'}(u,v) = d_G(u,v)$, and $d_{G'}(x,v) = 1 + d_G(a,v)$ for every $u,v \in V(G)$. Also notice that the degree of $a$ increases by 1, but all the other vertex degrees are not changed. It is clear that the contribution of $u,v \in V(G) \setminus \{a\}$ is the same in $\text{Gut}(G')$ and in $\text{Gut}(G)$. Hence,
\[
\text{Gut}(G') - \text{Gut}(G) = \sum_{v \in V(G) \setminus \{a\}} d_G(v)d_G(a,v) + \sum_{v \in V(G)} d_{G'}(v)(d_G(a,v) + 1) \\
= 2 \sum_{v \in V(G) \setminus \{a\}} d_G(v)d_G(a,v) + \sum_{v \in V(G)} d_G(v) + 1.
\]

Since $d_G(a,v) \geq 1$ and $d_G(v) \geq 1$ for every $v \in V(G) \setminus \{a\}$ and $\sum_{v \in V(G)} d_G(v) = 2|E(G)| \geq 2(n - 1)$, we infer $\text{Gut}(G') - \text{Gut}(G) \geq 4n - 3$. Moreover the equality holds if and only if $d_G(v) = 1$ for every $v \in V(G) \setminus \{a\}$, in which case $G = S_n$. \qed
From (3.13) and (3.14) we find that for every tree $T$ on $n$ vertices $\text{Gut}(T) = O(n^3)$. Together with Theorem 3.3.1, we obtain the following result.

**Corollary 3.3.2.** If $T$ is a tree on $n$ vertices, then

$$(n - 1)(2n - 3) = \text{Gut}(S_n) \leq \text{Gut}(T) \leq \text{Gut}(P_n) = \frac{(n - 1)(2n^2 - 4n + 3)}{3}.$$ 

### 3.3.2 Bounds on minimal Gutman index

In this section, we consider graphs with minimal Gutman index. First, we show lower and upper bounds for graphs with minimum degree at least two.

**Proposition 3.3.3.** A connected graph $G$ on $n$ vertices with minimum degree $\delta(G) = \delta \geq 2$ and minimal Gutman index satisfies

$$\delta(\delta + 1)n^2 > \text{Gut}(G) \geq \frac{\delta^2 n}{2} (2n - \delta - 2).$$

*Proof.* First, we show the lower bound

$$\text{Gut}(G) = \frac{1}{2} \sum_u d(u) \sum_v d(v) d(u, v) \geq \frac{n}{2} \min_u \left( d(u) \sum_v d(v) d(u, v) \right) \geq \frac{n \delta}{2} \min_u \left( d(u) \sum_v d(u, v) \right).$$

Since there are $d(u)$ vertices on distance one to $u$, and $n - d(u) - 1$ vertices on distance at least two to $u$, we have further

$$\text{Gut}(G) \geq \frac{n \delta}{2} \min_u \left( d(u)(d(u) + 2(n - d(u) - 1)) \right) = \frac{n \delta}{2} \min_u \left( d(u)(2n - d(u) - 2) \right).$$

The quadratic function $f(x) = x(2n - x - 2)$ with $\delta \leq x \leq n - 1$ has its minimum at $\delta$. Thus,

$$\text{Gut}(G) \geq \frac{n \delta}{2} \delta(2n - \delta - 2).$$

Now, we show the upper bound. By Erdős-Gallai theorem [47], there exists a graph $H$ on $n - 1$ vertices such that

(a) if at least one of $\delta$ or $n$ is odd, then $H$ is $\delta - 1$ regular graph; or

(b) if both $\delta$ and $n$ are even, a vertex $x$ is of degree $\delta$ and all others are of degree $\delta - 1$.
exists.

From \( H \), we construct the graph \( H^* \) by introducing a new vertex \( y \) adjacent to all vertices of \( H \). Observe that \( e_H = |E(H)| = \left\lceil \frac{(\delta - 1)(n - 1)}{2} \right\rceil \). The contribution of \( y \) to \( \text{Gut}(H^*) \) is

\[
\sum_{v \in V(H)} d_{H^*}(y)d_{H^*}(v)d_{H^*}(y, v) \leq (n - 1)((n - 2)\delta + \delta + 1).
\]

The contribution of \( x \) to \( \text{Gut}(H^*) \) is

\[
\sum_{v \in V(H)} d_{H^*}(x)d_{H^*}(v)d_{H^*}(x, v) \leq (\delta + 1)(\delta^2 + 2\delta(n - \delta - 2)),
\]

and the remaining vertices of \( H^* \) contribute

\[
\sum_{u,v \in V(H) \setminus \{x\}} d_{H^*}(u)d_{H^*}(v)d_{H^*}(u,v) = \delta^2 \left[ e_H - \delta + 2 \left( \frac{n - 2}{2} - e_H + \delta \right) \right].
\]

Thus,

\[
\text{Gut}(H^*) \leq (n - 1)((n - 2)\delta + \delta + 1) + (\delta + 1)(\delta^2 + 2\delta(n - \delta - 2)) + \delta^2 \left[ e_H - \delta + 2 \left( \frac{n - 2}{2} - e_H + \delta \right) \right] = (n - 1)(n\delta - \delta + 1) + (\delta + 1)(2n\delta - \delta^2 - 4\delta) + \delta^2 \left[ 2 \left( \frac{n - 2}{2} \right) - e_H + \delta \right] < \delta(\delta + 1)n^2 - \frac{1}{2}(\delta^3 + 5\delta - 2)n - \frac{\delta^2}{2}(\delta + 1) - 3\delta - 1 < \delta(\delta + 1)n^2.
\]

\[\square\]

**Corollary 3.3.4.** A connected graph \( G \) on \( n \) vertices with minimum degree at least \( \delta \geq 2 \) and minimal Gutman index satisfies

\[
\delta(\delta + 1)n^2 - O(n) \geq \text{Gut}(G) \geq \delta^2n^2 - O(n).
\]

Now, we show an upper bound for graphs with minimal Gutman index and maximum degree at most \( \Delta \).

**Proposition 3.3.5.** A connected graph \( G \) on \( n \) vertices with maximum degree at most \( \Delta > 2 \) and minimal Gutman index satisfies

\[
\text{Gut}(G) < 4(n^2 - 8n + 4) \log_{\Delta-1} n.
\]
**Proof.** Let $G$ be a $\Delta$-regular balanced tree. Let us denote its radius by $k$, hence $\text{diam}(G) = 2k$. If $\text{diam}(G) = 2k$, then the number of vertices $n = \Delta \frac{(\Delta - 1)^k - 1}{\Delta - 2} + 1$. This tree has $\Delta (\Delta - 1)^{k-1} = \frac{(\Delta - 2)n + 2}{\Delta - 1}$ leaves and $\frac{n - 2}{\Delta - 1}$ inner vertices. Notice that $\log_{\Delta-1} \frac{\Delta - 2}{\Delta} n < k < \log_{\Delta-1} n$.

Now $G$ has three types of vertex pairs: a pair of two leaves, a leaf and an inner vertex, and a pair of two inner vertices. Their contribution to the Gutman index is:

- **Two leaves:** the distance between two leaves is at most $\text{diam}(G) = 2k$, so their contribution to the Gutman index is at most
  \[
  \left( \frac{(\Delta - 2)n + 2}{\Delta - 1} \right)^2 2k < \left( \frac{(\Delta - 2)n + 2}{\Delta - 1} \right)^k.
  \]

- **A leave and an inner vertex:** since every inner vertex has degree $\Delta$, and the distance between any two vertices is at most $2k$, their contribution is less than
  \[
  \frac{(\Delta - 2)n + 2}{\Delta - 1} \cdot \frac{n - 2}{\Delta - 1} 2k \Delta.
  \]

- **Two inner vertices:** these pair contribute at most
  \[
  \left( \frac{n - 2}{2} \right)^2 2k \Delta^2 < \left( \frac{n - 2}{\Delta - 1} \right)^2 \Delta^2 k.
  \]

Now,

\[
\text{Gut}(G) < \left( \frac{(\Delta - 2)n + 2}{\Delta - 1} \right)^2 k + \frac{(\Delta - 2)n + 2}{\Delta - 1} \cdot \frac{n - 2}{\Delta - 1} 2k \Delta + \left( \frac{n - 2}{\Delta - 1} \right)^2 \Delta^2 k
= \frac{4k}{(\Delta - 1)^2}(\Delta - 1)^2 (n^2 - 8n + 4)
< 4(n^2 - 8n + 4) \log_{\Delta-1} n,
\]

and this proves the upper bound. \(\square\)

Note that if $G$ is a graph with maximum degree $\Delta \leq 2$, then $G$ is a path.

### 3.3.3 Bounds on maximal Gutman index

In this section, we consider graphs with maximal Gutman index. First, we show lower and upper bounds for graphs with maximum degree at most $\Delta$. 
**Proposition 3.3.6.** Let $G$ be a connected graph on $n$ vertices with maximum degree $\Delta(G) \leq \Delta$, and maximal Gutman index. Then, the following holds:

\[
\frac{(n + 1)^3}{27} \Delta^2 \leq \text{Gut}(G) \leq \left(\frac{n + 1}{3}\right) \Delta^2.
\]

**Proof.** For the lower bound we consider the graph $Q$ which is illustrated in Figure 3.4. To simplify the calculation, we assume that $s = (\Delta + 1)/3$, $bn$ and $3an/(\Delta + 1)$ are integers. The graph $Q$ has $n$ vertices, so $2an + bn = n$ holds.

![Figure 3.4](image)

Figure 3.4: The graph $Q$ consist of two identical parts $Q^L$ and $Q^R$ connected by path on $nb$ vertices. $Q^L$ (resp. $Q^R$) consists of a lexicographic product $P_p[K_s]$, $s = \frac{\Delta + 1}{3}$, plus all edges between the vertices of $K_{s,1}^L$ and $K_{s,p}^L$ (resp. $K_{s,1}^R$ and $K_{s,p}^R$) except the edge $x_Ly_L$ (resp. $x_Ry_R$). The vertices $x_L$ and $y_L$ (resp. $x_R$ and $y_R$) are adjacent to the vertex $v_1$ (resp. $v_{bn}$).

A pair $(x, y)$, where $x$ is a vertex from $Q^L$ and $y$ is a vertex from $Q^R$, contributes at least $\Delta^2(bn + 1)$ to $\text{Gut}(Q)$. Since there are $an$ vertices in each $Q^L$ and $Q^R$, the contribution of these vertices is $(an)^2\Delta^2(bn + 1)$. Under the constraint $2a + b = 1$, the expression $(an)^2\Delta^2(bn + 1)$ attains maximum for $a = (n + 1)/3n$ and $b = \frac{n-2}{3n}$. Finally we have

\[
\text{Gut}(Q) \geq \frac{(n + 1)^3}{27} \Delta^2.
\]

Now, we show the upper bound. From (3.14) and $\Delta(G) \leq \Delta$, it follows that

\[
\text{Gut}(G) \leq \sum_{u,v} \Delta^2 d(u, v) = \Delta^2 W(G) \leq \Delta^2 W(P_n) = \Delta^2 \left(\frac{n + 1}{3}\right).
\]
For graphs with bounded maximum degree, we obtain the following result.

**Corollary 3.3.7.** Let $G$ be a connected graph on $n$ vertices with bounded maximum degree $\Delta$. Then,

$$O(n^3) \geq \text{Gut}(G) \geq \Omega(n^2 \log n),$$

and those bounds can be attained.

**Proof.** The lower bound follows directly from Proposition 3.3.5 and the upper bound from Proposition 3.3.6. \hfill \Box

In the sequel, we consider lower and upper bounds for graphs with maximal Gutman index and minimum degree at least $\delta$. Dankelmann et al. [30] presented the following upper bound on Gutman index.

![Figure 3.5: The graph $L$ consists of $bn$ cliques $K^1_{\delta-1}, \ldots, K^m_{\delta-1}$ on $\delta - 1$ vertices, and $bn + 1$ other vertices $v_0, \ldots, v_{bn}$ such that every vertex of clique $K^i_{\delta-1}$ is adjacent to $v_{i-1}$ and $v_i$. Moreover, $v_0$ is adjacent to every vertex of a clique $K^1_{an}$ on $an$ vertices and $v_{bn}$ is adjacent to every vertex of other clique $K^2_{an}$ on $an$ vertices.](image)

**Theorem 3.3.8** (Dankelmann et al. [30]). Let $G$ be a connected graph on $n$ vertices. Then

$$\text{Gut}(G) \leq \frac{2^4}{5^5} n^5 + O\left(\frac{n^2}{\delta^5}\right),$$

and the coefficient of $n^5$ is the best possible.

Now, we present the lower bound.

**Proposition 3.3.9.** A connected graph $G$ on $n$ vertices with minimum degree at least $\delta$, and maximal Gutman index satisfies

$$\frac{2^5}{5^5} \left(\frac{n + \delta - 1}{\delta^5}\right) < \text{Gut}(G).$$
Proof. To show the bound consider the graph $L$ given in Figure 3.5.

To simplify the calculations, we assume that the parameters $a_n$ and $b_n$ of the graph $L$ are integers. Since $L$ has $n$ vertices, $2a_n + bn\delta + 1 = n$. We consider only the contribution of the pairs $(x, y)$ to $\text{Gut}(L)$, where $x \in V(K^1_{a_n})$, $y \in V(K^2_{a_n})$, which is more than $(a_n)^42(b_n + 1)$. Under the constrain $2a_n + bn\delta + 1 = n$, the expression $2(a_n)^4(b_n + 1)$ attains the maximum at $bn + 1 = \frac{n + \delta - 1}{5\delta}$ and $a_n = 2(b_n + 1)$. Thus, we obtain

$$\text{Gut}(G) > \frac{2^5(n + \delta - 1)^5}{5^5\delta^5}.$$
Chapter 4

Fullerenes

4.1 Fullerene graphs

A fullerene graph is a 3-connected 3-regular planar graph with only pentagonal and hexagonal faces. By Euler’s formula, it follows that the number of pentagonal faces is always twelve. Grünbaum and Motzkin [63] showed that fullerene graphs with \( n \) vertices exist for all even \( n \geq 24 \) and for \( n = 20 \). Although the number of pentagonal faces is negligible compared to the number of hexagonal faces, their layout is crucial for the shape of a fullerene graph. There are fullerene graphs where no two pentagons are adjacent, i.e., each pentagon is surrounded by five hexagons. Those fullerene graphs satisfy the isolated pentagon rule or shortly IPR, and they are the most stable fullerene compounds. If all pentagonal faces are equally distributed, we obtain fullerene graphs of icosahedral symmetry, whose smallest representative is the dodecahedron. The dodecahedron is the only icosahedral fullerene that does not satisfy the IPR.

On the other hand, there is a class of fullerene graphs of tubular shapes, called nanotubes. Nanotubical graphs or simply nanotubes are fullerene graphs with additional structural properties. They are cylindrical in shape, with the two ends capped with a subgraph containing six pentagons and possibly some hexagons. The construction of the nanotubes is shown on Figure 4.1, the Buckminsterfullerene \( C_{60} \) is the smallest nanotube of type \((5,5)\). The cylindrical part of the nanotube can be obtained from a planar hexagonal grid by identifying objects lying on two parallel lines. The way the grid is wrapped is represented by a pair of integers \((p_1, p_2)\). The numbers \( p_1 \) and \( p_2 \) denote the coefficients of the linear combination of the unit vectors \( a_1 \) and \( a_2 \) such that the vector \( p_1 a_1 + p_2 a_2 \) joins pairs of identified points, i.e., the integers \( p_1 \) and \( p_2 \) denote the number of unit vectors along two directions in the honeycomb crystal lattice of the nanotube (see Figure 4.2). Nanotubes
Figure 4.1: Buckminsterfullerene is the smallest nanotube of type (5, 5).

with $p_2 = 0$ are called zig-zag nanotubes, and the ones with $p_1 = p_2$ are called armchair nanotubes.

Figure 4.2: An example of a (2, 4) nanotube. The hexagons denoted equally overlap.

A polygon-hexagon patch or just patch is a 2-connected plane graph with only pentagonal or hexagonal faces, except maybe one face-the exterior face, all interior vertices of degree 3 and all boundary vertices of degree 2 or 3. A hexagonal patch is a simply connected set of hexagons in the (oriented) plane with all interior vertices having valency 3, at most two of the boundary vertices have valency 1 while all the other vertices have valency 2 or 3.

As mentioned before, the study of fullerene graphs has been motivated by a search for invariants that will correlate with their stability as a compound. Among the promising candidates for stability predictors are: the bipartite edge frustration, the saturation number,
the independence number, etc. The diameter of the graph can also be used as a measure of
the fullerene stability. Banhart et al [14] showed observed that a molecule structure with
sharp edges and facets are less stable than the structures with smooth curvature. In this
sense, a molecule graph with smaller diameter will be more spherical and therefore more
stable.

As it was shown in [7], the diameter of the nanotubes is linear in the number of vertices.
On the other hand, the diameter of a fullerene graph $G$ on $n$ vertices having icosahedral
symmetry is small, it is of order $\Theta(\sqrt{n})$.

In this thesis we establish lower and upper bounds for the diameter of fullerene graphs
and use the results to improve the upper bound on their saturation number and settling
the relationship between the independence number and the diameter. Later we determine
the diameter of an icosahedral fullerene graph with full icosahedral symmetry, and prove
that each pentagonal vertex is diametral. Hexagonal vertices on the other side are not
necessarily diametral. Even more, for an arbitrary vertex $x \in V(G)$ there is a pair of
diametral pentagonal vertices $u, v \in V(G) \setminus \{x\}$ and a diametral path between them
passing through $x$.

In order to determine the diameter of a fullerene graph with full icosahedral symmetry,
we consider the two cases: $(0, i)$- and $(i, i)$-icosahedral fullerene graphs, where $i > 0$.

As we conjecture the fullerenes with full icosahedral symmetry have the smallest diam-
eter.

The bipartite edge frustration of a graph $G$, denoted by $\varphi(G)$, is the smallest cardinality
of a set of edges of $G$ that need to be removed from $G$ in order to obtain a bipartite spanning
subgraph. Bipartite edge frustration of a fullerene graph $G$ can be efficiently computed by
finding a minimum-weight perfect matching in the pentagon-distance graph of $G$ [41]. In
the same reference it was shown that $\varphi(G) \geq 6$ for any fullerene graph $G$ and that this
bound is sharp. Furthermore, it was shown that the bipartite edge frustration of fullerene
graphs with icosahedral symmetry is proportional to the square root of the number of
vertices ([41], Proposition 11 and Corollary 12). The numerical computations reported
there suggested that it cannot behave worse than that, and prompted the authors to state
the following conjecture.

**Conjecture 4.1.1.** Let $G$ be a fullerene graph with $n$ vertices. Then $\varphi(G) \leq \sqrt{\frac{12}{5}n} = 1.549\sqrt{n}$.

First, Dvořák, Lidický, and Škrekovski [43] proved a theorem with a weaker multiplicativa-
centre.

**Theorem 4.1.1.** Let $G$ be a fullerene graph with $n$ vertices. Then $\varphi(G) \leq 39.29\sqrt{n}$. 
Later Faria, Klein and Stehlík proved the Conjecture 4.1.1 [51].

Another invariant investigated for its stability-predicting potential is the smallest eigenvalue of a fullerene graph. In [54] it was proven that the dodecahedron has maximum smallest eigenvalue among all fullerene graphs and it is equal to $-\sqrt{5}$. It was also shown that the buckminsterfullerene $C_{60}$ has the maximum smallest eigenvalue among all IPR fullerene graphs. This observation lead the authors to state the following conjecture on the smallest eigenvalue of fullerene graphs with at least 60 vertices.

**Conjecture 4.1.2.** Among all fullerene graphs with at least 60 vertices, the buckminster fullerene has the maximum smallest eigenvalue.

The Conjectures 4.1.1 and 4.1.2 are connected via a result on Laplacian eigenvalues from the monograph by Godsil and Royle ([59], pp. 293).

**Theorem 4.1.2.** Let $G$ be a graph with $n$ vertices. Then $\text{bip}(G) \leq \frac{n}{4} \mu_{\infty}(G)$.

Here $\text{bip}(G)$ denotes the maximum number of edges in a bipartite spanning subgraph of $G$ (hence the number of edges in $G$ minus the bipartite edge frustration), and $\mu_{\infty}(G)$ is the largest Laplacian eigenvalue of $G$. We refer the reader to Chapter 13 of the above monograph for more on Laplacian eigenvalues; it suffices for our purposes to note that for 3-regular graphs $\mu_{\infty}(G) = 3 - \lambda_n(G)$, where $\lambda_n(G)$ is the smallest eigenvalue of $G$.

Another invariant tested as a possible stability predictor is the independence number [50]. A set $I \subseteq V(G)$ is independent if no two vertices from $I$ are adjacent in $G$. The cardinality of any largest independent set in $G$ is called the independence number of $G$ and denoted by $\alpha(G)$. A sharp upper bound on the independence number of fullerene graphs was established in [39] as $\alpha(G) \leq \frac{n}{2} - 2$. It was obtained using the fact that all fullerene graphs are 2-extendable. No sharp lower bound on the independence numbers has been reported so far — the best known result $\alpha(G) \geq \frac{3}{8}n$ [73] is no better than the lower bound for triangle-free planar cubic graphs, and numerical evidence suggests that it is far from being sharp. In fact, numerical results suggest a bound of the type $\alpha(G) \geq \frac{n}{2} - C\sqrt{n}$. Those observations were formalized in a pair of conjectures in a recent Ph.D. thesis by S. Daugherty ([33, pp. 96]). The first one states that the minimum possible independence number is achieved on the icosahedral fullerenes that also figure prominently in Conjecture 4.1.1. The second one [33, Conjecture 5.5.2] states the precise form of the conjectured lower bound. Notice that the constant $3/\sqrt{15}$ is exactly one half of the constant $\sqrt{12/5}$ of Conjecture 4.1.1.
Conjecture 4.1.3. Let $G$ be a fullerene graph with $n$ vertices. Then

$$\alpha(G) \geq \frac{n}{2} - 3\sqrt{n/15}.$$ 

The relations between diameter and the independence number of fullerenes appear in Conjecture 912 of Graffiti [56]:

Conjecture 4.1.4. If $G$ is a fullerene graph, then

$$\alpha(G) \geq 2(diam(G) - 1).$$

For more on independence number in fullerenes and in particular in icosahedral fullerenes we refer the reader to [61, 62].

The last invariant considered here, the saturation number, is related to matchings. The existence of perfect (and hence maximum) matchings in fullerene graphs has been established long time ago, and there are many papers concerned with their structural and enumerative properties [39, 79, 83]. Another class of matchings, the maximal matchings, have received much less attention so far, in spite of being potentially useful as mathematical models of dimer absorption. A matching $M$ is maximal if it cannot be extended to a larger matching of $G$. The saturation number of $G$ is the cardinality of any smallest maximal matching of $G$. We denote it by $s(G)$. The saturation number of fullerene graph was studied in [39, 42], where the following bounds were established.

Theorem 4.1.3. There exists an absolute constant $C$ such that

$$\frac{3n}{10} \leq s(G) \leq \frac{n}{2} - C\log_2 n,$$

for any fullerene graph $G$ with $n$ vertices.

The upper bound of the above theorem will be improved using the results of Section 4.2.1.

4.2 Bounds on the diameter of fullerene graphs

4.2.1 Lower bound on the diameter

A well known result on the degree-diameter problem states that the number of vertices in a planar graph with maximum degree 3 grows at most exponentially with diameter [57].

Proposition 4.2.1. Let $G$ be a planar graph with maximum degree 3. Then, $G$ has at most $2^{diam(G)+1} - 1$ vertices.
This results in a logarithmic lower bound on the diameter in terms of the number of vertices.

**Corollary 4.2.2.** Let $G$ be a planar cubic graph with $n$ vertices. Then,
\[
\text{diam}(G) \geq \lceil \log_2(n + 1) \rceil - 1.
\]

![Figure 4.3: An example of $\Psi_3$.](image)

To illustrate Corollary 4.2.2, we refer to a Halin graph $\Psi$ obtained from a complete balanced 3-regular tree. A *Halin* graph is a planar graph constructed from a plane embedding of a tree $T$ having four or more vertices, and no vertices of degree two, by connecting all the leaves of the tree with a cycle, in the cyclic order defined by the embedding of the tree. Now, let $T_n$ to be a complete balanced 3-regular tree on $n$ layers with leaves be denoted by $t_1, t_2, ..., t_{3\cdot2^n-2}$. Let the Halin graph $\Psi_n$ be constructed by $T_n$. For any $n \in \mathbb{N}$, the graph $\Psi_n$ has $6 \cdot 2^{n-2} - 2$ vertices. It is easy to see, that when $n$ is big enough, the diameter of $\Psi_n$ is $2n$, which is logarithmic in terms of $|V(\Psi_n)|$. Figure 4.3 shows an example of $\Psi_3$. Note that for $n > 3$, the distance between $a_{2^n-1}, b_{2^n-1}$ is logarithmic.

The logarithmic character of the bound can be attributed to the presence of faces of large size. It would be reasonable to expect that better lower bounds exist for polyhedral graphs with bounded face size. Surprisingly, no such bounds seem to be available in the literature.

However, as mentioned above, fullerene graphs only have pentagonal and hexagonal faces, and we use this fact to show that the diameter is of order $\Omega(\sqrt{n})$. Crucial for our result is a fact that the infinite hexagonal grid is a graph of quadratic growth. In what follows we investigate how that behavior is affected by the presence of pentagonal defects. The basic idea is intuitively clear, but in order to formalize it we first introduce some terminology.
Let $G$ be a fullerene graph and let $N_k(x) = \{ v \in V(G) | d(v, x) = k \}$ be a set of vertices at distance $k$ from a vertex $x$. We call $N_k(x)$ a $k$-sphere and a vertex in a $k$-sphere is a $k$-sphere vertex. It is easy to see that for $k \geq 1$ it holds

\[ v \in N_k(x) \Rightarrow N(v) \subset N_{k-1}(x) \cup N_k(x) \cup N_{k+1}(x), \]

where $N(x)$ is the set of all neighbors of $x$ and $N_0(x) = \{ x \}$. For a chosen $x$ and an arbitrary $k$-sphere vertex $v \neq x$, we define the value of $v$ as

\[ \mu(v) = \sum_{u \in N(v) \cap N_{k+1}(x)} \frac{1}{|N(u) \cap N_k(x)|}, \]

where $k = d(v, x)$. Observe that the value $\mu(v)$ represents a measure of the number of vertices that $v$ contributes to the $(k+1)$-sphere. Hence, the number of vertices at distance $k$ from $x$ is

\[ |N_k(x)| = \sum_{v \in N_{k-1}(x)} \mu(v). \tag{4.1} \]

Notice that a $(k+1)$-sphere vertex $u$ adjacent to two $k$-sphere vertices contributes $\frac{1}{2}$ to the value of each neighbor in the $k$-sphere.

**Lemma 4.2.3.** Let $G$ be a fullerene graph and let $x \in V(G)$. Then,

\[ |N_k(x)| \leq |N_{k-1}(x)| + 3, \]

for $k \geq 1$.

**Proof.** The lemma obviously holds for $k = 1$, so we assume that $k \geq 2$ in the sequel. Let $G$ be a fullerene graph embedded in the plane and $x$ an arbitrary vertex of $G$. By (4.1), the statement of the lemma is equivalent to

\[ |N_k(x)| = \sum_{u \in N_{k-1}(x)} \mu(u) \leq |N_{k-1}(x)| + 3. \]

In the proof we will make use of the following observation. Let $P = uvwz$ be an induced path in $G$ such that $u$ is an $(i + 3)$-sphere vertex, $v$ an $(i + 2)$-, $w$ an $(i + 1)$-, and $z$ an $i$-sphere vertex, respectively. Moreover, let $P$ be incident with a face $f$. Then, the vertex $z$ has another $(i+1)$-sphere neighbor $w'$, and the vertex $u$ has another $(i+2)$-sphere neighbor $v'$ such that $v'$ is adjacent to $w'$, for otherwise the length of $f$ would be at least 7 (see Figure 4.44). We say that $u$ and $z$ are extreme for $f$.

Since every $k$-sphere vertex has at least one neighbor in the $(k-1)$-sphere, its value is at most 2. We show that only the neighbors of $x$ may have value 2.
Claim 1. Let $v$ be a vertex such that $\mu(v) = 2$. Then $d(v, x) = 1$.

Suppose, to the contrary, that $v$ is a $k$-sphere vertex, for $k > 1$, with $\mu(v) = 2$. Then, $v$ has precisely two neighbors $u_1$, $u_2$ in the $(k+1)$-sphere, and $v$ is the only $k$-sphere neighbor of $u_1$ and $u_2$. Let $w$ be the $(k-1)$-sphere neighbor of $v$. Consider the other two neighbors of $w$, $z_1$ and $z_2$. At least one of them, say $z_1$, is in the $(k-2)$-sphere. Now, consider the face $f$ incident to the vertices $v$, $w$, and $z_1$. Notice that either $u_1$ or $u_2$, say $u_1$, is also incident with $f$. Hence, $u_1$ and $z_1$ are extreme for $f$, thus $u_1$ has another $k$-sphere neighbor incident with $f$, a contradiction. This establishes Claim 1.

By Claim 1, the maximum value of a $k$-sphere vertex in $G$, for $k > 1$, is at most $1 + \frac{1}{2} = \frac{3}{2}$. We call a vertex $v$ with $1 < \mu(v) \leq \frac{3}{2}$ expansive. Furthermore, Claim 1 also implies that an expansive $k$-sphere vertex, for $k > 1$, has at most one expansive $(k+1)$-sphere neighbor. The following claims show that every expansive vertex has a unique expansive predecessor and at most one expansive successor. The only exception are the vertices in the 2-sphere, since the vertices of the 1-sphere are not expansive.

Claim 2. An expansive $k$-sphere vertex $v$ has an expansive $(k-1)$-sphere neighbor or there is an expansive $(k-2)$-sphere vertex $z$ such that $d(v, z) = 2$.

Suppose that the unique $(k-1)$-sphere neighbor $w$ of $v$ is not expansive. Let $u_1$, $u_2$ be the $(k+1)$-sphere neighbors of $v$. By Claim 1, we may assume that $u_1$, say, is adjacent to another $k$-sphere vertex, while $u_2$ is not. Next, let $z_1$, $z_2$ be the other two neighbors of $w$ and, without loss of generality, we assume that $z_1$ is a $(k-2)$-sphere vertex. Since $u_2$ has only one $k$-sphere neighbor it follows that $z_2$ is not a $(k-2)$-sphere vertex and the vertices $u_1$, $v$, $w$, and $z_1$ are all incident to some face $f$. Since $z_1$ is an extreme vertex for $f$ it has another $(k-1)$-sphere neighbor, which means that it is expansive.
Claim 3. An expansive $k$-sphere vertex $v$ has at most one expansive $(k + 2)$-sphere vertex at distance 2.

Suppose, to the contrary, that $v$ has two expansive $(k + 2)$-sphere vertices at distance 2. Let $u_1$ and $u_2$ be the two $(k + 1)$-sphere neighbors of $v$. By Claim 1, at least one of $u_1$ and $u_2$, say $u_2$, has another $k$-sphere neighbor $v'$. Now, we consider the $(k + 2)$-sphere neighbors of $u_1$ and $u_2$. If $u_2$ has no $(k + 2)$-sphere neighbor, we are done, since $u_1$ cannot have two expansive $(k + 2)$-sphere neighbors by Claim 1. Hence, we may assume that $u_2$ has an expansive $(k + 2)$-sphere neighbor $t$. Then, it has two $(k + 3)$-sphere neighbors $y_1$ and $y_2$. However, they are the extreme vertices of the two faces incident with $t$, $u_2$, $v$, and $t$, $u_2$, $v'$, respectively. That means that $y_1$ and $y_2$ both have two $(k + 2)$-sphere neighbors and the value of $t$ is at most 1, hence $t$ is not expansive. Recall that $u_1$ has at most one expansive $(k + 2)$-sphere neighbor, so Claim 3 holds.

Observe that all six vertices in the 2-sphere may be expansive, therefore, by Claims 2 and 3, it follows that there are at most six expansive vertices in every ring. Hence,

$$|N_k(x)| = \sum_{u \in N_{k-1}(x)} \mu(u) \leq 6 \cdot \frac{3}{2} + (|N_{k-1}(x)| - 6) \cdot 1 = |N_{k-1}(x)| + 3,$$

which concludes the proof.

The following theorem gives the lower bound for the diameter of fullerenes [7].

Theorem 4.2.4. Let $G$ be a fullerene graph. Then,

$$\text{diam}(G) \geq \frac{\sqrt{24n - 15} - 3}{6}.$$ 

Proof. Let $G$ be a fullerene graph with $n$ vertices. For every vertex $x \in V(G)$ there exists an integer $k$ such that there is no vertex at distance at least $k + 1$ from $x$, while a vertex at distance $k$ from $x$ exists. By Lemma 4.2.3, it is easy to see that the following inequality holds:

$$n = \sum_{i=0}^{k} |N_i(x)| \leq 1 + 3 + \sum_{i=2}^{k} |N_i(x)| = \frac{3}{2} k(k + 1) + 1.$$ 

Since the diameter of $G$ is at least $k$, we have that

$$\text{diam}(G) \geq k \geq \frac{\sqrt{24n - 15} - 3}{6}.$$ 

The function of the fullerene diameter is in $\Omega(\sqrt{n})$. However, there are many fullerene graphs with the diameter of order $\Theta(n)$, e.g., nanotubes. We discuss this in the next section.
4.2.2 Upper bound on the diameter

In this section we determine the upper bound on the diameter in fullerene graphs. In [7], we prove the following theorem.

**Theorem 4.2.5.** Let $F$ be a fullerene graph with $n$ vertices. Then,

$$\text{diam}(F) \leq \frac{n}{6} + \frac{5}{2},$$

unless $F$ is a $(5,0)$-nanotube. In that case, we have $n = 10k$, $k \in \mathbb{N}$ and

$$\text{diam}(F) = \begin{cases} 
\frac{n}{5} + 1, & k = 2; \\
\frac{n}{5}, & k \in \{3, 4\}; \\
\frac{n}{5} - 1, & k \geq 5.
\end{cases}$$

Before we continue, we present some additional notation and definitions. Let $F$ be a fullerene graph and let $v$ be an arbitrary vertex in $F$. We define $L^0_v = \{v\}$ as an initial layer and $F^0_v$ as a set of faces incident with $v$. Inductively, having defined the sets $L^i_{v-1}$ and $F^i_{v-1}$, $L^i_v$ is the set of vertices incident with $F^i_{v-1}$, not contained in $L^i_{v-1}$. Furthermore, $F^i_v$ is the set of faces incident with $L^i_v$ that are not contained in $F^i_{v-1}$. For an edge $e = uw$, where $u, w \in V(F)$, we say that it is an incoming edge to $L^i_v$ if $u \in L^i_{v-1}$ and $w \in L^i_v$. If $e$ is an incoming edge to $L^i_v$, then we also say that $e$ is an outgoing edge from $L^i_{v-1}$. The vertex $u$ is an outgoing vertex, and $w$ is an incoming vertex, respectively. Notice that a vertex cannot be outgoing and incoming at the same time, and also that the vertices in the last layer are never outgoing (it may also happen that such a vertex is neither incoming).

Recall that an edge-cut $C$ of $G$ is cyclic if each component of $G - C$ contains a cycle. A graph is cyclically $k$-edge-connected if at least $k$ edges must be removed to disconnect it into two components such that each contains a cycle. For fullerene graphs, Došlić [40] proved the following theorem.

**Theorem 4.2.6.** Every fullerene graph $F$ is cyclically 5-edge-connected.

Additionally, Kardoš and Škrekovski [80] proved that the cyclically 5-edge-connected fullerenes are of unique type.

We say that a cyclic 5-edge cut id trivial, if it separates only one pentagonal face.

**Theorem 4.2.7.** A $(5,0)$-nanotube is the only fullerene graph with a nontrivial cyclic 5-edge-cut.
In this sense we say that if $G$ is a fullerene graph which is not $(5, 0)$-nanotube, it is cyclically 6-edge-connected.

As every face in $F$ is of length 5 or 6 and every vertex has degree 3, we immediately infer that:

**Lemma 4.2.8.** For every vertex $x \in L_{i+1}^v$, $i \geq 1$, there exists a vertex $y \in L_i^v$ such that $d(x, y) \leq 2$.

The inequality in Lemma 4.2.8 is tight only when $x$ is an outgoing vertex, otherwise there is a vertex $y \in L_i^v$ adjacent to $x$. Also, note that if $x \in L_1^v$, then $d(x, v)$ could be 3 (see Figure 4.5). This together with Lemma 4.2.8 gives:

![Figure 4.5: The vertex $v$ is a starting vertex and $L_0^v = \{v\}$. Faces incident to $v$ belong to the set $F_0^v$. The vertices incident to $F_0^v$ different from $v$ form the first layer $L_1^v$. Distance between $v$ and $x \in L_1^v$ is three.](image)

**Lemma 4.2.9.** Let $x \in L_i^v$. Then $d(v, x) \leq 2i + 1$. Furthermore, if $d(v, x) = 2i + 1$, then $v$ is adjacent with at least one hexagon.

Now, we show that when $L_i^v$ is small enough, $L_{i+2}^v$ is empty, or in other words we reach the “end” of the fullerene.

**Lemma 4.2.10.** Let $i \geq 2$ and $|L_i^v| < 12$. Then, $L_{i+2}^v = \emptyset$.

**Proof.** Suppose first that $L_i^v$ induces an acyclic graph. Then, $F_i^v = \emptyset$ and therefore also $L_{i+1}^v = L_{i+2}^v = \emptyset$. Hence, we may assume that there exists a cycle $C$ in the graph induced by $L_i^v$. By Theorem 4.2.6, there are at least five incoming edges to $L_i^v$. If the number of incoming edges is precisely five, $C$ is a 5-face, for otherwise $F$ is a $(5, 0)$-nanotube. It follows that $L_{i+1}^v = L_{i+2}^v = \emptyset$.

On the other hand, if there are at least six incoming edges to $L_i^v$ and since $|L_i^v| < 12$ we have at most five outgoing edges from $L_i^v$, which also means, that there is at most
five incoming vertices to $L^v_{i+1}$. By the same argument we infer that the graph induced by $L^v_{i+1}$ is either acyclic or it contains a cycle $C'$ which is a 5-face in $F$. Either way, $L^v_{i+2}$ is empty.

The following lemma will determine the maximal distance from the last layer with at least 12 vertices $L^v_{k-1}$ to the vertices in the last layer.

**Lemma 4.2.11.** Let $x$ be a vertex from the last layer in our graph and let $k$ be the smallest number, such that $k \geq 2$ and $|L^v_k| < 12$. Then, there exists a vertex $z \in L^v_{k-1}$ such that $d(z, x) \leq 3$.

**Proof.** If $L^v_k$ is the last layer in our graph, we know by Lemma 4.2.8 that $d(z, x) \leq 2$. Now consider $L^v_{k+1} \neq \emptyset$. By Lemma 4.2.10, $L^v_{k+2}$ is an empty set. It follows that there are no outgoing vertices from $L^v_{k+1}$. Hence, every vertex in $L^v_{k+1}$ is adjacent to some vertex $y$ in $L^v_{k}$. Moreover, by Lemma 4.2.8 there is a vertex $z \in L^v_{k-1}$ such that $d(y, z) \leq 2$, hence $d(x, z) \leq 3$. Note that the vertex $y$ is an outgoing vertex.

Now we are ready to prove Theorem 4.2.5.

**Proof of Theorem 4.2.5.** Let $F$ be a fullerene graph. We divide the proof in two parts. In the first, we prove that if $F$ is not a $(5,0)$-nanotube, then the diameter of $F$ is at most $\frac{3}{2} + \frac{5}{2}$. In the later part, we prove the bound for $(5,0)$-nanotubes.

So, assume that $F$ is not a $(5,0)$-nanotube. Let $v$ be an arbitrary vertex of $F$. We will prove that $d(u, v) \leq \frac{3}{2} + \frac{5}{2}$ for every vertex $u \in V(F)$, which will establish the first part of the theorem.

Let $C_m$ be the number of vertices in $L_{k+1}^v \cup L_k^v$ and let $L_k^v$ be the first layer that contains less then 12 vertices (according to the vertex $v$), where $k \geq 2$. By Lemma 4.2.10, $L_k^v$ or $L_{k+1}^v$ is the last layer of the fullerene. Then, the order $n$ of fullerene $F$ is

$$n = |L_0^v| + |L_1^v| + \sum_{i=2}^{k-1} |L_i^v| + |L_k^v \cup L_{k+1}^v| \geq 1 + |L_1^v| + 12(k - 2) + C_m,$$

or

$$k \leq \frac{1}{12}(n + 23 - |L_1^v| - C_m). \tag{4.2}$$

We will now determine the distance from $v$ to an outgoing vertex $x \in L_{k-1}^v$. According to the choice of vertex $v$, there are two cases:
1. Let \( v \) be adjacent to pentagons only.

Obviously, \(|L^v_1| = 9\). It also follows from Lemma 4.2.9 and from (4.2), that:

\[
d(v, x) \leq 2k - 2 \leq \frac{1}{6}(n + 2 - C_m).
\] (4.3)

Later we will see, that this case gives us better bound, but it may happen, that there
is no such possible choice of \( v \).

2. Let \( v \) be adjacent to at least one hexagon.

Obviously \(|L^v_1| \geq 10\). It also follows from Lemma 4.2.9 and from (4.2), that:

\[
d(v, x) \leq 2k - 1 \leq \frac{1}{6}(n + 7 - C_m).
\] (4.4)

So now we have the distance from \( v \) to the last layer with at least 12 vertices for both
cases above. Determining the distance from an outgoing vertex of this layer to the “end”
will establish the proof.

Let \( d_M \) be the maximal distance between the vertices in the last layer and the outgoing
vertices of layer \( L^v_{k-1} \). By Lemma 4.2.11 it follows that \( 1 \leq d_M \leq 3 \). We will now consider
all three cases to bound the number of vertices in the last layers:

- \( d_M = 3 \): By Lemma 4.2.8, we immediately infer that \( L^v_{k+1} \neq \emptyset \), so \(|L^v_{k+1}| \geq 1\).
  Moreover, since \( L^v_{k+1} \neq \emptyset \), \( L^v_k \) is not acyclic. Now, by Theorem 4.2.7 there are at
  least six incoming vertices in \( L_k \). Since there is at least one vertex in \( L^v_{k+1} \) there are
  also at least three outgoing vertices in \( L_k \). Hence, we have \( C_m = |L^v_k \cup L^v_{k+1}| \geq 10 \).

- \( d_M = 2 \): It is obvious that in this case \( L^v_{k+1} = \emptyset \). Let \( x \in L^v_k \) be such a vertex that the
distance to the closest vertex in \( L^v_{k-1} \) is two. Since \( x \) cannot be an outgoing vertex
  and since \( \deg(x) = 3 \) it follows that \( N(x) \subseteq L^v_k \), so we have \( C_m = |L^v_k| \geq 4 \).

- \( d_M = 1 \): In this case it is obvious that in the last layer there is at least one vertex,
  i.e., \( C_m = |L^v_k| \geq 1 \).

Finally, we compute the upper bound of the distance between \( v \) and a vertex in the
last layer and we use that result to compute the bound of the diameter of \( F \).

\[
\text{diam}(F) \leq d(v, x) + d_M,
\] (4.5)

where \( x \) is an outgoing vertex of \( L^v_{k-1} \). By (4.3), (4.4), and (4.5) we again have two cases,
depending on the choice of \( v \).

\[
\text{diam}(F) \leq \frac{1}{6}(n + 2 - C_m) + d_M = \frac{n}{6} + C_1,
\] (4.6)

\[
\text{diam}(F) \leq \frac{1}{6}(n + 7 - C_m) + d_M = \frac{n}{6} + C_2.
\] (4.7)
Now, we determine the upper bound of the constants $C_1, C_2$ by plugging the values computed above in (4.6) and (4.7), respectively. We infer that $C_1 \leq \frac{5}{3}$ and $C_2 \leq \frac{5}{2}$. This establishes the first part of Theorem 4.2.5. Note, that if our fullerene contains diametral vertex, adjacent only to pentagons, then we can use the bound from (4.6) with constant $C_1$, which is better than $C_2$.

Figure 4.6: A $(5,0)$-nanotube.

Suppose now that $F$ is a $(5,0)$-nanotube with $n$ vertices. Notice that $n$ is multiple of 10, or $n = 10k$, $k \in \mathbb{N}$. The diameter of the graph is determined by the most distanced vertices, and in this case they belong to the different caps and are incident only to 5-faces. Now, it is easy to compute that the theorem holds for $k \in \{2, 3, 4, 5\}$. For $k > 5$, we prove the theorem by induction on the number of vertices. Let $k \geq 5$ and assume that the theorem holds for $(5,0)$-nanotubes. A $(5,0)$-nanotube $F'$ on $10(k+1)$ vertices can be constructed easily by adding an extra layer of hexagons between already existing hexagonal layers. This construction gives us a $(5,0)$-nanotube with additional 10 vertices (see Figure 4.6). By Lemma 4.2.8 and the comment after it, we have that the diameter increases by 2, i.e.,

$$\text{diam}(F') = \text{diam}(F) + 2 = \frac{10k}{5} - 1 + 2 = \frac{10(k+1)}{5} - 1,$$

and this completes the proof. \qed
4.3 Diameter of full icosahedral-symmetry fullerene graphs

4.3.1 Construction of icosahedral fullerene graphs

The common feature of all icosahedral fullerenes is their geometrical shape. The simplest icosahedral fullerene graph is the dodecahedron, $C_{20}$. Creating bigger icosahedral fullerene graphs means adding hexagons around each pentagon in $C_{20}$ wisely. Caspar and Klug [25] and Coxeter [28] suggested a method that works with the icosahedral fullerene graph dual: geodesic domes, i.e., triangulations of the sphere with vertices of degree 5 and 6. Their method is filling the triangular faces of the icosahedron with equilateral triangles from the hexagonal tessellation of the plane.

Goldberg [60] used a hexagonal lattice to determine the vertices of the icosahedron triangular faces. Even more, Goldberg showed that the number of vertices $n$ in a polyhedra of icosahedral symmetry can be related to two integers $i$ and $j$ by the following equation, conveniently called the Goldberg equation

$$n = 20(i^2 + ij + j^2). \quad (4.8)$$

The integers $i$ and $j$ in the Goldberg equation can be considered as components of a two-dimensional Goldberg vector $\vec{G} = (i, j)$. To avoid the mirror effect, we always assume that $0 \leq i \leq j$ and $0 < j$.

![Figure 4.7: Construction of a (2, 3)-triangle, the face of a (2, 3)-icosahedral fullerene graph. The vertices of the equilateral triangle $ABC$ are centers of pentagons.](image)

Soon after the discovery of $C_{60}$, Goldberg vector turned out to be very useful in constructing bigger icosahedral fullerenes. This vector determines the distance and positions of
the vertices of the \((i, j)\)-triangle in the hexagonal lattice. See Figure 4.7 for a construction method of an \((i, j)\)-triangle. Precisely 20 such \((i, j)\)-triangles produce an \((i, j)\)-icosahedral fullerene in a manner shown on Figure 4.8. In other words, Goldberg vector defines the way of adding hexagons around each pentagonal face. The vertices of the triangle are centers of the 12 pentagons in the fullerene. The pair of the triangles \(ABC\) and \(EB'C'\), as shown on Figure 4.8, is a pair of opposite triangles. There are exactly 10 such pairs. The pentagons with centers in \(A\) and \(E\) (Figure 4.8) are called antipodal pentagons (similarly, the pentagons with centers in \(B\) and \(B'\), as well as those with centers \(C\) and \(C'\) are antipodal).

Figure 4.8: A \((2, 3)\)-icosahedral fullerene. Its triangular faces are constructed as on Figure 1. The vertices with a same name coincide. The vertices of each triangular are centers of the pentagons. The pentagons with center \(A\) and center \(E\) are antipodal pentagons, and the triangles \(ABC\) and \(EB'C'\) form a pair of opposite triangles.

The icosahedral group \(I\) is a group of symmetries of order 60. This group is isomorphic to \(A_5\), the alternating group of even permutations of five objects. The full icosahedral group \(I_h\), is the point group of symmetries of the icosahedron and dodecahedron. This group is equivalent to the group direct product \(A_5 \times \mathbb{Z}_2\) of the alternating group \(A_5\) and cyclic group \(\mathbb{Z}_2\). The order of the full icosahedral group of symmetries is 120. The \((i, i)\)-and \((0, i)\)-icosahedral fullerene graphs, \(i > 0\), have full icosahedral symmetry group, i.e., every element of this class of graphs has a symmetry group \(I_h\).

A vertex \(v\) that belongs to the border of a pentagonal face is called a pentagonal vertex. A vertex that is not pentagonal is called hexagonal.

From the structure of the icosahedral fullerene graphs it is clear that the most distant
vertices are vertices in opposite triangles. Even more, the maximal distance between two pentagonal vertices will be achieved for antipodal pentagon vertices. Combining these observations leads to the main result.

In order to determine the diameter of full icosahedral-symmetry fullerene graphs, we apply Property 3 (defined later) and find vertices from the fullerene graph closer to a specific pentagonal vertex than to any other vertex from the same pentagon. There are also vertices equally distanced from two adjacent pentagonal vertices, $a$ and $b$, but closer to $a$ and $b$ than to any other vertex from the same pentagon. We show that every pentagonal vertex is diametral, but that does not hold for all hexagonal vertices.

**Some properties of a hexagonal lattice**

As we already saw in the previous section, icosahedral fullerenes can be represented in a hexagonal lattice. Due to this fact, we present some properties of a hexagonal lattice needed in the next sections.

Tilling a plane with hexagons, means adding hexagons in three different directions, denoted by $\vec{i}$, $\vec{j}$ and $\vec{k}$ on Figure 4.9. Notice that $\vec{k} = -\vec{i} - \vec{j}$. Without loss of generality we can assume that one of the directions is horizontal, say $\vec{k}$. Now, every vertex $a$ is incident to precisely one edge normal to $\vec{k}$, i.e., is incident to a vertical edge $e_a$. Also, $a$ is incident to a hexagonal face $h_a$, not containing $e_a$. We say that $a$ is a *top vertex* if the vertical edge $e_a$ is above the hexagon $h_a$. If the vertical edge $e_a$ is below the hexagon $h_a$, then we say that $a$ is a *bottom vertex*. For example in Figure 4.9 (a), the vertex $a$ is a top vertex, and the vertex $b$ is a bottom vertex.

Let $a$ and $b$ be two different vertices in a hexagonal lattice. We can assume that $a$ is up and left from $b$, or they are in a same line of hexagons (in some of the directions $\vec{i}$, $\vec{j}$ or $\vec{k}$). Let $h_a$ and $h_b$ be the hexagons defined above for $a$ and $b$ respectively. The lines parallel to $\vec{i}$, $\vec{j}$ and $\vec{k}$ passing trough the centers of $h_a$ and $h_b$ form three different parallelograms, the smallest one is the parallelogram determined by the vertices $a$ and $b$. In the case when $a$ and $b$ belong to the same line of hexagons, this parallelogram is a segment.

The parallelogram determined by the vertices $a$ and $b$ defines a unique (hexagonal) parallelogram patch. Depending on the type of the vertices $a$ and $b$, there are three types of (hexagonal) parallelogram patches, as shown on Figure 4.9.

The first property determines the distance, i.e., one of the shortest paths between any two vertices in a hexagonal lattice.

**Property 1.** Let $a$ and $b$ be two vertices in a hexagonal lattice, defining a (hexagonal) parallelogram patch $\mathcal{P}$. One of the shortest paths between the vertices $a$ and $b$ consists of
Figure 4.9: All three types of parallelogram patches defined by the vertices \(a\) and \(b\) in a hexagonal lattice. \textit{Type-a}: the vertex \(a\) is top vertex and \(b\) is bottom vertex. \textit{Type-b}: both of the vertices are of the same type. \textit{Type-c}: The vertex \(a\) is bottom vertex and the vertex \(b\) is top vertex.

Moreover, every vertex from the (hexagonal) parallelogram patch belongs to a shortest path between the vertices determining the patch.

**Property 2.** Let \(a\) and \(b\) be two vertices in a hexagonal lattice. Let \(x\) be a vertex from the (hexagonal) parallelogram patch determined by \(a\) and \(b\). Then, there is a shortest path between \(a\) and \(b\) that contains \(x\).

Notice that, if a vertex \(x\) does not belong to a (hexagonal) parallelogram patch determined by the vertices \(a\) and \(b\), then there is no shortest path between \(a\) and \(b\) containing \(x\).

A \textit{bisector} of an edge (a segment) in the hexagonal grid is the line orthogonal to the edge passing through its midpoint. Now, the final property of a hexagonal lattice needed is obvious.

**Property 3.** Let \(a\) and \(b\) be adjacent vertices in a hexagonal lattice. Let \(p\) be the bisector of the edge \(ab\) dividing the lattice into two sections. The section containing the vertex \(a\) also contains all the vertices closer to \(a\) than to \(b\) (and vice versa).

### 4.3.2 Diameter of \((0, i)\)-icosahedral fullerene graphs

First we calculate the diameter of a \((0, i)\)-icosahedral fullerene graph, \(i > 0\). In this case, unlike the others, every hexagonal vertex belongs to a diametral path between any pair of diametral pentagon vertices \([10]\).

**Theorem 4.3.1.** Let \(G\) be a \((0, i)\)-icosahedral fullerene graph, with \(i > 0\). Then \(\text{diam}(G) = 6i - 1\).
Proof. Let \( v \) be a pentagonal vertex. Due to symmetry, we can assume that \( v = a \) as shown on Figure 4.10. We want to determine the closest vertex (vertices) to the vertex \( a \) from the antipodal pentagon. In order to do that, we apply Property 3 twice, once on each edge incident to \( a \).

From the structure of a \((0, i)\)-icosahedral fullerene graphs, it is obvious that the bisector of the bordering edge of a pentagon overlaps with an edge of a \((0, i)\)-triangle. Therefore, we find two different bisectors of a pentagonal edge. As a result of this “phenomenon”, there are vertices that are equally distanced from the vertices \( a \) and \( b \), since they are at the same time on the “left” and on the “right” side from the bisector of the edge \( ab \).

Consider that the vertices of the fullerene are grouped in ten sections \( A, B, \ldots, CD \) and \( DE \) as depicted in Figure 4.10. All the vertices left from the bisector of the edge \( ab \), i.e., the sections \( A, AE, AB \) are closer to the vertex \( a \) than to \( b \). At the same time the vertices on the right side of the bisector (the sections \( B, AB, BC \)) are closer to \( b \). This implies that the vertices from the section \( AB \) are equally distant from the vertices \( a \) and \( b \).

The same analysis can be done for all five pentagonal vertices. By combining we conclude that the vertices from the section \( A \) are closer to the vertex \( a \) than to any other pentagonal vertex from the same pentagon. The vertices in the section \( AB \) (resp. \( AE \)) are at same distance from the vertex \( a \) and from the vertex \( b \) (resp. from the vertex \( a \) and the vertex \( e \)), but closer to \( a \) and \( b \) (resp. \( a \) and \( e \)) than to any other vertex from the same pentagon (Figure 4.10).

Now, it is clear that the closest antipodal pentagon vertices to the vertex \( a \) are \( c' \) and \( d' \). The union of sections \( A \) and \( AB \) is the parallelogram defined by the vertices \( a \) and \( d' \), respectively. The union of the sections \( A \) and \( AE \) is the parallelogram defined by the vertices \( a \) and \( c' \). Observe that the parallelogram patch defined by these vertices (\( a \) and \( d' \) or \( a \) and \( c' \)) is of type-\( a \). Due to the symmetry of the graph, the same holds for the vertices \( a \) and \( c' \).

By Property 2, for every vertex \( x \) from the sections \( A \) and \( AB \) there is a shortest path between \( a \) and \( d' \) that contains \( x \). From the above, Property 1, and the construction of \((0, i)\)-triangle (Figure 1), we conclude that the distance between two antipodal pentagons is equal to \( 6i - 3 \). Moreover the following holds:

Claim 1. The distance between a pentagonal vertex \( v \in V(G) \) and its closest vertices from the antipodal pentagon is \( 6i - 3 \). Moreover, there are precisely two such vertices.

Notice that a path between the vertices \( a \) and \( e' \) that goes trough \( b \) is comprised by the shortest path between \( b \) and \( e' \) and the edge \( ab \). This path is of length \( 6i - 2 \), and there
is no shorter path since the vertex $e'$ is closer to $b$ than to $a$. Clearly there are paths of length $6i - 1$ between the vertices $a$ and $a'$, and these paths are the shortest. If there is shorter path between $a$ and $a'$, then the distance between $b$ and $a'$, or between $e$ and $a'$ is $6i - 3$ what contradicts with Claim 1. So, we have that the following claim holds.

**Claim 2.** The maximum distance between two pentagonal vertices is $6i - 1$.

Observe that, for every pentagonal vertex $v$, there is a unique pentagonal vertex $u$ such that $d(u, v) = 6i - 1$. Next claim determines the upper bound of the distances between pentagonal and a hexagonal vertex.

**Claim 3.** Let $u$ and $v$ be pentagonal vertices at distance $6i - 1$. Let $w$ be an arbitrary vertex. There is a shortest path between $u$ and $v$ that goes trough $w$.

In order to prove this claim, let $v = a$ and $u = a'$. If $w$ is in the sections $A$ or $AB$, by Property 2, there is a path $P_1$ between $a$ and $d'$ of length $6i - 3$ that contains the vertex $w$, so the desired path is $P = P_1d'e'a'$. If $w$ is in the sections $B$ or $BC$, there is a path $P_2$ from $b$ to $e'$ trough $w$ of length $6i - 3$, i.e., $P = abP_2e'a'$ is a path of length $6i - 1$ between $a$ and $a'$ that contains $w$. If $w$ is in one of the sections $C$ or $CD$, then the required path comprised of the 2-path $abc$ and a path $P_3$ from $c$ to $a'$ containing $w$. By the symmetry of the graph, all the cases are covered, and that proves this claim.

Claim 3 implies that the distance between any pentagonal and hexagonal vertices is
less than $6i - 1$.

Let $w_1$ and $w_2$ are two hexagonal vertices. By Claim 3, we can fix pentagonal vertices $u$ and $v$ at distance $6i - 1$ and a pair of $u-v$ paths trough $w_1$ and $w_2$, respectively. The union of these two paths gives a closed walk of length $2(6i - 1)$. Therefore we have that the distance between any two hexagonal vertices is at most $6i - 1$.

**Claim 4.** The distance between any two hexagonal vertices is at most $6i - 1$.

Finally, this claim completes the proof of the Theorem 4.3.1.

By the icosahedral symmetry of the fullerene graph and the previous theorem follows:

**Corollary 4.3.2.** Let $G$ be a $(0,i)$-icosahedral fullerene graph, $i > 0$. Then, every pentagon vertex in $G$ is diametral. Even more for every pentagonal vertex, there is a unique (pentagonal) vertex at distance $\text{diam}(G)$.

![Figure 4.11: A (0,3)-icosahedral fullerene graph with diameter 17. The vertex $s$ is not diametral. Blue vertices are at distance 4 from $s$, white at distance 8, and green vertices are at distance 12. The most distanced vertices from $s$ are the vertices $d_1$, $d_2$, and $d_3$, which are on distance 15.](image)

On the other side, there are hexagonal vertices that are not diametral. Notice that the number of vertices at maximum distance from a hexagonal vertex is not necessarily one as shown in Example 4.1.

**Example 4.1.** By Theorem 4.3.1, the diameter of the $(0,3)$-icosahedral fullerene is 17. Let $s$ be a hexagonal vertex from the considered fullerene, as shown on Figure 4.11. The most distanced vertices from $s$ are $d_1$, $d_2$, and $d_3$ and $d(s, d_i) = 15$, $i = 1, 2, 3$. The vertex $s$ is not diametral, and there are three different vertices at maximal distance from $s$. 
4.3.3 Diameter of \((i, i)\)-icosahedral fullerene graphs

Another type of fullerene graphs with full icosahedral symmetry are fullerenes with Goldberg vector \(\vec{G} = (i, i)\) where \(i > 0\). In this section we determine the diameter of such graphs \([10]\).

**Theorem 4.3.3.** Let \(G\) be an \((i, i)\)-icosahedral fullerene graph, with \(i > 0\). Then \(\text{diam}(G) = 10i - 1\).

*Proof.* Similarly as in the proof of Theorem 4.3.1 we show that every pentagonal vertex is diametral. Due to the symmetry of the graph we can choose any pentagonal vertex, say vertex \(a\) as shown on Figure 4.12.

First we will determine the vertices closer to \(a\) than to any other vertex from the same pentagon. Apply Property 3 for vertices \(a\) and \(b\), later apply the same property for vertices \(a\) and \(e\). It is clear that vertices \(c'\) and \(d'\) are equally distanced from vertex \(a\), and at the same time they are the closest vertices to \(a\) from the antipodal pentagon (see Figure 4.12). The parallelogram patch defined by vertices \(a\) and \(c'\) (or \(d'\)) is of type-c.

The bisector of the edge \(ab\) passes through the center of a pentagon, in this case the point \(x_1\), and breaks into two lines. This can easily be seen if we rotate the triangle \(x_1x_3x_4\) such that the points \(x_4\) and \(x_5\) are identified. In such a way we get the vertices equally distanced form \(a\) and \(b\). Vertices right from the line \(x_2x_4\) do not belong in the parallelogram patch defined by \(a\) and \(d'\), but belong to the parallelogram patch defined by \(b\) and \(e'\), therefore they are closer to \(b\) than to \(a\). In the same manner we find vertices closer to \(a\) than to \(e\), as well as vertices equally distanced from them, but closer to \(a\) and \(e\) than to any other vertex from the same pentagon. The sections of vertices closer to a different pentagonal vertices of the same pentagon are illustrated on Figure 4.12. The construction of an \((i, j)\)-icosahedral fullerene graph, Property 1, and the previous observation give the following claim.

**Claim 1.** The distance between two antipodal pentagons is \(10i - 3\).

Notice, that by Property 2 all the vertices from the sections \(A\), \(AB\) and \(AE\), belong to a shortest path between \(a\) and \(c'\) or between \(a\) and \(d'\). So, there are paths of length \(10i - 1\) between \(a\) and \(a'\) and these paths are the shortest. One such path is comprised by a 2-path \(abc\) and one of the shortest paths between the vertices \(c\) and \(a'\). By this and Claim 1 we have the following.

**Claim 2.** The maximum distance between any two pentagonal vertices is \(10i - 1\).
Figure 4.12: A \((3,3)\)-icosahedral fullerene graph. Vertices in the section \(A\) are closer to vertex \(a\) than to any other vertex from the same pentagon. Vertices in the section \(AB\) (resp. \(AE\)) are equally distanced to \(a\) and \(b\) (resp. to \(a\) and \(e\)), but closer to \(a\) and \(b\) (resp. \(a\) and \(e\)) than to any other vertex from the same pentagon. The diametral vertex of the vertex \(a\) is \(a'\).

Notice that the distance between the vertex \(a\) and any other hexagonal vertex is less than \(10i - 1\). If the hexagonal vertex \(x\) belongs to the sections \(B\) or \(BC\) (resp. \(E\) or \(DE\)), the distance \(d(x,b) < 10i - 3\) (resp. \(d(x,e) < 10i - 3\)). So a shortest path between \(a\) and \(x\) is comprised by the edge \(ab\) (resp. \(ae\)) and a shortest path between \(b\) and \(x\) (resp. \(e\) and \(x\)). Similarly if vertex \(x\) belongs to sections \(C\) or \(CD\) (resp. \(D\) or \(CD\)), the shortest path between vertices \(a\) and \(x\) is comprised by the 2-path \(abc\) (resp. \(aed\)) and a shortest path between \(c\) and \(x\) (resp. \(d\) and \(x\)). Similarly as the case of \((0,i)\)-icosahedral fullerene graphs, \(i > 0\), for every pentagonal vertex \(v\) there is a unique antipodal vertex. The distance between these two vertices in \((i,i)\)-icosahedral fullerene graph \(i > 0\) is \(d(u,v) = 10i - 1\). Next we should determine the distance between any two hexagonal vertices.

**Claim 3.** Let \(F_0\) and \(F_1\) be antipodal pentagons. Then for any two hexagonal vertices \(w_1\) and \(w_2\), there is a pair of pentagonal vertices \(v \in V(F_0)\) and \(u \in V(F_1)\) at distance \(10i - 1\) such that there are shortest paths \(P_1\) and \(P_2\) between \(u\) and \(v\) containing \(w_1\) and \(w_2\) respectively.

To prove this claim, first let locate the vertices that belong to a shortest path between
Figure 4.13: The uncolored part of the fullerene contains the vertices that belong to a shortest path between \(a\) and \(a'\). This part is an union of the (hexagonal) parallelogram patches determined by the vertices: \(a\) and \(c'\), \(a\) and \(d'\), \(b\) and \(e'\), \(c\) and \(a'\), \(d\) and \(a'\), or the vertices \(e\) and \(b'\), since every vertex from these parallelograms belongs to a path of length \(10i - 1\) between the vertices \(a\) and \(a'\). The shaded parallelograms are the sections of vertices that do not belong to a shortest path between the vertices \(a\) and \(a'\). The vertices \(a\) and \(a'\). Clearly all the vertices from the sections \(A\), \(AB\) and \(AE\) belong to such a path. Further, we have that all the vertices that belong to a shortest path between vertices \(b\) and \(e'\) also belong to a path of length \(10i - 1\) between \(a\) and \(a'\). By Property 2, every vertex \(x\) from the (hexagonal) parallelogram patch determined by vertices \(b\) and \(e'\) belongs to a shortest path \(P_x\) between \(b\) and \(e'\), and the required path is \(abP_xe'a'\). Similarly, each vertex from the (hexagonal) parallelogram patch determined by vertices \(c\) and \(a'\) belongs to a shortest path between \(a\) and \(a'\). This path is comprised by the 2-path \(abc\) and a shortest path between \(c\) and \(a'\) containing the corresponding vertex. Due to the symmetry of the graph we find all the vertices that belong to a shortest path between \(a\) and \(a'\). These vertices belong to the uncolored section of the fullerene graph as illustrated on Figure 4.13. Respectively, the complement of this section contains vertices that do not belong to such a path.

By the symmetry of the graph we can find these sections for all five vertices on the border of \(F_0\) as shown on Figure 4.14. On Figure 4.13, we can see that if \(w_1\) or \(w_2\) do not belong to any of the shaded sections according to some vertex, let say \(a\), then we can choose \(v = a\) and \(u = a'\). If only one of the vertices belongs to a shaded section, say section \(S_1\), then \(v\) can be one of the vertices \(\{b, c, d\}\). Now, let both vertices belong to some of the shaded sections. There are ten such sections (Figure 4.14). Without loss of generality we can assume that \(w_1\) belongs to the section \(S_1\). We consider two cases:
Figure 4.14: The vertices from the sections sections $S_1$, $S_3$, $S_6$ and $S_8$ might not belong to a shortest path between $a$ and $a'$, as shown on Figure 4.13. Using the symmetry of the graph we find that sections of vertices that might not belong to a shortest path between the vertices: $b$ and $b'$ (sections $S_3$, $S_5$, $S_8$ and $S_{10}$), $c$ and $c'$ (sections $S_2$, $S_5$, $S_7$ and $S_{10}$), $d$ and $d'$ (sections $S_2$, $S_4$, $S_7$ and $S_9$), and $e$ and $e'$ (sections $S_1$, $S_4$, $S_6$ and $S_9$).

- If $w_2$ belongs to some of the sections $S_1$, $S_3$, $S_5$, $S_6$, $S_8$ or $S_{10}$, then we choose $v = d$ and $u = d'$.
- If $w_2$ belongs to some of the sections $S_2$, $S_4$, $S_7$ or $S_9$, then $v = b$ and $u = b'$.

This proves Claim 3. Notice that there are more different possibilities for the choices for $u$ and $v$.

Now, by Claim 3, we have that for every pair of hexagonal vertices, there is a closed walk of length at most $2(10i - 1)$ going through both of the vertices. That gives the following claim.

**Claim 4.** The distance between any two hexagonal vertices is not greater than $10i - 1$.

This claim establishes the theorem. }

Theorem 4.3.1 and Theorem 4.3.3 can be combined together. Then we obtain the theorem for a diameter of fullerene graphs with full icosahedral symmetry [10].

**Theorem 4.3.4.** Let $G$ be an $(i, j)$-icosahedral fullerene graph, such that $0 = i < j$ or $0 < i = j$. Then, the diameter of $G$ is given by

$$
\text{diam}(G) = 4i + 6j - 1.
$$
Applying Goldberg equation (4.8) and Theorem 4.3.4 we conclude that the diameter of a fullerene graph with full icosahedral symmetry is of order $\Theta(\sqrt{n})$. If we consider an $(i,i)$-icosahedral fullerene $G$ ($i > 0$) then by (4.8), $n = 60i^2$. By Theorem 4.3.4, $\text{diam}(G) = 10i - 1$, i.e., $\text{diam}(G) = 10\sqrt{\frac{n}{60}} - 1 = \sqrt{\frac{5n}{3}} - 1$. As we believe that the icosahedral fullerenes have the smallest diameter, it leads us to conjecture the following:

**Conjecture 4.3.1.** Let $G$ be a fullerene graph on $n$ vertices. Then

$$\text{diam}(G) \geq \left\lfloor \sqrt{\frac{5n}{3}} \right\rfloor - 1.$$

### 4.4 Bounds on some related invariants

#### 4.4.1 Lower bound on the independence number

Independence number of fullerene graphs attracted a lot of attention not only as a potential stability predictor [50], but also in the context of study of independent sets as possible models for addition of bulky segregated groups such as free radicals or halogen atoms [17]. Sharp upper bounds on the independence number of $n/2 - 2$ for general fullerenes and $n/2 - 4$ for those with isolated pentagons follow by simple counting argument [53]. Lower bounds were gradually improved from (almost) trivial $\alpha(G) \geq n/3$ valid for all 3-chromatic graphs to $\alpha(G) \geq \frac{3}{8}n$ mentioned in section 2 [73]. A better lower bound of type $\alpha(G) \geq \frac{n}{2} - C\sqrt{n}$, for some constant $C$, was established for icosahedral fullerenes [61]. Using Theorem 4.1.1, it can be shown that such a bound holds for all fullerene graphs [7], which goes in favor to Conjecture 4.1.3.

**Theorem 4.4.1.** Let $G$ be a fullerene graph with $n$ vertices. Then

$$\alpha(G) \geq \frac{n}{2} - 78.58 \sqrt{n}.$$

**Proof.** Let $G$ be a fullerene graph with $n$ vertices. By the upper bound $\varphi(G) \leq 39.29 \sqrt{n}$ [43], it follows that the removal of at most $39.29 \sqrt{n}$ edges from $G$ results in a bipartite spanning subgraph $G'$. At least one of the two partition classes of $G'$, call it $W'$, is of size at least $\frac{n}{2}$, and it is an independent set in $G'$. We know that the set $M$ of removed edges forms a matching [41], and that each edge from $M$ connects two vertices from the same partition class of $G'$. Even if each edge of $M$ connects two vertices from $W'$ in $G$, there are at most $39.29 \sqrt{n}$ edges in $M$, and hence the vertices of $W'$ not incident to any edge from $M$ form an independent set in $G$ of cardinality at least $\frac{n}{2} - 2 \cdot 39.29 \sqrt{n} = \frac{n}{2} - 78.58 \sqrt{n}$. \qed
Theorem 4.2.5 and Theorem 4.4.1 imply the next corollary.

**Corollary 4.4.2.** Let $G$ be a fullerene graph with $n$ vertices. If $n$ is sufficiently large, then

$$\alpha(G) \geq 2(diam(G) - 1).$$

**Proof.** Using the bounds in Theorem 4.2.5 and Theorem 4.4.1 it is not hard to compute that when $n \geq 617,502$, the following series of inequalities holds:

$$\alpha(G) \geq \frac{n}{2} - 78.58 \sqrt{n} \geq 2 \left( \frac{n}{5} + 1 \right) - 1 \geq 2(diam(G) - 1).$$

Hence, Corollary 4.4.2 settles Conjecture 4.1.4, for all fullerenes of sufficiently large order.

### 4.4.2 Upper bound on the smallest eigenvalue

Recall that the smallest eigenvalue $\lambda_n(G)$ of a 3-regular graph $G$ and the largest Laplacian eigenvalue $\mu_\infty(G)$ of $G$ are related via the following relation ([59, pp. 280]):

$$\lambda_n(G) = 3 - \mu_\infty(G).$$

By plugging this into Theorem 4.1.2 and noting that $\text{bip}(G) = \frac{3}{2}n - \varphi(G)$ we obtain an upper bound on $\lambda_n(G)$ in terms of the bipartite edge frustration of $G$ of the form $\lambda_n(G) \leq -3 + \frac{4}{n} \varphi(G)$. By taking into account an upper bound on $\varphi(G)$ we immediately obtain the following upper bound on the smallest eigenvalue of a fullerene graph with $n$ vertices [7].

**Theorem 4.4.3.** Let $G$ be a fullerene graph with $n$ vertices. Then,

$$\lambda_n(G) \leq -3 + \frac{157.16}{\sqrt{n}}.$$

Since the smallest eigenvalue of $C_{60}$ is $-\phi^2$, where $\phi$ is the golden ratio $\frac{1+\sqrt{5}}{2}$, an immediate consequence is that Conjecture 4.1.2 is true for all fullerene graphs with at least 169,291 vertices.
4.4.3 Upper bound on the saturation number

In this subsection we improve the upper bound on the saturation number \( s(G) \) in fullerene graphs. Using the obtained lower bound on the diameter we are able to improve the logarithmic additive correction of Theorem 4.1.3 and to prove the following result [7].

**Theorem 4.4.4.** Let \( G \) be a fullerene graph with \( n \) vertices. Then,

\[
s(G) \leq \frac{n}{2} - \frac{1}{4} (\text{diam}(G) - 2).
\]

In particular,

\[
s(G) \leq \frac{n}{2} - \frac{\sqrt{24n - 15} - 15}{24}.
\]

**Proof.** Let \( G \) be a fullerene graph with \( n \) vertices and diameter \( k \). Let \( x \) and \( y \) be a pair of diametral vertices of \( G \), i.e., \( d(x, y) = k \). By Theorem 4.2.4, we have that \( k \geq \frac{\sqrt{24n - 15} - 3}{6} \).

Let \( P = xv_1v_2 \cdots v_{k-1}y \) be a shortest path between \( x \) and \( y \). Notice that vertices \( v_i \), for every even \( i \) such that \( 1 \leq i < k \), form an independent set \( I \). We call a vertex \( v \) *even* if \( v \in I \), and *odd* if \( v \in V(P) \setminus I \). In what follows, we will construct a maximal matching \( M \) in \( G - I \) such that it will cover all the vertices adjacent to \( I \). The idea is to choose a set of independent edges covering all neighbors of \( I \) with no vertex of \( I \) being covered and then extend it to a maximal matching \( M \).

For \( i \in \{1, 2, \ldots, k - 1\} \), let \( u_i \) be the third neighbor of \( v_i \) distinct from \( v_{i-1} \) and \( v_{i+1} \) (for convenience, we define \( v_0 = x \) and \( v_k = y \)), and let \( w^1_i, w^2_i \) be the two neighbors of \( u_i \) distinct from \( v_i \).

![Figure 4.15: An independent set with three unmatched vertices \( v_2, v_4, \) and \( v_6 \).](image)

First, we show that all the vertices \( u_i \) are distinct. It is easy to see that we obtain a cycle of length less than 5 if \( u_i \) is adjacent to \( v_j \), for \( j \in \{i - 2, i - 1, i + 1, i + 2\} \), which violates the girth condition of fullerene graphs. Moreover, since vertices \( v_i \) are on the shortest path between \( x \) and \( y \), we have that \( i - 1 \leq d(x, u_i) \leq i + 1 \), and so \( u_i \) is not adjacent to \( v_j \), if
$|j-i| > 2$. Hence, all $u_i$'s are distinct and the edges $u_i v_i$ independent. We add the edges $u_i u_i$, for every odd $v_i$, to the matching $M$.

In order to match all neighbors of vertices labeled with even number, it remains to add either the edge $u_i w_i^1$ or the edge $u_i w_i^2$ to $M$, for all even $v_i$. First, notice that a vertex $u_i$ may be adjacent to some $u_j$, for $j \in \{i-3, i+3\}$, that means the edge $u_i u_j$ cannot be in $M$, since $u_j$ is already covered. Fortunately, since $P$ is a shortest path, both edges $u_i u_{i-3}$ and $u_i u_{i+3}$ cannot appear in $G$. Therefore, for all such $u_i$, let $w_i \in \{w_i^1, w_i^2\}$ be distinct from $u_j$ and add the edge $u_i w_i$ to $M$.

Now, let $H$ be the subgraph of $G$ induced by the edges $u_i w_i^j$, where $i$ is even, $j \in \{1, 2\}$, and $w_i^j \neq u_{i \pm 3}$ (observe, that it may happen, that $w_i^j = u_{i \pm 2}$, see Figure 4.15). We claim that $H$ has the following properties:

1. $\Delta(H) \leq 2$.

(2) No path component of $H$ starts and ends with $u_i$'s.

We prove each claim separately. Observe that vertex $u_i$ cannot be of degree 3, since it is adjacent to $v_i$ which is not a vertex of $H$. So, suppose that some $w_i^j$ is of degree 3 in $H$. Then, $w_i^j$ must be adjacent to $u_{i-2}$, $u_i$, and $u_{i+2}$ as $P$ is a shortest path. But, since no separating cycles of size 5 or 6 exist in fullerene graphs, we infer that $w_i^j$ is of degree at most 2. This proves (1).

Now we show claim (2). Suppose that $P'$ is a path that starts with a vertex $u_a$ and ends with a vertex $u_b$, for some $a, b \in \{1, 2, \ldots, k-1\}$. We assume that $a < b$. A vertex $u_i$ has degree 1 in $H$ only if it is adjacent to $u_{i-3}$ or $u_{i+3}$ in $G$. Thus $u_a$ is adjacent to $u_{a-3}$ or $u_{a+3}$. Since $G$ has no separating cycles of length at most 6, we conclude that $u_a$ must be adjacent to $u_{a-3}$. Similarly, $u_b$ must be adjacent to $u_{b+3}$. So, the path $v_{a-3} u_{a-3} P' u_{b+3} v_{b+3}$ is shorter than the path $v_{a-3} v_{a-2} \ldots v_{b+3}$, contradicting the fact that the path $P$ is a shortest path between $x$ and $y$.

Finally, we find a matching $M'$ in $H$ that covers all $u_i$'s in $H$. We consider every component $C$ of $H$ separately. By (1), they are only paths and cycles. If $C$ is a path in $H$ that does not start nor end with $u_i$, we add every second edge of $C$ to $M'$. Otherwise, we start with the edge incident to $u_i$ with which $C$ starts or ends. By (2), it follows that all $u_i$'s of $C$ are covered. If $C$ is an even cycle, we simply add every second edge of $C$ to $M'$. In case when $C$ is an odd cycle, it contains an edge $u_i u_{i+2}$ for some $i$. We add $u_i u_{i+2}$ to $M'$ and choose the edges of the path $C - u_i u_{i+2}$ as described above.

In this way, every $u_i$ in $H$ is matched and we add the edges of $M'$ to $M$. Hence, we have matched all the neighbors of the even vertices. Next, extend $M$ to a maximal matching in
Since no even vertex is matched by the edges in $M$, its size is at most

$$|M| \leq \frac{n - |I|}{2} = \frac{n}{2} - \frac{1}{2} \left[ \frac{\text{diam}(G) - 2}{2} \right] \leq \frac{n}{2} - \frac{\text{diam}(G) - 2}{4} \leq \frac{n}{2} - \frac{\sqrt{24n - 15} - 15}{24},$$

which establishes the theorem.

\[ \square \]

### 4.5 Further work

We have established new lower and upper bounds on the diameter of fullerene graphs and combined it with recently established upper bounds on the bipartite edge frustration to derive improved bounds on the independence number, the smallest eigenvalue, and the saturation number of fullerene graphs.

The main motivation for exploring fullerenes is finding appropriate invariants that can predict the stability of the molecule. Not all fullerenes that can be drawn as graphs, or those that can be constructed in laboratories can be found in nature. Chemists believe that some conditions must be fulfilled for a physical existence of the particular fullerene. All fullerene obtained by a leapfrog construction are satisfying this condition \([59]\), but outside of this group very few fullerenes do. Another condition for a fullerene to exist in nature is satisfying the isolated pentagons rule. Chemists believe that these fullerenes are more stable. Theorem 4.2.5 tells us that the among all fullerenes on $n$ vertices (5,0)-nanotube has the longest diameter, and this fullerene is not IPR.

This observation combined with some other fullerene graph properties made us believe that the IPR fullerene graphs have smaller diameter. Even more we found that the following holds \([2]\).

**Theorem 4.5.1.** Let $G$ be a IPR fullerene graph on $n$ vertices. Then there exists a constant $C > 0$ such that

$$\text{diam}(G) \leq \frac{n}{10} + C.$$
Appendix A.
Asymptotic notation

The important definitions for dealing with lower and upper bounds are the $O$, $\Omega$ and $\Theta$ notations.

$O$-notation: For non-negative functions, $f(n)$ and $g(n)$, if there exists an integer $n_0$ and a constant $c > 0$ such that for all integers $n > n_0$, $f(n) \leq c \cdot g(n)$, then $f(n) = O(g(n))$.

$\Omega$-notation: For non-negative functions, $f(n)$ and $g(n)$, if there exists an integer $n_0$ and a constant $c > 0$ such that for all integers $n > n_0$, $f(n) \geq c \cdot g(n)$, then $f(n) = \Omega(g(n))$.

$\Theta$-notation: For non-negative functions, $f(n)$ and $g(n)$, $f(n)$ is theta of $g(n)$ if and only if $f(n) = O(g(n))$ and $f(n) = \Omega(g(n))$. This is denoted as $f(n) = \Theta(g(n))$. 
Bibliography


[48] S. Fajtlowicz, Written on the Wall (A List of Conjectures of Graffiti), *(available from the author on request).*


[92] S. Nikolić, G. Kovačević, A. Milčević, N. Trinajstić, The Zagreb indices 30 years after, 


[96] D. Stevanović, Remarks on Fowler–Manolopoulos predictor of fullerene stability, 


[104] D. Vukičević, A. Graovac, Comparing Zagreb $M_1$ and $M_2$ indices: Overview of the results, manuscript.


Daljši povzetek

V doktorskem delu se bomo osredotočili na del teorije grafov, ki se uporablja v kemiji. Od XVII stoletja je znano, da imajo molekule posebno strukturo, zgodovinsko so se te strukture predstavljale na različne načine. Ena taka predstavitev je z grafom. V tej predstavitvi je vsak atom predstavljen kot vozlišče in vezi med njimi kot povezave grafa. Omenimo, da nas tukaj ne zanimajo vrste atomov, ki nastopajo v molekuli, temveč le kateri atomi so medseboj povezani tako da si delijo vsaj en skupen elektron. V tem smislu se teorija grafov uporablja za matematično modeliranje molekul iz katerih bi radi pridobili fizikalne lastnosti molekul.

Molekulski deskriptor je količina, ki jo izračunamo iz grafa kemijske spojine in za katero verjamemo (včasih pa lahko tudi argumentiramo), da odraža pomembne strukturne lastnosti molekule. Kakšnih 20 let nazaj je bilo znanih nekaj deset molekulskih deskriptorjev, od tega le nekaj uporabnih v kemiji. Število indeksov, ki so se izkazali pri odkrivanju farmacevtsko pomembnih spojinch, je do današnjega dne naraslo [36, 99].


Zagrebški indeks


$$M_1(G) = \sum_{v \in V} d(v)^2 \quad \text{in} \quad M_2(G) = \sum_{uv \in E} d(u)d(v).$$

Zaradi enostavnosti se pogostokrat uporabljata okrajšave $M_1$ in $M_2$.

Leta 2003 je članek [92] populariziral Zagrebška indeksa in od takrat je bilo opravljeno veliko raziskav na tem področju. Za več rezultatov v povezavi z Zagrebškima indeksoma glej [89, 104].

Primerjava vrednosti teh indeksov je zelo naravna in še vedno daje zanimive rezultate. Najprej je bila predlagana naslednja računalniško ustvarjena domneva [22]:

**Domneva 1.** Za vse enostavne grafe $G$ velja,

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \quad (1)$$

**Domneva 1.** Za vse enostavne grafe $G$ velja,

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}$$

in enakost velja za polne grafe.

Če je graf regularen, potem velja enakost. Enakost velja tudi, če je $G$ zvezda. Neenakost (1) velja za drevesa [103], za grafe s maksimalno stopnjo 4, t.j. tako imenovane kemijske grafe [72] in tudi za uniciklične grafe [24]. Neenačba pa v splošnem ne velja.

Za graf $G$ rečemo, da je dober, če velja neenakost (1). Ker za drevesa in uniciklične grafe velja $M_1/n \leq M_2/m$, so ti grafi dobri. V delu sta oba rezultata dokazana na krajišni način [5]. Pokazali smo, da je vsak graf z ciklotrojnim številom največ 2 podgraf dobre biciklične grafe.

Včasih, da bi ugotovili ali velja neenakost oz. kdaj velja neenakost, obravnavamo kdaj je razlika $M_2/m - M_1/n$ negativna. Naj bo $m_{i,j}$ število povezav, ki povezujejo vozlišča stopnje $i$ z vozlišči stopnje $j$ v grafu $G$. Vukičević je pokazal [72] da velja:

$$\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i \leq j, k \leq l \in \mathbb{N}^2 \atop (i,j),(k,l) \in \mathbb{N}^2}} \left[ i j \left( \frac{1}{k} + \frac{1}{l} \right) + kl \left( \frac{1}{i} + \frac{1}{j} \right) - i - j - k - l \right] m_{i,j} m_{k,l}. \quad (2)$$

Da poenostavimo izraz (2), definirajmo naslednjo funkcijo $f$ in si poglejmo njene lastnosti. Za cela števila $i, j, k, l$ naj bo

$$f(i, j, k, l) = i j \left( \frac{1}{k} + \frac{1}{l} \right) + kl \left( \frac{1}{i} + \frac{1}{j} \right) - i - j - k - l.$$
Zdaj lahko (2) zapišemo kot
\[
\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i,j,k,l \in N^2 \atop (i,j),(k,l) \in N^2}} f(i,j,k,l)m_{i,j}m_{k,l}.
\]
Opazimo, da se funkcija \( f \) prepiše v
\[
f(i,j,k,l) = (ij - kl) \left( \frac{1}{k} + \frac{1}{l} - \frac{1}{i} - \frac{1}{j} \right)
\]
in ima nekaj simetrijskih lastnosti.

Označimo z \( D(G) \) množico stopnjen vozlišč grafa \( G \),
\[
D(G) = \{ d(v) \mid v \in V \}.
\]
Pravimo, da je množica celih število \( S \) dobra, če za vsak graf \( G \) za katerega je \( D(G) \subseteq S \) velja neenakost (1). V nasprotnem primeru je \( S \) slaba množica.

Kot smo že omenili, je domneva 1 v splošnem neveljavna, velja pa za regularne grafe. Lahko se vprašamo, če velja tudi za ”skoraj regularne” grafe, t.j. za grafe samo z nekaj različnimi stopnjami vozlišč. Preverili smo da velja za grafe z le dvema stopnjama vozlišč. Tudi vsak interval dolžine 3 je dober. Še več, velja naslednje:

**Trditev 1.** Naj bosta \( s, x \in \mathbb{N} \). Za vsak graf \( G \) z n vozlišči, m povezavami, in je \( D(G) \subseteq \{ x-s, x, x+s \} \), neenakost (1) drži.

Naš naslednji cilj je odkriti dolge dobre intervale, če sploh obstajajo. Naslednji izrek nam zagotovi dobre intervale vseh velikosti. Pravzaprav je ta rezultat karaketrizacija dobrih in slabih intervalov [3]:

**Izrek 1.** Za vsako pozitivno celo število \( n \) je interval \([a, a+n]\) dober, če in samo če je \( a \geq \frac{n(n-1)}{2} \) ali \([a, a+n] = [1, 4]\).

**Trditev 2.** Če \( f(i,j,k,l) < 0 \) za neka pozitivna števila \( i, j, k, l \in [a, b], \) potem je \([a, b]\) slab interval.


**Izrek 2.** Obstaja neskončno grafov \( G \) z maksimalno stopnjo \( \geq 5 \) za katere je
\[
\frac{M_1}{n} > \frac{M_2}{m}.
\]
Obravnavamo še odločitveni problem, ali je dana skupina pozitivnih celih števil $S$ moči $s$ dobra. Z uporabo nekaj preprostih algoriščnih prijemov smo uspeli pokazati [3], da obstaja algoritem s časovno zahtevnostjo $O(s^2 \log s)$.

**Izrek 3.** Obstaja algoritem s časovno zahtevnostjo $O(s^2 \log s)$ in prostorsko kompleksnostjo $O(s)$, ki ugotovi ali je podana množica naravnih števil $S$ dobra.

Kljub obsežnim raziskavam neenakosti (1), je bilo le malo pozornosti posvečene enakosti oz. grafom za katere velja

$$ M_1/n = M_2/m. \quad (3) $$

V disertaciji podamo razrede grafov, ki izpolnjujejo enakost (3).

Podobno kot neenakost (1), lahko analiziramo neenakost

$$ \frac{\lambda M_1(G)}{n} \leq \frac{\lambda M_2(G)}{m}. \quad (4) $$

Vukičević [101] je analiziral neenakost (4) in pokazal, da ta neenakost ne velja za $\lambda \in [\sqrt{2}/2, 1]$. V istem članku je dan nepopoln dokaz naslednjega izreka:

**Izrek 4.** Za vse grafe $G$ in vsak $\lambda \in [0, \frac{1}{2}]$, velja

$$ \frac{\lambda M_1}{n} \leq \frac{\lambda M_2}{m}. $$

Celoten dokaz zgornjega izreka izpeljemo z uporabo Karamatove enakosti v [9].

**$R'$ indeks**

Leta 1975 je Randić [94] predstavil topološki indeks povezljivosti $R(G)$. Za graf $G$ je indeks $R$ določen kot vsota uteži $(d_G(u)d_G(v))^{-\frac{1}{2}}$ po vseh povezavah $uv \in E(G)$,

$$ R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}, $$


Ne tako dolgo nazaj so Dvořák in soavtorji [44] pokazali, da za vsak povezan graf $G$ velja

$$ R(G) \geq \frac{\text{rad}(G)}{2}, $$

pri čemer je $\text{rad}(G)$ širina grafen.
kjer je \( \text{rad}(G) \) polmer grafa \( G \). Glavna ideja je bila uvedba novega indeksa \( R'(G) \) definiranega kot:

\[
R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_G(u), d_G(v)\}}.
\]

Uporaba indeksa \( R' \) v kemiji doslej ni znana. Ta indeks je še vedno zelo koristen z matematičnega vidika, saj je veliko lažje slediti spremembam \( R' \) kot spremembam Randićevega indeksa. Z uporabo tega indeksa, so Cygan in soavtorji [29] dokazali, da za vse povezane grafe \( G \) z maksimalno stopnjo kvečjemu 4, ki ni pot s sodim številom vozlišč vlja

\[
R(G) \geq \text{rad}(G).
\]

Zaradi tega so rešili domnevo \( R(G) \geq \text{rad}(G) - 1 \), ki jo je postavil Fajtlowicz [49] leta 1988 za primer, ko je \( G \) kemijski graf (graf ki ima maksimalno stopnjo največ 4). Pokazali so, da za vsak kemijski graf \( G \) neenakost

\[
R'(G) \geq \text{rad}(G) - \frac{1}{2}
\]
drži.

Obravnavamo osnovne lasnosti \( R' \), v nadaljevanju pa določimo spodnjo in zgornjo mejo \( R' \) za splošne grafe.

**Trditev 3.** Za vsak graf \( G \) z \( n \) vozlišči, \( n > 1 \), velja neenakost \( R'(G) \leq R(G) \leq \frac{n}{2} \). Poleg tega je \( R'(G) = \frac{n}{2} \), če in samo če je \( G \) regularen graf.

**Posledica 1.** Za vsak graf \( G \) z vsaj dvema vozliščema velja \( R'(G) \geq 1 \). Poleg tega je \( R'(G) = 1 \), če in samo če je \( G \) zvezda.

Če ima graf \( G \) z \( n \) vozlišči maksimano stopnjo manjšo ali enako \( n - \delta(G) \), takrat je spodnja meja za \( R'(G) \) kar \( \delta(G) \). Kot posledico dobimo spodnjo mejo za grafe brez trikotnikov, ki je dosežena za \( K_{k,n-k} \) [8].

**Izrek 5.** Naj bo \( G \) enostaven graf z \( n \) vozlišči in \( \delta(G) = k, k \geq 1, \Delta(G) \leq n - k, n > 2k \), ter z minimalnim \( R'(G) \). Takrat je

\[
R'(G) = k \quad \text{in} \quad G = K_{k,n-k}.
\]

**Posledica 2.** Naj bo \( G \) graf brez trikotnikov z \( n \) vozlišči in \( \delta(G) = k, k \geq 1 \). Potem je \( R'(G) \geq k \) in enakost velja, če in samo če je \( G = K_{k,n-k} \).

**Gutmanov indeks**

Wienerjev index, \( W(G) = \sum_{u,v \in V(G)} d(u, v) \), za povezan graf \( G \) je zelo študirana grafovská invarianta v matematiki in kemiji. Za podrobnosti glej [18, 37, 45, 64, 66, 68]. Osredotočili
se bomo na različico Wienerjevega indeksa imenovano Schultzev indeks druge vrste [64], enako znan kot Gutmanov indeks [99].

Gutmanov indeks je v povezanem grafu $G$ definiran z

$$\text{Gut}(G) = \sum_{u,v \in V(G)} d(u)d(v)d(u,v).$$

Obravnavali bomo grafe z minimalno vrednostjo Gutmanovega indeksa [6].

**Posledica 3.** Za vsako drevo $T$ z $n$ vozlišči velja

$$(n - 1)(2n - 3) = \text{Gut}(S_n) \leq \text{Gut}(T) \leq \text{Gut}(P_n) = \frac{(n - 1)(2n^2 - 4n + 3)}{3}.$$

Gledali bomo grafe z minimalno vrednostjo Gutmanovega indeksa. Prvič bomo pokazali spodnjo in zgornjo mejo za grafe z minimalno stopnjo vsaj dva.

**Trditev 4.** Povezan graf $G$ z $n$ vozlišči in minimalno stopnjo vsaj $\delta \geq 2$ ter minimalnim Gutmanovim indeksom izpolnjuje

$$\delta(\delta + 1)n^2 \geq \text{Gut}(G) \geq \frac{\delta^2 n}{2} (2n - \delta - 2).$$

Nadalje bomo ugotovili spodnjo in zgornjo mejo Gutmanovega indeksa za grafe z maksimalno stopnjo največ kot $\Delta$.

**Trditev 5.** Za povezan graf $G$ z $n$ vozlišči, maksimalno stopnjo $\Delta > 2$ in minimalnim Gutmanovim indeksom velja

$$\text{Gut}(G) < 4(n^2 - 8n + 4) \log_{\Delta-1} n.$$

**Trditev 6.** Naj bo $G$ povezan graf z $n$ vozlišči, maksimalno stopnjo $\Delta(G) \leq \Delta$ in maksimalnim Gutmanovim indeksom. Potem velja zveza:

$$\frac{(n + 1)^3}{27} \Delta^2 \leq \text{Gut}(G) \leq \left(\frac{n + 1}{3}\right)^2 \Delta^2.$$

Za grafe z omejeno maksimalno stopnjo smo dobili naslednja rezultata.

**Posledica 4.** Naj bo $G$ povezan graf z $n$ vozlišči in omejeno maksimalno stopnjo $\Delta$. Potem je

$$O(n^3) \geq \text{Gut}(G) \geq \Omega(n^2 \log n),$$

in meji lahko dosežemo.

**Trditev 7.** Za povezan graf $G$ z $n$ vozlišči, minimalno stopnjo vsaj $\delta$ in maksimalnim Gutmanovim indeksom velja

$$\frac{2^5 (n + \delta - 1)^5}{5^5 \delta^5} < \text{Gut}(G).$$
Fulereni


Fuleren je molekula sestavljena iz ogljikovih atomov, ki so razporejeni v obliki sfere, elipsoida ali cevi, kjer trivalentni atomi ogljika tvorijo petkotnike in šestkotnike. Fulerenski grafi so 3-povezani 3-regularni ravninski grafi, ki imajo le lica velikosti 5 in 6. S pomočjo Eulerjeve formule pokažemo, da ima vsak fulerenski graf natanko 12 petkotnikov in poljubno število šestkotnikov.

Matematični opis fulerenskih grafov opisuje razred grafov, ki bi lahko v naravi predstavljale molekulo iz samih ogljikov. Stabilnost takšne molekule je lahko odvisna od določenih grafovskih invariant. Po drugi strani smo motivirani za iskanje novih grafovskih invariant, ki bi bile v dobri zvezi s stabilnostjo fulerenskih molekul. Naj omenim nekaj fulerenskih lastnosti, ki so v precej dobri korelaciji s stabilnostjo molekul:

- izoliranost petkotnikov (isolated pentagon rule IPR): nobena dva petkotnika nista sosedja v fulerenskem grafu,
- uravnoteženost incidenčne matrike: v incidenčni matriki fulerena je polovica lastnih vrednosti pozitivnih (oz. negativnih),
- število polnih prirejanj, itd.

Nanocevke tvorijo podrazred fulerenov, ki imajo cilindrično obliko, na vsaki strani pa se zaključijo s sferično strukturo. Fulerenski graf je nanocevka, če ga lahko ločimo na cilindrični del, ki vsebuje le šestkotnike in dva krovna grafa - kapici, izmed katerih vsak vsebuje natanko šest petkotnikov ter morebiti tudi kakšni šestkotniki. V krovnem grafu se mora vsaj eden od petkotnikov dotikati cilindričnega dela. Cilindričien del se lahko definira z vektorjem $(p_1, p_2)$, kjer je $p_1 \geq p_2 \geq 0$ in $p_2 > 0$. 
Drug zanimiv razred fulerenskih grafov so ikosaedrični fulereni. *(Popolna) ikosaedrična grupa* $I_h$ je grupa simetrije ikosaedra in dodekaedra. Grupa $I_h$ je ekvivalentna direktnemu produktu grupe $A_5 \times Z_2$, ker je $A_5$ je alternirajoča grupa, $Z_2$ pa je ciklična grupa. Fulereni grafi, ki imajo grupo simetrije $I_h$, se imenujejo *fulereni s popolno ikosaedersko simetrijo*. Najmanjši ikosaedričen fulerenski graf je dodekaeder $C_{20}$. Goldberg [60] je uporabil šestkotniške mreže, da bi določil pozicije petkotniških lic v fulerskem grafu, ki ima popolno simetrijo. Še več, Goldberg je pokazal, da je število vozlišč $n$ poliedra, ki ima ikosaedrično simetrijo povezano z celima številoma $i$ in $j$ z naslednjo relacijo:

$$n = 20(i^2 + ij + j^2), \quad (5)$$

$0 \leq i \leq j$ in $0 < j$. Enačba (5) se danes imenuje *Goldbergova enačba*, in urejeni par $\vec{G} = (i, j)$ se imenuje *Goldbergov vektor*.

**Premer fulerenskih grafov**

Najprej bomo v prvem razdelku obravnavali spodnjo mejo premera fulerenov, nato pa si bomo v naslednjih razdelkih s pomočjo te nove spodnje meje podrobneje pogledali še nekatere druge lastnosti fulerenov, kot so nedvodelnost grafa, neodvisnostno število grafa ter nasičenostno število grafa. Premer nekega fulerena je povezan z njegovo obliko: premer fulerenov z ikosaedrično simetrijo je manjši, po drugi strani pa je premer nanocevke linearen glede na število vozlišč.

Za vsak graf z omogočeno maksimalno stopnjo število vozlišč raste kvečjemu eksponentno odvisnosti od premera. Logaritemsko obnašanje premera je namreč tesno povezano s prisotnostjo velikih lic. Zelo intuitivno se je torej vprašati, če za fulerenke grafe, ki imajo velikost lic omejeno s 6, morebiti ne obstaja boljša spodnja meja premera.

Prav zaradi omejitve velikosti lic nam je uspelo pokazati, da je v fulerenskih grafih premer vsaj reda $\Omega(\sqrt{n})$. Za ta rezultat je ključno opaziti, da je neskončna šestkotniška mreža graf linearne rasti.

**Izrek 6.** Naj bo $G$ poljuben fuleren. Potem velja

$$\text{diam}(G) = \Omega(\sqrt{|V(G)|}).$$

Pri nanocevkah je premer pogosto veliko večji, celo asimptotično linearen glede na število vozlišč. Za zgornjo mejo premera velja:
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Izrek 7. Naj bo $G$ fuleren na $n$ vozliščih. Potem je $\text{diam}(G) \leq \frac{n}{6} + \frac{5}{2}$ razen v primeru, če je $G$ nanocevka tipa $(5,0)$. V tem primeru lahko izrazimo $n$ kot $n = 10k$, $k \in \mathbb{N}$, ter velja:

$$
\text{diam}(G) = \begin{cases} 
\frac{n}{5} + 1, & k = 2 \\
\frac{n}{5}, & k \in \{3,4\} \\
\frac{n}{5} - 1, & k \geq 5.
\end{cases}
$$

Kot smo že ugotovili v izreku 6, imajo vsi fulereni z $n$ vozlišči premer vsaj $\Omega(\sqrt{|V(G)|})$. Dodatno smo se vprašali, če obstaja fulerenski grah, ki ima premer $\Omega(\sqrt{|V(G)|})$. Zato smo obravnavali ikosaedrične fulerenske grafe s popolno simetrijo in dobili smo:

Izrek 8. Naj bo $G$ ikosaedričen fulerenski graf tipa $(0,i)$, $i > 0$. Potem je premer grafa $G$ enak $\text{diam}(G) = 6i - 1$.

Izrek 9. Naj bo $G$ ikosaedričen fulerenski graf tipa $(i,i)$, $i > 0$. Potem je premer grafa $G$ enak $\text{diam}(G) = 10i - 1$.

Za ikosaedrične fulerenske grafe tipa $(0,i)$ in $(i,i)$, $i > 0$, rečemo, da imajo popolno simetrijo. Prejšna dva izreka lako kombiniramo in dobimo naslednji izrek.

Izrek 10. Naj bo $G$ ikosaedričen fulerenski graf tipa $(i,j)$, $0 \leq i \leq j$ in $0 < j$. Potem velja $\text{diam}(G) = 4i + 6j - 1$.

Če uporabimo Goldbergovo enačbo (5) in izrek 10, bomo prišli do zaključka, da je premer fulerenskega grafa s popolno ikosaedrično simetrijo reda $\Theta(\sqrt{n})$. Če imamo ikosaedrični fulerenski graf $G$ tipa $(i,i)$, $(i > 0)$, potem iz (5) sledi $n = 60i^2$. Po izreku 10 je $\text{diam}(G) = 10i - 1$, oziroma $\text{diam}(G) = 10\sqrt{\frac{5}{60}} - 1 = \sqrt{\frac{5n}{3}} - 1$. Ker verjamemo, da imajo ikosaedrični fulerenski grafi najmanjši premer, nas to vodi k naslednji domnevi:

Domneva 2. Za vsak fulerenski graf $G$ z $n$ vozlišči velja $\text{diam}(G) \geq \left\lfloor \sqrt{\frac{5}{3}n} \right\rfloor - 1$. 

Druge grafovske invariante

Poljuben graf je $k$-nedvodelen, če obstaja taka množica povezav $E_0$ moči $k$, da je $G - E_0$ dvodelen graf. *Nedvodelnost* grafa $G$, $\varphi(G)$, je najmanjše tako število $k$, da je graf $G$ $k$-nedvodelen. V [41] so predlagali naslednjo hipotezo:

**Domneva 3.** Naj bo $G$ fulerenski graf. Potem velja:

$$\varphi(G) \leq \sqrt{\frac{12n}{5}}.$$


**Izrek 11.** Naj bo $G$ fulerenski graf z $n$ vozlišči. Potem je

$$\varphi(G) = O(\sqrt{n}).$$

Ta izrek bomo v nadaljnjih razdelkih uporabili pri dokazovanju nekaterih drugih izboljšanih mej.

Kar se tiče neodvisnostnega števila fulerenskih grafov sta znani naslednji hipotezi podani v [33] in [56].

**Domneva 4.** Naj bo $G$ fulerenski graf. Potem je

$$\alpha(G) \geq \frac{n}{2} - 3\sqrt{\frac{|V(G)|}{15}}.$$

**Domneva 5.** Za vsak fulerenski graf $G$ velja

$$\alpha(G) \geq 2(\text{diam}(G) - 1).$$

V splošnem smo za vse dovolj velike fulerenske grafe potrdili domnevi 4 in 5.

**Izrek 12.** Obstaja takšna konstanta $c > 0$, da za vsak fulerenski graf $G$ z $n$ vozlišči velja zveza $\alpha(G) \geq \frac{n}{2} - c\sqrt{n}$.

**Trditev 8.** Naj bo $G$ fulerenski graf z $n$ vozlišči. Če je $n$ dovolj velik, potem je

$$\alpha(G) \geq 2(\text{diam}(G) - 1).$$

Z uporabo novega rezultata o spodnji mejni premera fulerenskih grafov smo izboljšali zgornjo mejo za nasičenostno število.

**Izrek 13.** Naj bo $G$ poljuben fulerenski graf z $n$ vozlišči. Potem obstaja taka konstanta $c > 0$, da je

$$s(G) \leq \frac{2}{n} - c\sqrt{n}.$$
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Podpis: . . . . . . . . . . . . . . . . . . . . . . . . . . . .