摘 要

在历史上，图论与化学有着非常紧密的联系。化学结构可以很简单地表示成图的形式，这样的图也称为化学图，或者分子图。分子的拓扑指标是从化学图集合到实数集合的一个映射，理论化学家和数学家提出了众多的拓扑指标并进行研究。本文主要研究一种广受化学家和数学家关注的拓扑指标—— Randić 指标，研究 Randić 指标与图的其它若干不变量之间的关系，如色数，半径，直径，最小度，最大度，阶数和边数，等等。

1975 年著名理论化学家、数学化学家 Randić 提出了连通性指标，即 Randić 指标。(化学) 图 G 的 Randić 指标定义为 $R(G)=\sum_{uv\in E(G)}(d(u)d(v))^{-\frac{1}{2}}$，其中 $d(u)$ 表示图 G 中顶点 u 的度数。Randić 指标与分子的物理化学性质，如沸点、表面积等，都有着紧密的联系。1998 年，著名数学家 Bollobás 和 Erdös 将 $R(G)$ 中的 $-\frac{1}{2}$ 替换为任意的实数 α，从而提出了广义 Randić 指标的定义。理论化学家和数学家对广义 Randić 指标进行研究，并且得到了很多重要而深刻的结果。

第一章是引言部分，介绍了 Randić 指标的定义、研究背景，以及本文中涉及到的相关概念和基本知识。以下五章为本文的主要贡献：

在第二章中，我们指出了 Hansen 和 Mélot 的文章 [Variable neighborhood search for extremal graphs 6: Analyzing bounds for the connectivity index, J. Chem. Inf. Comput. Sci. 43(2003), 1–14] 中两个定理证明的错误，并给出了正确的证明。这两个定理刻画了化学树的 Randić 指标和叶子点数之间的联系。

在第三章中，我们讨论了图 G 的 Randić 指标 $R(G)$ 和最小度 $\delta(G)$ 之间的关系，并部分解决了 Bollobás 和 Erdös 提出的公开问题。1988 年，Shearer 证明了如果图的最小度 $\delta(G)\geq 1$，那么 $R(G)\geq\sqrt{n}/2$，几个月后 Alon 将这个界改进到 $\sqrt{n}-8$。1998 年，Bollobás 和 Erdös 证明，如果 $\delta(G)\geq 1$，则有 $R(G)\geq\sqrt{n-1}$，其中等号成立当且仅当 G 是星图。Bollobás 和 Erdös 提出如下问题：给定图 G 的最小度 $\delta(G)$，$R(G)$ 的最小值是多少？在 2002 年，Delorme, Favaron 和

Rautenbach 针对这一问题提出了如下猜想：如果图 G 的最小度 $\delta(G) \geq k$，那么 $R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1}$，其中等号成立当且仅当图 G 是由完全二部图 $K_{k,n-k}$ 做如下变换得到：在 $K_{k,n-k}$ 含有 k 个顶点的那部分内的任意两个顶点连一条边。提出猜想后，他们证明了 $k=2$ 时猜想是成立的。我们验证了 $k=3$ 时猜想的正确性，由此很容易地得到猜想中的不等式对所有的化学图也是成立的。更进一步，我们证明了当 $k \geq 4$ 时，如果图的顶点数满足 $n \geq \frac{3}{2}k^3$，则猜想是成立的。

在第四章的第一部分，我们完全解决了 Caporossi 和 Hansen 提出的关于图的 Randić 指标和色数的猜想：对顶点数 $n \geq 2$ 的连通图 G，$R(G) \geq \frac{\chi(G)-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{\chi(G)-1} + n - \chi(G)\right)$，而且对所有的 n 以及 $2 \leq \chi(G) \leq n$，这个界是紧的，其中图 G 的色数 $\chi(G)$ 是指使得图 G 有正常顶点着色（相邻顶点所着颜色不同）的最小颜色数目。在第二部分中我们考虑了 Fajtlowicz 提出的关于图的 Randić 指标和半径的猜想：对任意连通图 G，$R(G) \geq r(G)-1$，其中图 G 的半径 $r(G) = \min_{v\in G}\max_{u\in(G)} d(u,v)$。根据 Erdös 等人的关于图的半径和最小度的结果，我们证明了若 G 是具有 n 个顶点，最小度为 $\delta(G)$ 的连通图，如果 $\delta(G) \geq \frac{n}{5}$ 且 $n \geq 25$，则猜想成立；更进一步，对任意实数 $0 < \varepsilon < 1$，如果 $\delta(G) \geq \varepsilon n$，则对充分大的 n，猜想都是成立的。

在第五章中，我们考虑了具有 n 个顶点、m 条边的化学图的广义零阶 Randić 指标的极值问题，其中广义零阶 Randić 指标定义为 ${}^0R_\alpha(G) = \sum_{u\in V(G)} d(u)^\alpha$。对任意的实数 α，我们用图的顶点数和边数给出了广义零阶 Randić 指标的严格上界和下界，刻画了相应的极图。

在第六章中，我们研究了图 G 的反比度 $I(G)$ 和直径 $D(G)$ 的关系，其中反比度的定义为 $I(G) = {}^0R_{-1}(G) = \sum_{u\in V(G)} \frac{1}{d(u)}$。Erdös, Pach 和 Spencer 证明，对具有 n 个顶点的连通图 G，若 $I(G) \geq 3$，则有

$$\left(\frac{2}{3}\lfloor r/3 \rfloor + o(1)\right)\frac{\log n}{\log\log n} \leq \mu(n,r) \leq D(n,r) \leq (6r + o(1))\frac{\log n}{\log\log n},$$

其中 $\mu(G)$ 是图 G 的平均距离，$\mu(n,r) = \max\{\mu(G) : I(G) \leq r\}$，$D(n,r) = \max\{D(G) : I(G) \leq r\}$。Dankelmann 等人将此上界改进了 2 倍，即 $D(G) \leq (3I(G) + 2 + o(1))\frac{\log n}{\log\log n}$。针对树和单圈图，我们将 Dankelmann 等人的上界改进了 $\frac{4}{3}\cdot\frac{\log n}{\log\log n}$ 倍，并且证明此时的界是最好的，确定了达到此上界的极图。

关键词：Randić 指标，图的不变量，极图，化学图，线性规划，度序列，色数，直径，半径，反比度

Abstract

Historically, graph theory has a close relation with chemistry. A chemical structure can be conveniently represented by a graph, which is called a chemical graph or a molecular graph. A topological index is a map from the set of chemical graphs to the set of real numbers. Various topological indices are proposed and researched by both theoretical chemists and mathematicians. This thesis consider one popular topological index—Randić index, and study the relations of Randić index and some other graph invariants, such as the chromatic number, the radius, the diameter, the minimum degree, the maximum degree, the order and the size, etc.

The Randić index (or the connectivity index) $R(G)$ of a (chemical) graph G was introduced by the chemist Randić in 1975 as $R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-\frac{1}{2}}$, where $d(u)$ denotes the degree of a vertex u in G. Randić index has a good correlation with several physicochemical properties of alkanes: boiling points, chromatographic retention times, enthapies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc. Later, in 1998 Bollobás and Erdös generalized this index by replacing $-1/2$ with any real number α, which is called the general Randić index. It has been extensively studied by both theoretical chemists and mathematicians. Many important mathematical properties have been established.

In Chapter 1, we introduce the definition and the background of the Randić index, and give the basic notations and terminology related to this thesis. The succeeding five chapters are the main contributions of this thesis:

In Chapter 2, we point out the mistakes in the proofs of two theorems in the paper of Hansen and Mélot [Variable neighborhood search for extremal graphs

6: Analyzing bounds for the connectivity index, J. Chem. Inf. Comput. Sci. 43(2003), 1–14]. In the two theorems, they studied the relation of the Randić index and the number of pendent vertices of chemical trees. We present the corrected proofs.

In Chapter 3, we study the relation between the Randić index $R(G)$ and the minimum degree $\delta(G)$ of graphs and partially solve the open problem proposed by Bollobás and Erdös. In 1988, Shearer proved $R(G) \geq \sqrt{n}/2$ if $\delta(G) \geq 1$. A few months later, Alon improved this bound to $\sqrt{n} - 8$. In 1998, Bollobás and Erdös proved that $R(G) \geq \sqrt{n-1}$ if $\delta(G) \geq 1$, with equality if and only if G is a star. Bollobás and Erdös asked for the minimum value of the Randić index for graphs with given minimum degree. In 2002, Delorme, Favaron and Rautenbach proposed the conjecture: if $\delta(G) \geq k$, then $R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1}$, with equality if and only if G is obtained from a complete bipartite graph $K_{k,n-k}$ by joining each pair of vertices in the part with k vertices by a new edge. They showed that the conjecture is true for $k = 2$. We verify this conjecture for $k = 3$, which can easily lead to the conclusion that the inequality of the conjecture holds for all chemical graphs. Furthermore, we prove that for $k \geq 4$, the conjecture is true for any graph of order $n \geq \frac{3}{2}k^3$.

In the first part of Chapter 4, we give a complete proof to a conjecture on the relation between the Randić index $R(G)$ and the chromatic number $\chi(G)$ proposed by Caporossi and Hansen: for any connected graph G of order $n \geq 2$, $R(G) \geq \frac{\chi(G)-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{\chi(G)-1} + n - \chi(G)\right)$, the bound is sharp for all n and $2 \leq \chi(G) \leq n$, where the chromatic number of G is defined as the minimum number of colors that are needed to color the vertices of G properly, i.e., no tow adjacent vertices share a same color. In the second part, we consider the conjecture on the relation between the Randić index $R(G)$ and the radius $r(G)$ proposed by Fajtlowicz: for any connected graph G, $R(G) \geq r(G) - 1$, where $r(G)$ denotes the radius of G. From a result on the radius and the minimum degree of graphs given by Erdös *et al.*, we prove that for any connected graph G of order n with minimum degree $\delta(G)$, the conjecture holds for $\delta(G) \geq \frac{n}{5}$ and $n \geq 25$, furthermore, for any arbitrary real number $0 < \varepsilon < 1$, if $\delta(G) \geq \varepsilon n$, the conjecture holds for sufficiently large n.

In Chapter 5, we consider the extremal values of the zeroth-order general Randić index of chemical graph G, which is defined as ${}^0R_\alpha(G) = \sum_{u\in V(G)} d(u)^\alpha$, where α is an arbitrary real number. We give the sharp upper and lower bounds of ${}^0R_\alpha(G)$ by using the order n and the size m of G, and characterize the respective extremal graphs.

In Chapter 6, we investigate the inverse degree $I(G)$ and the diameter $D(G)$ of graph G, where the inverse degree $I(G) = {}^0R_{-1}(G) = \sum_{u\in V(G)} \frac{1}{d(u)}$. Erdös, Pach and Spencer proved that, if G is a connected graph of order n and $I(G) \geq 3$, then

$$\left(\frac{2}{3}\lfloor r/3\rfloor + o(1)\right)\frac{\log n}{\log\log n} \leq \mu(n,r) \leq D(n,r) \leq (6r + o(1))\frac{\log n}{\log\log n},$$

where $\mu(G)$ is the average distance, $\mu(n,r) = \max\{\mu(G) : I(G) \leq r\}$ and $D(n,r) = \max\{D(G) : I(G) \leq r\}$. Dankelmann *et al.* improved the upper bound by a factor of 2,

$$D(G) \leq (3I(G) + 2 + o(1))\frac{\log n}{\log\log n}.$$

We give the sharp upper bounds for trees and unicyclic graphs, which improve the above upper bound by a factor of approximately $\frac{4}{3}\cdot\frac{\log n}{\log\log n}$.

Keywords: Randić index, graph invariant, extremal graph, chemical graph, linear programming, degree sequence, chromatic number, diameter, radius, inverse degree

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Chapter 1

Introduction and Historical Notes

This chapter recalls and defines some important notions of graph theory. It is assumed that the reader is familiar with this material in all the subsequent chapters.

We follow in general what is considered by many graph theorists to be of common use. The standard textbooks of Bondy and Murty [16, 17] and Bollobás [13] are the main references for such terminology.

1.1 Graph theory and chemical graph theory

Graph theory finds its roots in the famous Königsberg Bridge Problem. In the eighteenth century, two branches of the River Pregel meet in the Eastern Prussia city of Königsberg, to flow into the Baltic Sea. Seven bridges connect the various parts of the city which are separated by water. Some of the citizens wondered if it were possible to take a journey across all seven bridges without having to cross any bridge more than once. This problem raised the curiosity of the mathematician Euler. He proved in 1736 [37] that such a journey was impossible. This structure composed of land areas and bridges can be represented with a graph. Each vertex is a land area and an edge is a bridge between two of them. The initial problem can be reformulated as follows: given a graph, one has to find a sequence of vertices and edges which crosses each edge exactly once, returning to its starting vertex.

Euler [37] gave a condition for when it is possible on any graph: each vertex has to be incident with an even number of edges. He proved that this condition is necessary and sufficient.

Actually, graph theory has a lot of applications, for details see [16, 42, 43]. Much of the present-day interest in the subject is due to the fact that, quite apart from being an elegant mathematical discipline in its own right, graph theory is playing an ever-increasing role in such a wide range of subjects as electrical engineering and industrial engineering, physics and biologies, operational research and crystallography, probability and genetics, and sociology, economics, geography, linguistics and numerical analysis.

Historically, graph theory has a close relation with chemistry. A chemical structure can be, of course, conveniently represented by a graph: atoms are vertices and chemical bonds are edges of the graph, which is called the chemical graph or the molecular graph. Chemical applications in graph theory are numerous. The field of research that we nowadays call *chemical graph theory* originated in the 1870s, when the great British mathematician Cayley published the paper "On the mathematical theory of isomers" [23], followed by some half a dozen of other chemicomathematical treatises. At about the same time, the British-American mathematician Sylvester published a note (in *Nature* **17** (1877–1878), 284) entitled "Chemistry and Algebra" [93], where he introduced the name "graph" for this kind of mathematical structure, and he took this name from the chemistry. The paper deals with graph invariants and mentions the connection to chemistry.

On the side of chemistry a lot of activities was devoted to the enumeration of chemical isomers. In a paper of Lunn and Senior the first connection between this kind of a problem and group theoretic methods were mentioned. But the main clarification is due to the famous paper of Pólya: "Anzahlbestimmungen für Gruppen, Graphen und Chemische Verbindungen" [87]. This paper can be considered as the foundation of graphical enumeration, more generally, of algebraic combinatorics.

Prelog just before winning the Nobel Prize in chemistry in 1975 made a simple but profound comment about graphs and graph theory:

"Pictorial representations of graphs are so easily intelligible that chemists are

often satisfied with inspecting and discussing them without paying to attention to their algebraic aspects, but it is evident that some familiarity with the theory of graphs is necessary for deeper understanding of their properties."

In theoretical chemistry atomic connectivity belongs to basic facts and, for this reason, graph theoretical considerations have always played a role in chemistry. There are relevant physical and chemical questions, in particular for large systems, to whose solutions graph theory can make insightful contributions.

In chemistry, people want to find some new molecules with desired physico-chemical properties, for example, boiling points, molecular volumes, flavor threshold concentration antiviral activity, energy levels, electronic populations, etc. And these properties can be quantitatively represented by some values of a certain index. The notion of a "topological index" appears first in a paper of the Japanese chemist Hosoya [54], who investigated the surprising relation between the physico-chemical properties of a molecule and the number of its independent edge subsets (matchings). A *topological index* is a map from the set of chemical graphs to the set of real numbers. Therefore a topological index is a numeric quantity that is mathematically derived in a direct and unambiguous manner form the structural graph of a molecule. Since isomorphic graphs possess identical values for any given topological index, these indices are referred to as graph invariants. Topological indices usually reflect both molecular size and shape. The advantage of topological indices is that they may be used directly as simple numerical descriptors in a comparison with physical, chemical, or biological parameters of molecules in quantitative structure-property relationships (QSPR) and in quantitative structure-activity relationships (QSAR).

Graphs representing molecular structures often have a maximum degree Δ which is bounded. In particular, we recall that

Definition 1.1.1 *A chemical graph is a graph with the maximum degree* $\Delta \leq 4$.

It comes from the fact that the carbon atom has a valency of 4. For instance, the fullerenes are molecules composed entirely of carbon, which take the form of a hollow sphere, ellipsoid, or tube.

Various topological indices, more than 1000, have been studied, for example, the Wiener index, the Balaban index, the Randić index, the Zagreb index, the Hosoya index, the Merrified and Simmons index, etc. Some of them are distance based indices, some are degree based indices, some others are structure based indices, such as matchings or independent sets, etc. Different indices have different use in chemistry, i.e., different indices can indicate different chemical information and describe different properties of chemicals. With the increase of interest in QSPR/QSAR, numerous results in this area have been published. For more details about chemical graph theory and graph invariants, one can see [7, 8, 48, 51, 58, 78, 82, 90, 91, 94, 95, 96].

1.2 Notations and definitions

In this thesis, we consider only finite, undirected simple graphs.

Let $G = (V, E)$ be a finite, undirected simple graph. Let u be a vertex of G, then we write $u \in G$ instead of $u \in V$. The *order* of G is the number of vertices in G, denoted by $|G|$, and thus $|G| = |V(G)|$. A graph of order n is also called an *n-vertex graph*. The *size* of G is the number of edges in G. Similarly, $G(n, m)$ denotes an arbitrary graph of order n and size m, which is also denoted by an (n, m)-graph. A graph of order n and size $\binom{n}{2}$ is called a *complete graph* and is denoted by K_n. A *tree* T is a connected acyclic graph, then a tree of order n has size $m = n - 1$. Let P_n or C_n be the *path* or the *cycle* of order n, respectively. A *bipartite graph* $B_{p,q}$ is composed of two independent sets of vertices (partitions), with p and q vertices respectively, and some edges joining pairs of vertices u and v such that u and v are not in the same partition. If one bipartite graph contains such edges for all pairs, then it is called a *complete bipartite graph*, denoted by $K_{p,q}$. The graph $K_{1,n-1}$ is also called a *star* of order n, denoted by S_n.

Two isomorphic graphs share several properties which can be expressed in terms of invariants. A *graph invariant* is a numerical value which is preserved by isomorphism. The order n and the size m of a graph G are the simplest examples of graph invariants.

There exist many invariants describing specific characteristics of graphs. Some of them are based on the notions of degree, distance, colors, and so on. In the following, we introduce some graph invariants related in this thesis, such as the minimum degree, the maximum degree, the diameter, the radius, the chromatic number, etc.

For any vertex $v \in G$, denote by $N(v)$ the *neighborhood* of v and $d(v)$ the *degree* of v. The *minimum degree* of G is denoted by $\delta(G)$, while the *maximum degree* is denoted by $\Delta(G)$. A vertex of degree 0 is said to be an *isolated vertex*. A vertex of degree 1 is called a *leaf vertex* (or simply, a *leaf*), sometimes is also called a *pendent vertex*, and the edge incident with the leaf is called a *pendent edge*. Denote by $\pi(G) = [d_1, d_2, \ldots, d_n]$ the degree sequence of graph G, where d_i stands for the degree of the i-th vertex of G, and $d_1 \geq d_2 \geq \cdots \geq d_n$. For convenience, sometimes we denote $\pi(G) = [d_1^{\alpha_1}, d_2^{\alpha_2}, \ldots, d_s^{\alpha_s}]$, where $d_1 > d_2 > \cdots > d_s$ and $d_i^{\alpha_i}$ denotes that the number of vertices with degree d_i is α_i.

The *length* of a path is the number of edges in the path. The *distance* $d(u, v)$ between two vertices u and v is the length of a shortest path between u and v. If G has no such path between vertices u and v, then $d(u, v) = \infty$. A graph G is *connected* if there exists a path between every pair of vertices in G. The *diameter* $D(G)$ of G is the maximum distance between any pair of vertices of G, i.e., $D(G) = max_{u,v \in V(G)} d(u, v)$. The *eccentricity* of a vertex u, written $\epsilon(u)$, is $\max_{v \in V} d(u, v)$. Note that the diameter equals the maximum of the vertex eccentricities. The *radius* of a graph G is $r(G) = min_{u \in V} \epsilon(u)$. For a given graph G, a vertex coloring of G is called *proper* if any two adjacent vertices are assigned different colors. The *chromatic number* $\chi(G)$ of G is the minimum number of colors that are needed to color G properly.

1.3 Overview of the thesis

For a (chemical) graph $G = (V, E)$, the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d(u)d(v))^\alpha$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u of G, i.e.,

$$R_\alpha(G) = \sum_{uv \in E} (d(u)d(v))^\alpha$$

where α is an arbitrary real number.

In 1975, the chemist Randić [89] proposed a topological index R (R_{-1} and $R_{-\frac{1}{2}}$) under the name "*the branching index*", which is now also called "*the Randić index*" or "*the connectivity index*", suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Later, in 1998 Bollobás and Erdös [14] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the general Randić index.

The *zeroth-order Randić index*, conceived by Kier and Hall [57, 59], is defined as,

$$^0R(G) = {}^0R_{-1/2}(G) = \sum_{u \in G} d(u)^{-\frac{1}{2}}$$

where the summation goes over all vertices of G. In analogy to the Randić index, Li and Zheng [74] defined the *zeroth-order general Randić index* $^0R_\alpha(G)$ of a graph G,

$$^0R_\alpha(G) = \sum_{u \in G} d(u)^\alpha,$$

where α is an arbitrary real number.

Already Randić noticed that there is a good correlation between the Randić index R and several physicochemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc. In subsequent years countless applications of R were reported, most of them concerned with medicinal and pharmacological issues. A turning point in the mathematical examination of the Randić and general Randić index happened in the second half of the 1990s, when a significant and ever growing research on this matter started, resulting in numerous publications. As the chemist Gutman in [46] mentioned that: "In chemical graph theory, the connectivity index achieved a rapid and enormous success. It soon became the most popular and most frequently employed structure descriptor, used in innumerable QSPR and QSAR studies. It was soon generalized (to 'higher-order connectivity indices') and parametrized (so as to be applicable to heteroatom-containing species)."

Recently, the Randić index was studied by both mathematicians and theoretical chemists, who established a few of its fundamental mathematical properties. For a survey of results, we refer to the book [62] written by Li and Gutman and the survey [67].

Note that the Randić index and the zeroth-order Randić index are both graph invariants. Graph theory contains a large number of relations between graph invariants. Some of them are equalities, most of them are inequalities, often nonlinear in one or more parameters. The relations between the Randić index and some other graph invariants are listed as follows.

1.3.1 Randić index and the number of pendent vertices of chemical trees

A chemical graph (tree) is a graph (tree) in which the maximum degree is no more than 4. Let T be a chemical tree of order n with n_1 pendent vertices. There are many results on the relation between the randić index $R(T)$ and n_1, one can see [69, 73, 97, 99].

In fact, in 2003, Hansen and Mélot [52] studied the relation of $R(T)$ and the number of pendent vertices. In [52], the authors introduced two classes of chemical trees $L_e(n, n_1)$ and $U(n, n_1)$ (see Chapter 2). Two theorems are stated as follows:

Theorem 1.3.1 (Hansen and Mélot, [52]) *Let T be a chemical tree of order n with $n_1 \geq 5$ pendent vertices. Then*

$$R(T) \geq \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}, \tag{1.3.1}$$

with equality if and only if n_1 is even and T is isomorphic to $L_e(n, n_1)$.

Theorem 1.3.2 (Hansen and Mélot, [52]) *Let T be a chemical tree of order n with $n_1 \geq 3$ pendent vertices. Then*

$$R(T) \leq \frac{n}{2} - a_0' n_1,$$

where $a_0' = \frac{7}{6} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \approx 0.0513$, with equality if and only if T is isomorphic to $U(n, n_1)$.

However, we found some mistakes in their proofs. In Chapter 2, we will give the corrected proofs.

1.3.2 Randić index and the minimum degree

In 1988, Shearer proved $R(G) \geq \sqrt{n}/2$ if $\delta(G) \geq 1$. A few months later Alon improved this bound to $\sqrt{n} - 8$. Bollobás and Erdös [14] proved that among all graphs of order n with $\delta(G) \geq 1$, the star S_n attains the minimum Randić index $\sqrt{n-1}$. Bollobás and Erdös asked for the minimum value of the Randić index for graphs with given minimum degree. Delorme, Favaron and Rautenbach [32] gave an answer of $k = 2$ and proposed the following conjecture.

Conjecture 1.3.3 (Delorme, Favaron and Rautenbach, [32]) *Let $G = (V, E)$ be a graph of order n with $\delta(G) \geq k$. Then*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1},$$

with equality if and only if $G = K^*_{k,n-k}$, where $K^*_{k,n-k}$ is a graph obtained from a complete bipartite graph $K_{k,n-k}$ by joining each pair of vertices in the part with k vertices by a new edge.

In [3] Aouchiche and Hansen found examples showing that the conjecture is not true, and gave a modified form. In Chapter 3, we will consider Conjecture 1.3.3. We verify this conjecture for $k = 3$, which can easily lead to the conclusion that the inequality of the conjecture holds for all chemical graphs. Furthermore, we prove that for $k \geq 4$, the conjecture is true for any graph of order $n \geq \frac{3}{2}k^3$.

1.3.3 Randić index and the chromatic number, the radius

Caporossi and Hansen [21] proposed the following conjecture on the relation between Randić index and the chromatic number, which is also referred in [62]. In the first part of Chapter 4, we will give a positive proof to Conjecture 1.3.4.

Conjecture 1.3.4 (Caporossi and Hansen, [21]) *For any connected graph G of order $n \geq 2$ with chromatic number $\chi(G)$ and Randić index $R(G)$,*

$$R(G) \geq \frac{\chi(G)-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{\chi(G)-1} + n - \chi(G)\right).$$

Moreover, the bound is sharp for all n and $2 \leq \chi(G) \leq n$.

In [38], Fajtlowicz proposed the following conjecture on the relation between the Randić index and the radius, which is also referred in [62].

Conjecture 1.3.5 (Fajtlowicz, [38]) *For any connected graph G,*

$$R(G) \geq r(G) - 1,$$

where $r(G)$ denotes the radius of G.

Caporossi and Hansen [21] proved that for all trees T, $R(T) \geq r(T) + \sqrt{2} - \frac{3}{2}$, and for trees T except even paths, $R(T) \geq r(T)$. In [76], the conjecture is verified for unicyclic graphs, bicyclic graphs and connected graphs of order $n \leq 9$ with $\delta(G) \geq 2$. Recently, You and Liu [98] proved that the conjecture is true for biregular graphs, tricyclic graphs and connected graphs of order $n \leq 10$.

In the second part of Chapter 4, we will prove that for any connected graph G of order n with minimum degree $\delta(G)$, the conjecture holds for $\delta(G) \geq \frac{n}{5}$ and $n \geq 25$, furthermore, for any arbitrary real number $0 < \varepsilon < 1$, if $\delta(G) \geq \varepsilon n$, Conjecture 1.3.5 holds for sufficiently large n.

1.3.4 The zeroth-order (general) Randić index

It should be noted that the zeroth-order general Randić index is sometimes referred to as " the general first Zagreb index" [81, 101], in view of the fact that $\sum_u (d(u))^2$ is sometimes called "the first Zagreb index". For $\alpha = -1$, it is also called "the inverse degree", sometimes denoted by "$I(G)$" (see [36, 38, 79]).

In fact, there are many researches on this index, which has many useful applications in information theory and network reliability, and received considerable attentions also in graph theory (see [1, 11, 12, 26, 31, 80, 88]).

Pavlović [83] determined the sharp upper bound of the zeroth-order Randić index ${}^0R_\alpha$ of (n,m)-graphs. In [72] Li and Zhao gave the sharp upper and lower bounds of ${}^0R_\alpha$ of trees, with the exponent α equal to m, $-m$, $\frac{1}{m}$ and $-\frac{1}{m}$, where $m \geq 2$ is an integer. Later, Li and Zheng [74] gave an alternative proof for general real number α. Zhang and Zhang [101] determined the sharp upper and lower bounds of ${}^0R_\alpha$ of unicyclic graphs, while Zhang, Wang and Cheng [100] determined the sharp upper and lower bounds of bicyclic graphs. In [55, 66], the authors considered the extremal values of ${}^0R_\alpha$ for the connected (n, m)-graphs. And they gave the sharp lower bound of ${}^0R_\alpha$ for $\alpha < 0$ or $\alpha > 1$, and the sharp upper bound of ${}^0R_\alpha$ for $\alpha < 1$. There are also some gaps.

For chemical trees, Li and Zhao [72] determined the sharp and lower bounds of ${}^0R_\alpha$ for any α. In Chapter 5, we will investigate the zeroth-order general Randić index for chemical (n, m)-graphs, i.e., connected simple graphs with n vertices, m edges and maximum degree at most 4. We will give the sharp upper and lower bounds of ${}^0R_\alpha$ for any α.

1.3.5 The inverse degree and the diameter

We denote the inverse degree ${}^0R_{-1}(G)$ by $I(G)$. There is a Graffiti conjecture $\mu(G) \leq I(G)$ (see [38, 41]), where $\mu(G)$ is the average distance of G. However, the conjecture was refuted by Erdös, Pach and Spencer in [36]. They proved that, if G is a connected graph of order n and $I(G) \geq 3$, then

$$\left(\frac{2}{3}\lfloor r/3 \rfloor + o(1)\right) \frac{\log n}{\log\log n} \leq \mu(n, r) \leq D(n, r) \leq (6r + o(1))\frac{\log n}{\log\log n},$$

where $\mu(n, r) = \max\{\mu(G) : I(G) \leq r\}$ and $D(n, r) = \max\{D(G) : I(G) \leq r\}$. Dankelmann *et al.* [30] improved the upper bound by a factor of 2,

$$D(G) \leq (3I(G) + 2 + o(1))\frac{\log n}{\log\log n},$$

which is also an upper bound on the average distance since $\mu(G) \leq D(G)$.

In Chapter 6, we will give the sharp upper bounds for trees and unicyclic graphs, which improve the above upper bound by a factor of approximately $\frac{4}{3} \cdot \frac{\log n}{\log\log n}$. We show that for a tree T of order n

$$D(T) \leq \frac{3n - 2I(T) + 1 - \sqrt{4I(T)^2 - (4n-4)I(T) + n^2 - 2n - 7}}{2},$$

while for a unicyclic graph G of order n

$$D(G) \leq \frac{3n - 2I(G) - 1 - \sqrt{4I(G)^2 - (4n-12)I(G) + n^2 - 6n + 1}}{2}.$$

Chapter 2

Randić Index and the Number of Pendent Vertices of Chemical Trees

In this chapter, we point out the mistakes in the proofs of two theorems in the paper of Hansen and Mélot, in which they studied the relation of the Randić index and the number of pendent vertices of chemical trees. We present the corrected proofs.

2.1 Bounds of Hansen and Mélot

The *Randić index* $R(G)$ of a graph G, also called the connectivity index, was introduced by the chemist Randić under the name "*the branching index*" in 1975 as the sum of $1/\sqrt{d(u)d(v)}$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G, i.e.,

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

A vertex of degree 1 is called a *leaf vertex* (or simply, a *leaf*), sometimes is also called a *pendent vertex*.

As an important class of trees, trees with a given number of pendent vertices are considered frequently, for details see [52, 69, 73, 97, 99].

In 2003, Hansen and Mélot [52] studied the relation of $R(T)$ and the number of pendent vertices. In [52], the authors introduced two classes of chemical trees $L_e(n, n_1)$ and $U(n, n_1)$, which were founded by the system *AutoGraphix (AGX)* of Caporossi and Hansen (further papers describing mathematical applications of AGX are in [2], [18], [19], [21], [22]).

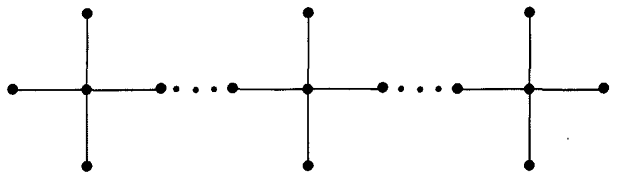

Figure 2.1: Structure of $L_e(n, n_1)$.

The structure of $L_e(n, n_1)$ (n_1 is even) is depicted in Figure 2.1. These trees are composed by subgraphs which are the stars S_5 and these stars are connected by paths (the dotted lines in the figure), for which the lengths can be zero. The configuration is complete if $n \geq 9$ and $6 \leq n_1 \leq \lfloor \frac{n+3}{2} \rfloor$ (and even).

We can compute $R(L_e(n, n_1))$. We see in Figure 2.1 that $L_e(n, n_1)$ is formed by $\frac{n_1-2}{2}$ stars S_5. This chemical tree has n_1 pendent edges of weight $\frac{1}{2}$, $n_1 - 4$ edges between the centers of the stars and the paths joining these stars of weight $\frac{1}{\sqrt{8}}$. The other edges are on the paths between the stars and have a weight of $\frac{1}{2}$ also. Since any tree has $n-1$ edges, there are $n - 2n_1 + 3$ edges of this type (and so n_1 has to be less than or equal to $\lfloor \frac{n+3}{2} \rfloor$). Thus, the Randić index of tree $L_e(n, n_1)$ is

$$\begin{aligned} R(L_e(n, n_1)) &= \frac{n_1}{2} + \frac{n_1 - 4}{2\sqrt{2}} + \frac{n - 2n_1 + 3}{2} \\ &= \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}\,. \end{aligned}$$

The tree $U(n, n_1)$ has a subgraph of $n_1 - 2$ vertices of degree 3 which is a tree; we denote its vertex set by V_3. In Figure 2.2, the vertices of V_3 are on a path, but in general case this may be different. All these vertices are connected to another vertex of V_3 or to a path of length at least 2. The number of paths adjacent to the vertices of V_3 is $|V_3| + 2$, and the number of vertices of degree 2 is $n - 2n_1 + 2$. This configuration is complete if $n \geq 7$ and $3 \leq n_1 \leq \lfloor \frac{n+2}{3} \rfloor$.

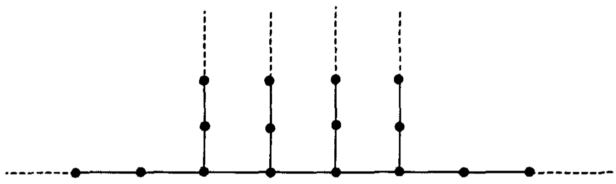

Figure 2.2: Structure of $U(n, n_1)$

We can compute $R(U(n,n_1))$. We see in Figure 2.2 that $U(n,n_1)$ has n_1 pendent edges of weight $\frac{1}{\sqrt{2}}$, n_1 edges connecting paths and the vertices of V_3 of weight $\frac{1}{\sqrt{6}}$, $n_1 - 3$ edges joining the vertices of V_3 of weight $\frac{1}{3}$. The $n_3 n_1 + 2$ other edges are the inner edges of the paths (the dotted lines) of weight $\frac{1}{2}$ (and thus $n_1 \leq \lfloor \frac{n+2}{3} \rfloor$). So, the Randić index of $U(n,n_1)$ is

$$R(U(n,n_1)) = \frac{n}{2} + n_1 \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} - \frac{7}{6} \right).$$

The paper [52] contains 8 theorems, 2 propositions, 2 corollaries and 1 lemma, in which many results were mentioned. Two theorems are stated as follows:

Theorem 2.1.1 (Theorem 8, [52]) *Let T be a chemical tree of order n with $n_1 \geq 5$ pendent vertices. Then*

$$R(T) \geq \frac{n}{2} + \frac{n_1}{2} \left(\frac{1}{\sqrt{2}} - 1 \right) + \frac{3}{2} - \sqrt{2} \tag{2.1.1}$$

with equality if and only if n_1 is even and T is isomorphic to $L_e(n,n_1)$.

In the proof of Theorem 8 of [52], expression (21):

$$R(T - v_1v_2) \geq \frac{n}{2} + \frac{n_1}{2} \left(\frac{1}{\sqrt{2}} - 1 \right) + \frac{3}{2} - \sqrt{2} + \frac{1}{2} - \frac{1}{\sqrt{2}}$$

was mis-calculated and should be

$$R(T - v_1v_2) \geq \frac{n}{2} + \frac{n_1}{2} \left(\frac{1}{\sqrt{2}} - 1 \right) + \frac{3}{2} - \sqrt{2} - \frac{1}{2\sqrt{2}}.$$

Then combining expressions (21) and (22) there:

$$R(T) - R(T - v_1v_2) \geq \frac{3}{2} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{8}},$$

we get

$$R(T) \geq \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2} + \frac{3}{2} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}}.$$

But, this time we have

$$\frac{3}{2} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} < 0,$$

which does not lead to the proof of the theorem.

Although we find mistakes in their proof, we still believe that the theorem is true. In Section 2.2, we will give the corrected proof.

Theorem 2.1.2 (Theorem 10, [52]) *Let T be a chemical tree of order n with $n_1 \geq 3$ pendent vertices. Then*

$$R(T) \leq \frac{n}{2} - a_0' n_1,$$

where

$$a_0' = \frac{7}{6} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \approx 0.0513$$

with equality if and only if T is isomorphic to $U(n, n_1)$.

In the proof of Theorem 10 of [52], one can not obtain expression (58): $x_{23} - x_{13} = n_1$, since by (54): $x_{22} = n - \frac{1}{2}(5n_1 + x_{23} - x_{13}) + 2 + n_4$, we only have that $5n_1 + x_{23} - x_{13}$ is even for all n_1, i.e., $x_{23} - x_{13}$ has the same parity as n_1, or $x_{23} - x_{13} = n_1 + 2k$, but not $x_{23} - x_{13} = (2k+1)n_1$. Note that the last two expressions are not equivalent.

However, the upper bound in Theorem 2.1.2 is sharp for $n \geq 3n_1 - 2$ but not for $n < 3n_1 - 2$. Thus, Theorem 2.1.2 can be modified as follows.

Theorem 2.1.3 *Let T be a chemical tree of order n with $n_1 \geq 3$ pendent vertices satisfying that $n \geq 3n_1 - 2$. Then*

$$R(T) \leq \frac{n}{2} - a_0' n_1,$$

where

$$a_0' = \frac{7}{6} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \approx 0.0513$$

with equality if and only if T is isomorphic to $U(n, n_1)$.

In Section 2.3, we will give the proof of Theorem 2.1.3.

2.2 Corrected proof of Theorem 2.1.1

Our proof is shorter, and uses linear programming approach, which is widely used in chemical graph theory.

Let T be a chemical tree of order n with n_1 pendent vertices. Denote by x_{ij} the number of edges joining the vertices of degrees i and j, and n_i the number of vertices of degree i in G. Thus, there is another description for the Randić index of T,

$$R(T) = \sum_{1 \le i \le j \le 4} \frac{x_{ij}}{\sqrt{ij}} \,. \tag{2.2.1}$$

Note that $x_{11} = 0$ whenever $n \ge 3$, and therefore the case $i = j = 1$ needs not be considered any further. Consequently, the right–hand side of (2.2.1) is a linear function of the following nine variables $x_{12}, x_{13}, x_{14}, x_{22}, x_{23}, x_{24}, x_{33}, x_{34}, x_{44}$. Firstly,

$$n_1 + n_2 + n_3 + n_4 = n \,. \tag{2.2.2}$$

Counting the edges terminating at vertices of degree i $(i = 1, 2, 3, 4)$, we obtain

$$x_{12} + x_{13} + x_{14} = n_1 \tag{2.2.3}$$

$$x_{12} + 2x_{22} + x_{23} + x_{24} = 2n_2 \tag{2.2.4}$$

$$x_{13} + x_{23} + 2x_{33} + x_{34} = 3n_3 \tag{2.2.5}$$

$$x_{14} + x_{24} + x_{34} + 2x_{44} = 4n_4 \,. \tag{2.2.6}$$

Another linearly independent relation of this kind is

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1) \,. \tag{2.2.7}$$

Now we will solve the linear programming

$$min \;\; R(T) = \sum_{1 \le i \le j \le 4} \frac{x_{ij}}{\sqrt{ij}}$$

with constraints (2.2.2) – (2.2.7).

By elementary calculations, we have

$$x_{22} = \frac{2n - 5n_1 + 6}{2} - \frac{1}{2}x_{12} + \frac{1}{6}x_{13} + \frac{1}{2}x_{14} - \frac{1}{3}x_{23} + \frac{1}{3}x_{33} + \frac{2}{3}x_{34} + x_{44} \tag{2.2.8}$$

$$x_{24} = 2n_1 - 4 - \frac{2}{3}x_{13} - x_{14} - \frac{2}{3}x_{23} - \frac{4}{3}x_{33} - \frac{5}{3}x_{34} - 2x_{44} \tag{2.2.9}$$

Substituting (2.2.8) and (2.2.9) into (2.2.1), we have

$$\begin{aligned} R(G) &= \frac{2n+(2\sqrt{2}-5)n_1+6-4\sqrt{2}}{4} + c_{12}\,x_{12} + c_{13}\,x_{13} + c_{14}\,x_{14} \\ &+ c_{23}\,x_{23} + c_{33}\,x_{33} + c_{34}\,x_{34} + c_{44}\,x_{44} \qquad (2.2.10) \end{aligned}$$

where

$$\begin{aligned} c_{12} &= 1/\sqrt{2} - 1/4 \approx 0.45711 \\ c_{13} &= 1/\sqrt{3} + 1/12 - \sqrt{2}/6 \approx 0.42498 \\ c_{14} &= 3/4 - 1/\sqrt{8} \approx 0.39645 \\ c_{23} &= 1/\sqrt{6} - 1/6 - \sqrt{2}/6 \approx 0.00588 \\ c_{33} &= 1/2 - \sqrt{2}/3 \approx 0.02860 \\ c_{34} &= 1/\sqrt{12} + 1/3 - 5\sqrt{2}/12 \approx 0.03275 \\ c_{44} &= 3/4 - 1/\sqrt{2} \approx 0.04289\ . \end{aligned}$$

Because all coefficients c_{ij} on the right–hand side of (2.2.10) are positive–valued, it is clear that for fixed n and n_1, $R(T)$ will be minimum if the parameters x_{12}, x_{13}, x_{14}, x_{23}, x_{33}, x_{34} and x_{44} are all equal to zero (provided this is possible). However, a tree must have at least two pendent vertices, and so we have

$$x_{12} + x_{13} + x_{14} > 0. \qquad (2.2.11)$$

Since $c_{14} < c_{13} < c_{12}$, considering the minimum of $R(T)$, the best solution of (2.2.11) is that all pendent vertices are adjacent to vertices with degree 4, i.e., $x_{14} = n_1$.

Thus, we get

$$\begin{aligned} R(T) &\geq \frac{2n+(2\sqrt{2}-5)n_1+6-4\sqrt{2}}{4} + \left(\frac{3}{4} - \frac{1}{\sqrt{8}}\right) n_1 \\ &= \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}, \end{aligned}$$

equality holds if and only if $x_{12} = x_{13} = x_{23} = x_{33} = x_{34} = x_{44} = 0$, $x_{14} = n_1$ and $n_3 = 0$. The proof is complete. ∎

2.3 Proof of Theorem 2.1.3

The proof of our result is carried out mainly by the following lemma [20].

Lemma 2.3.1 (Caporossi *et al.*, [20]) *Let G be a connected graph with n vertices. Then*

$$R(G) = \frac{n}{2} - \sum_{e \in E(G)} \omega^*(e),$$

where

$$\omega^*(e) = \frac{1}{2}\left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}}\right)^2$$

for $e = uv$. ∎

In fact, it can be considered as another expression of the Randić index. It is important to notice that, the weight ω^* of edges which connected the two vertices with the equal degree is zero.

A path $v_1v_2 \dots v_{s-1}v_s$ is called a *pendent path*, if $d(v_1) = 1$, $d(v_s) \geq 3$ and $d(v_2) = \cdots = d(v_{s-1}) = 2$.

Lemma 2.3.2 *Let T be the chemical tree which attains the maximum Randić index among all chemical trees of order n with n_1 ($n_1 \geq 3$) pendent vertices. For each $v \in V(T)$, if $d(v) = 2$, then v must be on a pendent path.*

Proof. By contradiction. Let $v \in V(T)$ and $d(v) = 2$. Suppose v is not on any pendent path. There must be a path $v_1v_2 \dots v_svw_t \dots w_2w_1$ ($s \geq 1$ and $t \geq 1$) such that $d(v_1) = p \geq 3$, $d(w_1) = q \geq 3$ and $d(v_2) = \cdots = d(v_s) = d(w_t) = \cdots = d(w_2) = 2$. Let x be a pendent vertex of T and y its neighbor with $d(y) = l \geq 2$. Let $T' = T - v_1v_2 - w_2w_1 + v_1w_1 + xv_2$. Then T' is also a tree with n vertices and n_1 pendent vertices. We have

$$\begin{aligned} R(T) - R(T') &= \frac{1}{\sqrt{2p}} + \frac{1}{\sqrt{2q}} + \frac{1}{\sqrt{l}} - \frac{1}{\sqrt{pq}} - \frac{1}{\sqrt{2l}} - \frac{1}{\sqrt{2}} \\ &= \left(\frac{1}{\sqrt{p}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{q}}\right) + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{l}}\right) < 0, \end{aligned}$$

a contraction. ∎

Now we are at the point to give the proof of Theorem 2.1.3.

Proof. Let T be a chemical tree of order n with n_1 ($n_1 \geq 3$) pendent vertices. By Lemma 2.3.2, we assume that all vertices of T with degree two are on pendent paths, then $x_{12} = x_{23} + x_{24}$. Note that $x_{12} + x_{13} + x_{14} = n_1$, and by Lemma 2.3.1,

$$\begin{aligned}
R(T) &= \frac{n}{2} - \sum_{e \in E(T)} \omega^*(e) \\
&= \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 x_{12} - \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{3}}\right)^2 x_{13} + \left(1 - \frac{1}{2}\right)^2 x_{14}\right] \\
&\quad -\frac{1}{2}\left[\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 x_{23} + \left(\frac{1}{\sqrt{2}} - \frac{1}{2}\right)^2 x_{24}\right] - \frac{1}{2}\left(\frac{1}{\sqrt{3}} - \frac{1}{2}\right)^2 x_{34} \\
&\leq \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 x_{12} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)^2 (x_{13} + x_{14}) \\
&\quad -\frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 (x_{23} + x_{24}) \\
&= \frac{n}{2} - \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right] x_{12} \\
&\quad -\frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)^2 (x_{13} + x_{14}) \\
&= \frac{n}{2} - \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right] n_1 \\
&\quad +\frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 - \left(1 - \frac{1}{\sqrt{3}}\right)^2\right] (x_{13} + x_{14}) \\
&= \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)n_1}{6} - \left(1 - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)(x_{13} + x_{14}) \\
&\leq \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)n_1}{6}.
\end{aligned}$$

The equality holds if all the equalities in the above inequalities hold. Thus $x_{13} = x_{14} = x_{24} = x_{34} = 0$. Then $x_{44} = 0$ since T is a tree. The proof is complete. ∎

Chapter 3

Randić Index and the Minimum Degree

In this chapter, we will consider the relation between the Randić index and the minimum degree.

3.1 Introduction

In 1988, Shearer proved if G has no isolated vertices then $R(G) \geq \sqrt{n}/2$. It is the first proof that Randić index goes to infinity together with n. A few months later Alon improved this bound to $\sqrt{n} - 8$ (see [40]). In 1998, Bollobás and Erdös [14] proved that the Randić index of a graph G of order n without isolated vertices is at least $\sqrt{n-1}$, with equality if and only if G is a star. Bollobás and Erdös asked for the minimum value of the Randić index for graphs with given minimum degree $\delta(G)$. In 2002, Delorme, Favaron and Rautenbach [32] gave the following conjecture:

Conjecture 3.1.1 (Delorme, Favaron and Rautenbach, [32]) *Let $G = (V, E)$ be a graph of order n with $\delta(G) \geq k$. Then*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1}$$

with equality if and only if $G = K^*_{k,n-k}$, where $K^*_{k,n-k}$ is obtained from a complete bipartite graph $K_{k,n-k}$ by joining each pair of vertices in the part with k vertices by a new edge.

At the same time, they showed that the conjecture is true for $k = 2$. Using the linear programming, Pavlović [84] verified the conjecture for the case of $k = 2$. In [3] Aouchiche and Hansen found examples showing that the conjecture is not true, and gave a modified form. There are many researches about this conjecture, such as [77, 84, 85, 86].

In this chapter, by using the linear programming we verify this conjecture for $k = 3$, which can easily lead to the conclusion that the inequality of the conjecture holds for all chemical graphs, i.e., graphs with maximum degree at most 4. Furthermore, we prove that for $k \geq 4$, the conjecture is true for any graph of order $n \geq \frac{3}{2}k^3$.

Denote by $x_{i,j}$ the number of edges joining the vertices of degrees i and j.

3.2 Some Lemmas and elementary results

Lemma 3.2.1 (Bollobás and Erdös, [14]) *Let x_1x_2 be an edge with the maximum weight in a graph G, then*

$$R(G - x_1x_2) < R(G).$$

Lemma 3.2.2 *Let G be the graph with the minimum Randić index among all simple graphs with order n and the minimum degree $\delta \geq k \geq 2$. Then the minimum degree of G must be k.*

Proof. Suppose $\delta(G) > k$, we construct a new graph G' from G by deleting an edge of maximum weight of G. It is easy to see $\delta(G') \geq k$. By Lemma 3.2.1, we have $R(G') < R(G)$, contradicting to the choice of G. Thus, $\delta(G) = k$. ∎

From Lemma 3.2.2, we can rewrite Conjecture 3.1.1 as the following equivalent form, and consider Conjecture 3.2.1 only in the sequel.

Conjecture 3.2.1 *Let $G = (V, E)$ be a graph of order n with $\delta(G) = k$. Then*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1}$$

with equality if and only if $G = K^*_{k,n-k}$, *where* $K^*_{k,n-k}$ *is obtained from a complete bipartite graph* $K_{k,n-k}$ *by joining each pair of vertices in the part with* k *vertices by a new edge.*

Lemma 3.2.3 *Let* k, p, n *be nonnegative integers, for* $k \geq 4$, $0 \leq p \leq k-1$ *and* $n \geq \frac{3}{2}k^3$, *we have*

$$(i).\ g(k,p,n) = (k-p)\cdot \left(\frac{n+k-2p-2}{k} - \frac{2(n-p-2)}{\sqrt{k(n-2)}} + \frac{2p}{\sqrt{k(n-1)}} - \frac{2p}{\sqrt{(n-1)(n-2)}}\right) > 0;$$

$$(ii)\ a(k,p,n) = \frac{1}{n-2} + \frac{2p}{(n-p-2)\sqrt{(n-2)(n-1)}} - \frac{2}{n+k-2p-2}\cdot \left(\frac{p}{\sqrt{k(n-1)}} + \frac{p(k-p)}{(n-p-2)\sqrt{(n-2)(n-1)}} + \frac{k-p}{\sqrt{k(n-2)}}\right) > 0;$$

$$(iii)\ s(k,p,n) = \frac{\binom{p}{2}}{n-1} - \left(\binom{k}{2}\frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}}\right) + \frac{n-p}{n+k-2p-2}\cdot \left(\frac{p(n-p-2)}{\sqrt{k(n-1)}} + \frac{p(k-p)}{\sqrt{(n-1)(n-2)}} + \frac{(k-p)(n-p-2)}{\sqrt{k(n-2)}}\right) > 0.$$

Proof. (i) Let $g_1(k,p,n) = \frac{k\sqrt{(n-1)(n-2)}}{k-p} g(k,p,n)$, i.e.,

$$\begin{aligned} g_1(k,p,n) =& (n+k-2p-2)\sqrt{(n-1)(n-2)} - \\ & 2(n-p-2)\sqrt{k(n-1)} + 2p\sqrt{k(n-2)} - 2pk. \end{aligned}$$

Since

$$\frac{\partial g_1(k,p,n)}{\partial p} = -\sqrt{n-1}\left(\sqrt{n-2} - \sqrt{4k}\right) - \sqrt{n-2}\left(\sqrt{n-1} - \sqrt{4k}\right) - 2k,$$

$g_1(k,p,n)$ is a strict decreasing function in p when $n \geq \frac{3}{2}k^3$ and $k \geq 4$. And then

$$\begin{aligned} g_1(k,p,n) &> g_1(k,k,n) \\ &= (n-k-2)\sqrt{n-1}\left(\sqrt{n-2} - 2\sqrt{k}\right) + 2k\sqrt{k}\left(\sqrt{n-2} - \sqrt{k}\right) > 0, \end{aligned}$$

since when $n \geq \frac{3}{2}k^3$ and $k \geq 4$,

$$\sqrt{(n-2)} - \sqrt{k} > \sqrt{n-2} - \sqrt{4k} > 0.$$

Then $g(k,p,n) > 0$.

(ii) Let

$$a_1(k,p,n) = (n-2)(n+k-2p-2)(n-p-2)\sqrt{k(n-1)}\ a(k,p,n),$$

i.e.,

$$\begin{aligned} a_1(k,p,n) =& (n+k-2p-2)(n-p-2)\sqrt{k(n-1)} \\ &+ 2p(n+k-2p-2)\sqrt{k(n-2)} - 2p(n-2)(n-p-2) \\ &- 2p(k-p)\sqrt{k(n-2)} - 2(k-p)(n-p-2)\sqrt{(n-1)(n-2)}. \end{aligned}$$

Then we have

$$\begin{aligned} & a_1(k,p,n) \\ > & (n+k-2p-2)(n-p-2)\sqrt{k(n-2)} + 2p(n+k-2p-2)\sqrt{k(n-2)} \\ & - 2p(n-1)(n-p-2) - 2p(k-p)\sqrt{k(n-2)} - 2(k-p)(n-p-2)(n-1) \\ = & (n-p-2)\left((n+k-2)\sqrt{k(n-2)} - 2k(n-1)\right) \\ > & (n-p-2)(n-1)\sqrt{k}\left(\sqrt{n-2} - \sqrt{4k}\right) > 0, \end{aligned}$$

since when $n \geq \frac{3}{2}k^3$ and $k \geq 4$, $\sqrt{n-2} - 2\sqrt{k} > 0$. So $a(k,p,n) > 0$.

(iii) Let

$$s_1(k,p,n) = (n-1)(n+k-2p-2)\sqrt{k(n-2)}\ s(k,p,n),$$

we have

$$\begin{aligned} & s_1(k,p,n) \\ = & \binom{p}{2}(n+k-2p-2)\sqrt{k(n-2)} + p(n-p)(n-p-2)\sqrt{(n-1)(n-2)} \\ & + p(k-p)(n-p)\sqrt{k(n-1)} + (n-p-2)(k-p)(n-p)(n-1) \\ & - \binom{k}{2}(n+k-2p-2)\sqrt{k(n-2)} \\ & - k(n-k)(n+k-2p-2)\sqrt{(n-1)(n-2)}. \end{aligned}$$

Then

$$\begin{aligned}
s_1(k,p,n) > &\frac{\sqrt{k(n-2)}}{2}\cdot \\
&[p(p-1)(n+k-2p-2)+2p(k-p)(n-p)-k(k-1)(n+k-2p-2)] \\
&+[p(n-p)(n-p-2)-k(n-k)(n+k-2p-2)]\sqrt{(n-1)(n-2)} \\
&+(n-1)(n-p)(k-p)(n-p-2) \\
=&\frac{(k-p)\sqrt{k(n-2)}}{2}\left[(p+1-k)n+pk+3k-2-k^2\right] \\
&+(k-p)[-n^2+2n(p+1)-p^2-pk-2k-2p+k^2]\sqrt{(n-1)(n-2)} \\
&+(n-1)(n-p)(k-p)(n-p-2).
\end{aligned}$$

Since when $0 \le p \le k-1$ and $n \ge \frac{3}{2}k^3$,

$$-n^2+2n(p+1)-p^2-pk-2k-2p+k^2 < 0 \quad \text{and} \quad \sqrt{(n-1)(n-2)} \le \frac{2n-3}{2},$$

then we have

$$\begin{aligned}
&s_1(k,p,n) \\
\ge &\frac{(k-p)\sqrt{k(n-2)}}{2}\left[(p+1-k)n+pk+3k-2-k^2\right]+(k-p)\cdot \\
&\Big((-n^2+2n(p+1)-p^2-pk-2k-2p+k^2)\frac{2n-3}{2}+ \\
&(n-1)(n-p)(n-p-2)\Big) \\
=&\frac{(k-p)}{2}\big[n^2+2(k^2-pk-2k-p-1)n-3k^2+3pk+6k+p^2+2p \\
&+\big((p+1-k)n+pk+3k-2-k^2\big)\sqrt{k(n-2)}\big] \\
>&\frac{(k-p)}{2}\left[n^2+2(k^2-k^2-2k-k)n-3kn+(-kn-k^2)\sqrt{kn}\right] \\
=&\frac{(k-p)\sqrt{n}}{2}\left[n\sqrt{n}-9k\sqrt{n}-(kn+k^2)\sqrt{k}\right].
\end{aligned}$$

Let $t(n,k) = (n\sqrt{n}-9k\sqrt{n})^2 - \left((kn+k^2)\sqrt{k}\right)^2 = n^3-(k^3+18k)n^2+(81k^2-2k^4)n-k^5$. Since $n \ge \frac{3}{2}k^3$,

$$\frac{\partial t(n,k)}{\partial n} = 3n^2-2k(k^2+18)n-k^2(2k^2-81) > 0,$$

then when $k \ge 6$,

$$t(n,k) > t(\frac{3}{2}k^3,k) = k^5\left(\frac{9}{8}k^4-\frac{87}{2}k^2+\frac{241}{2}\right) > 0,$$

which implies $s(k,p,n) > 0$ for $k \geq 6$.

For the cases of $k = 4$ and 5, we can verify that when $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, $s(k,p,n) > 0$ by considering all possible values of p. ∎

3.3 Some approaches to Conjecture 3.2.1

Let G be a simple graph of order n with $\delta(G) = k \geq 3$. At first, we will give some linear equalities. Mathematical description of the problem is as follows:

$$min\ R(G) = \sum_{\substack{k\leq i\leq n-1\\ i\leq j\leq n-1}} \frac{x_{i,j}}{\sqrt{ij}}$$

subject to:

$$\begin{array}{rcl}
2x_{k,k} + x_{k,k+1} + x_{k,k+2}+ & \cdots & +x_{k,n-1} = kn_k \\
x_{k+1,k} + 2x_{k+1,k+1} + x_{k+1,k+2}+ & \cdots & +x_{k+1,n-1} = (k+1)n_{k+1} \\
x_{k+2,k} + x_{k+2,k+1} + 2x_{k+2,k+2}+ & \cdots & +x_{k+2,n-1} = (k+2)n_{k+2} \\
 & \vdots & \\
x_{n-1,k} + x_{n-1,k+1} + x_{n-1,k+2}+ & \cdots & +2x_{n-1,n-1} = (n-1)n_{n-1}
\end{array} \tag{3.3.1}$$

and

$$n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-1} = n. \tag{3.3.2}$$

These constraints do not completely determine the problem. In order to have a better description for this problem we have to add the next constraints: $x_{i,n-1} = n_i n_{n-1}$ for $i = k, k+1, \ldots, n-2$ and $x_{n-1,n-1} = \binom{n_{n-1}}{2}$, which much more complicate the problem. Now the problem becomes a quadratic programming. To avoid the complexity of these quadratic inequalities, we will consider all the possible values of n_{n-1} and solve the problem.

We only consider the case of $k \leq n-2$, since the graph is unique when $k = n-1$.

Theorem 3.3.1 *For a given minimum degree $\delta(G) = k \geq 4$, the conjecture is true when the order of the graph $n \geq \frac{3}{2}k^3$. That is, for a given minimum degree $\delta(G) = k \geq 4$ and $n \geq \frac{3}{2}k^3$, we have*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1},$$

with equality if and only if G is a graph with $n_k = n-k$, $n_{n-1} = k$, $n_{k+1} = \cdots = n_{n-2} = 0$, $x_{k,n-1} = k(n-k)$, $x_{n-1,n-1} = \binom{k}{2}$ and all other $x_{i,j}$ and $x_{i,i}$ being equal to 0, i.e., $G \cong K^*_{k,n-k}$.

Proof. Since the minimum degree is k, we have $n_{n-1} \leq k$. So, we will consider two cases: $n_{n-1} = k$ and $n_{n-1} = p$, where p is an integer such that $0 \leq p \leq k-1$. Let G be a graph with order n and $\delta(G) = k \geq 4$. Denote G by $G^{(i)}$ if $n_{n-1}(G) = i$ $(i = 0, 1, \ldots, k)$. Let $R^{(i)} = R(G^{(i)})$.

Case 1: $n_{n-1} = k$

Since $x_{i,n-1} = kn_i$ for $i = k, k+1, \ldots, n-2$ and $x_{n-1,n-1} = \binom{k}{2}$, the constraints in (3.3.1) become:

$$x_{j,k} + \cdots + x_{j,j-1} + 2x_{j,j} + x_{j,j+1} + \cdots + x_{j,n-2} = (j-k)n_j,$$

for $j = k, k+1, \ldots, n-2$. Then we have

$$\begin{aligned}
R^{(k)} &= \sum_{\substack{k\leq i\leq n-1\\ i\leq j\leq n-1}} \frac{x_{i,j}}{\sqrt{ij}} = \sum_{j=k}^{n-2} \frac{kn_j}{\sqrt{j(n-1)}} + \binom{k}{2}\frac{1}{n-1} \\
&\quad + \frac{1}{2}\sum_{j=k}^{n-2}\left(\frac{x_{j,k}}{\sqrt{jk}} + \cdots + \frac{x_{j,j-1}}{\sqrt{j(j-1)}} + \frac{2x_{j,j}}{\sqrt{jj}} + \frac{x_{j,j+1}}{\sqrt{j(j+1)}} + \cdots + \frac{x_{j,n-2}}{\sqrt{j(n-2)}}\right) \\
&\geq \sum_{j=k}^{n-2} \frac{kn_j}{\sqrt{j(n-1)}} + \binom{k}{2}\frac{1}{n-1} \\
&\quad + \frac{1}{2}\sum_{j=k}^{n-2} \frac{x_{j,k} + \cdots + x_{j,j-1} + 2x_{j,j} + x_{j,j+1} + \cdots + x_{j,n-2}}{\sqrt{j(n-1)}} \\
&= \binom{k}{2}\frac{1}{n-1} + \frac{1}{2\sqrt{n-1}}\sum_{j=k}^{n-2}\left(\sqrt{j} + \frac{k}{\sqrt{j}}\right)n_j \\
&= \binom{k}{2}\frac{1}{n-1} + \frac{1}{2\sqrt{n-1}}\left(\sqrt{k} + \frac{k}{\sqrt{k}}\right)n_k + \frac{1}{2\sqrt{n-1}}\sum_{j=k+1}^{n-2}\left(\sqrt{j} + \frac{k}{\sqrt{j}}\right)n_j.
\end{aligned}$$

By substituting $n_k = n - k - (n_{k+1} + n_{k+2} + \cdots + n_{n-2})$ into the last equality, we have

$$R^{(k)} \geq \binom{k}{2}\frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}} + \frac{1}{2\sqrt{n-1}}\sum_{j=k+1}^{n-2}\left(\sqrt{j} + \frac{k}{\sqrt{j}} - 2\sqrt{k}\right)n_j.$$

Since

$$\sqrt{j} + \frac{k}{\sqrt{j}} - 2\sqrt{k} > 2\sqrt{k} - 2\sqrt{k} = 0$$

for $k+1 \leq j \leq n-2$, this function attains the minimum for $n_j = 0$, $j = k+1, k+2, \ldots, n-2$. Therefore, when $n_{n-1} = k$, the minimum value of the Randić index is

$$R^{*(k)} = \binom{k}{2}\frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}}.$$

The extremal graph must have $n_k = n-k$, $n_{k+1} = n_{k+2} = \cdots = n_{n-2} = 0$, $n_{n-1} = k$, $x_{k.n-1} = k(n-k)$, $x_{n-1,n-1} = \binom{k}{2}$ and all other $x_{i,j}$ and $x_{i,i}$ are equal to 0, i.e., $G = K^*_{k,n-k}$.

Case 2: $n_{n-1} = p$ $(0 \leq p \leq k-1)$

By substituting $x_{i,n-1} = pn_i$ for $i = k, k+1, \ldots, n-2$ and $x_{n-1,n-1} = \binom{p}{2}$ (if $p = 0, 1$, $\binom{p}{2} = 0$) into the constraints in (3.3.1), they become (3.3.3)

$$\begin{aligned}
2x_{k,k} + x_{k,k+1} + x_{k,k+2} + \cdots + x_{k,n-2} &= (k-p)n_k \\
x_{k+1,k} + 2x_{k+1,k+1} + x_{k+1,k+2} + \cdots + x_{k+1,n-2} &= (k+1-p)n_{k+1} \\
x_{k+2,k} + x_{k+2,k+1} + 2x_{k+2,k+2} + \cdots + x_{k+2,n-2} &= (k+2-p)n_{k+2} \\
&\vdots \\
x_{n-2,k} + x_{n-2,k+1} + x_{n-2,k+2} + \cdots + 2x_{n-2,n-2} &= (n-2-p)n_{n-2}
\end{aligned} \tag{3.3.3}$$

Since $n_{n-1} = p$, equality (3.3.2) becomes (3.3.4)

$$n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-2} = n - p. \tag{3.3.4}$$

We have the next problem: minimize $R^{(p)}$ subject to (3.3.3) and (3.3.4). It is easy to express n_i for $i = k+1, k+2, \ldots, n-3$ from the constraints in (3.3.3) as follows

$$n_i = \frac{x_{i,k} + \cdots + x_{i,i-1} + 2x_{i,i} + x_{i,i+1} + \cdots + x_{i,n-2}}{i-p}. \tag{3.3.5}$$

Using the first and the last constraint of (3.3.3), (3.3.4) and constraint (3.3.5), by some calculations, we can obtain

$$n_k = \frac{(n-p-2)(n-p)}{n+k-2p-2} + \frac{2x_{k,k}}{n+k-2p-2} - \sum_{j=k+1}^{n-3} \frac{(n-j-2)x_{k,j}}{(j-p)(n+k-2p-2)}$$
$$- \sum_{\substack{k+1\le i\le n-2\\ i\le j\le n-2}} \left(\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p}\right) \frac{x_{i,j}}{n+k-2p-2}, \tag{3.3.6}$$

$$n_{n-2} = \frac{(n-p)(k-p)}{n+k-2p-2} - \sum_{\substack{k\le i\le n-3\\ i\le j\le n-3}} \left(\frac{k-p}{i-p} + \frac{k-p}{j-p}\right) \frac{x_{i,j}}{n+k-2p-2}$$
$$- \sum_{i=k+1}^{n-3} \left(\frac{k-p}{i-p} - 1\right) \frac{x_{n-2,i}}{n+k-2p-2} + \frac{2x_{n-2,n-2}}{n+k-2p-2}, \tag{3.3.7}$$

$$x_{k,n-2} = \frac{(n-p-2)(n-p)(k-p)}{n+k-2p-2} - \sum_{j=k}^{n-3} \frac{(n-p-2)(k+j-2p)}{(j-p)(n+k-2p-2)} x_{k,j}$$
$$- \sum_{\substack{k+1\le i\le n-2\\ i\le j\le n-2}} \left(\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p}\right) \frac{(k-p)x_{i,j}}{n+k-2p-2}. \tag{3.3.8}$$

By substituting $x_{i,n-1} = pn_i$ $(i = k, k+1, \ldots, n-2)$, $x_{n-1,n-1} = \binom{p}{2}$, (3.3.5), (3.3.6), (3.3.7) and (3.3.8) into $R^{(p)}$, we have

$$R^{(p)} = \overline{R^{(p)}} + \sum_{j=k}^{n-3} a_{k,j} x_{k,j} + \sum_{\substack{k+1\le i\le n-2\\ i\le j\le n-2}} a_{i,j} x_{i,j}$$

where

$$\overline{R^{(p)}} = \frac{\binom{p}{2}}{n-1} + \frac{n-p}{n+k-2p-2} \cdot \left(\frac{p(n-p-2)}{\sqrt{k(n-1)}} + \frac{p(k-p)}{\sqrt{(n-1)(n-2)}} + \frac{(k-p)(n-p-2)}{\sqrt{k(n-2)}}\right)$$

and

$$a_{i,j} = \frac{1}{\sqrt{ij}} - \frac{p}{\sqrt{k(n-1)}} \cdot \frac{\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p}}{n+k-2p-2} - \frac{p}{\sqrt{(n-1)(n-2)}} \cdot \frac{\frac{k-p}{i-p} + \frac{k-p}{j-p}}{n+k-2p-2}$$
$$- \frac{k-p}{\sqrt{k(n-2)}} \cdot \frac{\frac{n-p-2}{i-p} + \frac{n-p-2}{j-p}}{n+k-2p-2} + \frac{\frac{p}{i-p}}{\sqrt{i(n-1)}} + \frac{\frac{p}{j-p}}{\sqrt{j(n-1)}}.$$

We will prove that all functions $a_{i,j}$ are nonnegative for corresponding i and j.

Let

$$f(i,j) = (n+k-2p-2)(i-p)(j-p)a_{ij},$$

then

$$\begin{aligned} f(i,j) = &\frac{(n+k-2p-2)(i-p)(j-p)}{\sqrt{ij}} - \frac{p(n-p-2)(i+j-2p)}{\sqrt{k(n-1)}} \\ &- \frac{p(k-p)(i+j-2p)}{\sqrt{(n-1)(n-2)}} - \frac{(k-p)(n-p-2)(i+j-2p)}{\sqrt{k(n-2)}} \\ &+ \frac{p(n+k-2p-2)(j-p)}{\sqrt{i(n-1)}} + \frac{p(n+k-2p-2)(i-p)}{\sqrt{j(n-1)}}. \end{aligned}$$

We have

$$\begin{aligned} \partial^2 f(i,j)/\partial j^2 &= \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}}\left(\frac{3p}{\sqrt{n-1}} - \frac{j+3p}{\sqrt{i}}\right) \\ &\leq \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}}\left(\frac{3p}{\sqrt{n-1}} - \frac{i+3p}{\sqrt{i}}\right) \\ &\leq \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}}\left(\frac{3p}{\sqrt{n-1}} - 2\sqrt{3p}\right) \\ &= \frac{(n+k-2p-2)(i-p)}{4\sqrt{j^5}} \cdot \frac{\sqrt{3p}}{\sqrt{n-1}}(\sqrt{3p} - 2\sqrt{n-1}) < 0, \end{aligned}$$

since $\frac{i+3p}{\sqrt{i}} = \sqrt{i} + \frac{3p}{\sqrt{i}} \geq 2\sqrt{3p}$ and $n-1 > k > p$. Thus, $f(i,j)$ is concave in j. We have to check that $a_{i,i}$ and $a_{i,n-2}$ are nonnegative in order to conclude that $a_{i,j} \geq 0$ for $k \leq i \leq n-2$ and $i \leq j \leq n-2$. Let

$$g(i,p,n) = (n+k-2p-2)(i-p)a_{i,i},$$

then

$$\begin{aligned} g(i,p,n) = &\frac{(n+k-2p-2)(i-p)}{i} - \frac{2p(n-p-2)}{\sqrt{k(n-1)}} - \frac{2p(k-p)}{\sqrt{(n-1)(n-2)}} \\ &- \frac{2(k-p)(n-p-2)}{\sqrt{k(n-2)}} + \frac{2p(n+k-2p-2)}{\sqrt{i(n-1)}}. \end{aligned}$$

We have

$$\frac{\partial g(i,p,n)}{\partial i} = \frac{p(n+k-2p-2)}{\sqrt{i^3}}\left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{n-1}}\right) > 0,$$

then for $i \geq k$, $g(i,p,n) \geq g(k,p,n)$, where

$$\begin{aligned} &g(k,p,n) \\ &= (k-p)\left(\frac{n+k-2p-2}{k} - \frac{2(n-p-2)}{\sqrt{k(n-2)}} + \frac{2p}{\sqrt{k(n-1)}} - \frac{2p}{\sqrt{(n-1)(n-2)}}\right). \end{aligned}$$

By Lemma 3.2.3 (i), for $k \geq 4$, $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, we have $g(k,p,n) > 0$, then $a_{i,i} > 0$.

Let

$$q(i,p,n) = (n+k-2p-2)(i-p)a_{i,n-2},$$

then

$$\begin{aligned} q(i,p,n) = &\frac{(n+k-2p-2)(i-p)}{\sqrt{(n-2)i}} - \frac{p(n-2p-2+i)}{\sqrt{k(n-1)}} \\ &- \frac{p\left(k-p+\frac{(k-p)(i-p)}{n-p-2}\right)}{\sqrt{(n-1)(n-2)}} - \frac{(k-p)(n-2p-2+i)}{\sqrt{k(n-2)}} \\ &+ \frac{p(n+k-2p-2)}{\sqrt{(n-1)i}} + \frac{p(n+k-2p-2)(i-p)}{(n-p-2)\sqrt{(n-1)(n-2)}}. \end{aligned}$$

Since

$$\partial^2 q(i,p,n)/\partial i^2 = -\frac{n+k-2p-2}{4\sqrt{i^5}}\left(\frac{i+3p}{\sqrt{n-2}} - \frac{3p}{\sqrt{n-1}}\right) < 0,$$

and $q(k,p,n) = 0$, we only need to prove

$$\begin{aligned} a_{n-2,n-2} = &\frac{1}{n-2} + \frac{2p}{(n-p-2)\sqrt{(n-2)(n-1)}} - \frac{2}{n+k-2p-2} \\ &\cdot\left(\frac{p}{\sqrt{k(n-1)}} + \frac{p(k-p)}{(n-p-2)\sqrt{(n-2)(n-1)}} + \frac{k-p}{\sqrt{k(n-2)}}\right) \geq 0. \end{aligned}$$

By Lemma 3.2.3 (ii), for $k \geq 4$, $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, we have $a_{n-2,n-2} > 0$, then $a_{i,n-2} > 0$.

Since $a_{i,j} \geq 0$ for $k \leq i \leq n-2$ and $i \leq j \leq n-2$, then $R^{(p)}$ attains the minimum if we put $x_{k,j} = 0$ for $j = k, k+1, \ldots, n-3$ and $x_{i,j} = 0$ for $k+1 \leq i \leq n-2$, $i \leq j \leq n-2$. The minimum value is $\overline{R^{(p)}}$ and

$$n_k = \frac{(n-p-2)(n-p)}{n+k-2p-2}, \quad n_{n-2} = \frac{(n-p)(k-p)}{n+k-2p-2}, \quad n_{n-1} = p, \quad n_i = 0$$

for $i = k+1, \ldots, n-3$. This solution may not correspond to any graph, and the real graphical solution $R^{*(P)} \geq \overline{R^{(p)}}$. Now we only need to show that $\overline{R^{(p)}} \geq R^{*(k)}$. Let

$$s(k,p,n) = \overline{R^{(p)}} - R^{*(k)} = \frac{\binom{p}{2}}{n-1} + \frac{n-p}{n+k-2p-2} \cdot \left(\frac{p(n-p-2)}{\sqrt{k(n-1)}} + \frac{p(k-p)}{\sqrt{(n-1)(n-2)}} + \frac{(k-p)(n-p-2)}{\sqrt{k(n-2)}} \right) - \left(\binom{k}{2} \frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}} \right).$$

By Lemma 3.2.3 (iii), for $k \geq 4$, $0 \leq p \leq k-1$ and $n \geq \frac{3}{2}k^3$, we have $s(k,p,n) > 0$. The proof is thus complete. ∎

Theorem 3.3.2 *Let G be a simple graph of order n with minimum degree $k = 3$. Then we have*

$$R(G) \geq \frac{3(n-3)}{\sqrt{3(n-1)}} + \binom{3}{2} \frac{1}{n-1},$$

with equality if and only if $G = K^*_{k,n-k}$.

Proof. By the proof of Theorem 3.3.1, we only need to prove the inequalities $g(k,p,n) \geq 0$, $a_{n-2,n-2} \geq 0$ and $s(k,p,n) \geq 0$ for $k = 3$ and $0 \leq p \leq 2$. In the following we only consider $n \geq 6$, since the graph with 4 vertices and $k = 3$ is unique, the number of graphs with 5 vertices and $k = 3$ are only two (see Figure 3.1). Now we consider all the possible values of p.

Case 1: $p = 0$

We have

$$g(3,0,n) = n+1 - \frac{6(n-2)}{\sqrt{3n-6}} \geq g(3,0,6) > 0;$$

$$a_{n-2,n-2} = \frac{1}{n-2} - \frac{6}{(n+1)\sqrt{3(n-2)}} = \frac{1}{\sqrt{n-2}} \left(\frac{1}{\sqrt{n-2}} - \frac{2\sqrt{3}}{n+1} \right) \geq 0;$$

$$s(3,0,n) = \frac{\sqrt{3}n(n-1)\sqrt{n-2} - 3(n+1) - \sqrt{3}(n-3)(n+1)\sqrt{n-1}}{(n+1)(n-1)}.$$

Let

$$\begin{aligned} s_0(n) &= \sqrt{3}n(n-1)\sqrt{n-2} - 3(n+1) - \sqrt{3}(n-3)(n+1)\sqrt{n-1} \\ &= \sqrt{3}n\left((n-1)\sqrt{n-2} - \sqrt{3} - (n-2)\sqrt{n-1}\right) + 3\sqrt{3}\sqrt{n-1} - 3. \end{aligned}$$

By simple calculation, we can prove that $3\sqrt{3}\sqrt{n-1}-3 > 0$ and $(n-1)\sqrt{n-2} - \sqrt{3} - (n-2)\sqrt{n-1} > 0$ for $n \geq 14$, i.e., $s_0(n) \geq 0$ for $n \geq 14$. We can directly verify that $s_0(n) \geq 0$ for $6 \leq n \leq 13$.

Case 2: $p = 1$

We have

$$g(3,1,n) = \frac{2\sqrt{n-1}\left((n-1)\sqrt{n-2} - 2\sqrt{3}(n-3)\right) + 4\sqrt{3}\left(\sqrt{n-2} - \sqrt{3}\right)}{3\sqrt{(n-1)(n-2)}}.$$

For $n \geq 6$, we have $\sqrt{n-2} - \sqrt{3} > 0$. Let

$$g_1(n) = (n-1)\sqrt{n-2} - 2\sqrt{3}(n-3),$$

we have

$$g_1'(n) = \frac{1}{2\sqrt{n-2}} + \frac{3}{2}\sqrt{n-2} - 2\sqrt{3} > \frac{1}{2\sqrt{n-2}} > 0$$

for $n \geq 9$, then $g_1(n)$ is a strictly increasing function in $n \geq 9$. So $g_1(n) > g_1(9) = 8\sqrt{7} - 12\sqrt{3} > 0$. By some calculations we obtain that $g(3,1,n) > 0$ for $6 \leq n \leq 8$.

$$\begin{aligned} a_{n-2,n-2} &= \frac{1}{n-2} - \frac{2}{\sqrt{3}(n-1)}\left(\frac{1}{\sqrt{n-1}} + \frac{2}{\sqrt{n-2}}\right) + \frac{2}{(n-1)\sqrt{(n-1)(n-2)}} \\ &\geq \frac{1}{n-2} - \frac{2}{\sqrt{3}(n-1)} \cdot \frac{3}{\sqrt{n-2}} = \frac{1}{\sqrt{n-2}}\left(\frac{1}{\sqrt{n-2}} - \frac{2\sqrt{3}}{n-1}\right). \end{aligned}$$

For $n \geq 12$, $\frac{1}{\sqrt{n-2}} - \frac{2\sqrt{3}}{n-1} > 0$, i.e., $a_{n-2,n-2} > 0$. For smaller n, we can verify it easily.

Let $s_1(n) = \sqrt{3}(n-1)\sqrt{n-2}\ s(3,1,n)$, i.e.,

$$s_1(n) = -2(n-3)\sqrt{(n-1)(n-2)} + 2\sqrt{3}\sqrt{n-1} + 2(n-3)(n-1) - 3\sqrt{3}\sqrt{n-2}.$$

By some calculations, we have

$$\begin{aligned} s_1(n) &> 2(n-3)\left(n-1-\sqrt{(n-1)(n-2)}\right) - \sqrt{3}\sqrt{n-2} \\ &> \sqrt{3(n-2)}\left[\sqrt{n-2}\left(n-1-\sqrt{(n-1)(n-2)}\right) - 1\right] > 0, \end{aligned}$$

since $2(n-3) > \sqrt{3}(n-2)$ and $\sqrt{n-2}\left(n-1-\sqrt{(n-1)(n-2)}\right)-1>0$ for $n \geq 10$. Thus, $s(3,1,n) > 0$ for $n \geq 10$. We can directly verify that $s(3,1,n) \geq 0$ for $6 \leq n \leq 9$.

Case 3: $p = 2$

Suppose $n \geq 8$. We have

$$\begin{aligned} g(3,2,n) &= \frac{(n-3)\sqrt{(n-1)(n-2)} - 2\sqrt{3}(n-4)\sqrt{n-1} + 4\sqrt{3}\sqrt{n-2} - 12}{3\sqrt{(n-1)(n-2)}} \\ &\geq \frac{(n-3)(n-2) - 2\sqrt{3}(n-4)\sqrt{n-1} + 4\sqrt{3}\sqrt{n-2} - 12}{3\sqrt{(n-1)(n-2)}} \\ &= \frac{g_2(n)}{3\sqrt{(n-1)(n-2)}}, \end{aligned}$$

where $g_2(n) = (n-3)(n-2) - 2\sqrt{3}(n-4)\sqrt{n-1} + 4\sqrt{3}\sqrt{n-2} - 12$. Since

$$\begin{aligned} g_2'(n) &= n-2+n-3-2\sqrt{3}\sqrt{n-1} - \frac{\sqrt{3}(n-4)}{\sqrt{n-1}} + \frac{2\sqrt{3}}{\sqrt{n-2}} \\ &> 2n-5-2\sqrt{3}\sqrt{n-1} - \sqrt{3}\sqrt{n-1} = 2n-5-3\sqrt{3}\sqrt{n-1}, \end{aligned}$$

and for $n \geq 11$, $g_2'(n) \geq g_2'(11) > 0$, we have $g_2(n) \geq g_2(11) = 60 + 12\sqrt{3} - 14\sqrt{30} > 0$. By some calculations for smaller n, we have $g(3,2,n) > 0$ for $n \geq 8$.

$$\begin{aligned} a_{n-2,n-2} &= \frac{1}{n-2} - \frac{2}{\sqrt{3}(n-3)}\left(\frac{2}{\sqrt{n-1}} + \frac{1}{\sqrt{n-2}}\right) + \frac{4}{(n-3)\sqrt{(n-1)(n-2)}} \\ &\geq \frac{1}{n-2} - \frac{2}{\sqrt{3}(n-3)}\,\frac{3}{\sqrt{n-2}} = \frac{1}{\sqrt{n-2}}\left(\frac{1}{\sqrt{n-2}} - \frac{2\sqrt{3}}{n-3}\right). \end{aligned}$$

For $n \geq 16$, $\frac{1}{\sqrt{n-2}} - \frac{2\sqrt{3}}{n-3} > 0$, i.e., $a_{n-2,n-2} > 0$. For smaller n, we can verify it easily.

Let $s_2(n) = \sqrt{3}(n-1)(n-3)\sqrt{n-2}\ s(3,2,n)$, where

$$\begin{aligned} s_2(n) = &(n-2)(n-1)(n-4) + 2\sqrt{3}(n-2)\sqrt{n-1} - 2\sqrt{3}(n-3)\sqrt{n-2} \\ &- (n^2-6n+11)\sqrt{(n-1)(n-2)}. \end{aligned}$$

Since $2\sqrt{3}(n-2)\sqrt{n-1} - 2\sqrt{3}(n-3)\sqrt{n-2} > 0$ for $n \geq 8$, we have

$$s_2(n) \geq (n-2)(n-1)(n-4) - (n^2-6n+11)\sqrt{(n-1)(n-2)}.$$

Then we only need to prove

$$((n-2)(n-1)(n-4))^2 > \left((n^2-6n+11)\sqrt{(n-1)(n-2)}\right)^2,$$

i.e., $(n-1)(n-2)\big((n-3)(n^2-13n+29)-2\big) > 0$. By some calculations, we have $(n-3)(n^2-13n+29)-2>0$ when $n \geq 11$. Thus, $s(3,2,n) > 0$ for $n \geq 8$, since we can verify easily for $8 \leq n \leq 10$.

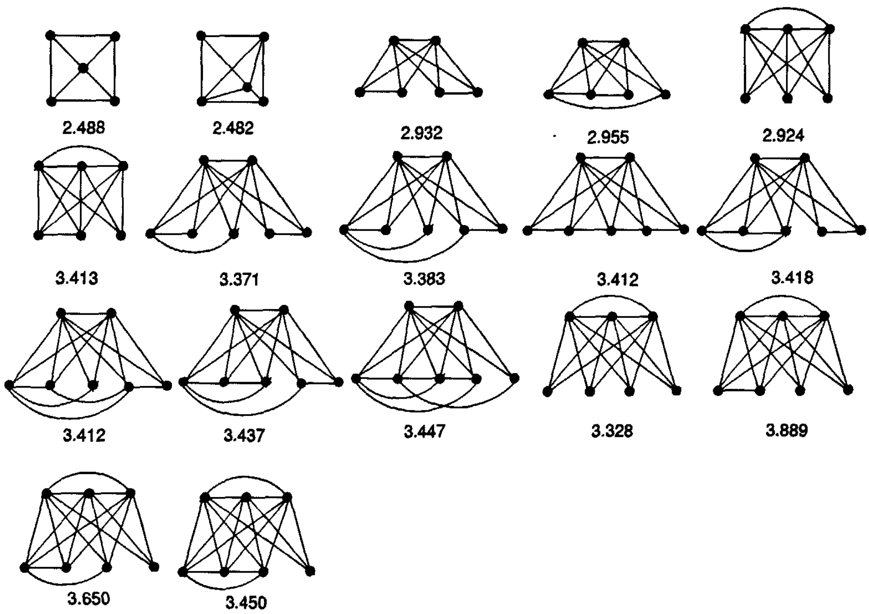

Figure 3.1: The graphs of order $5 \leq n \leq 7$ with the minimum degree $k=3$ and $2 \leq p \leq 3$.

For $6 \leq n \leq 7$, all the graphs with minimum degree 3 and $2 \leq p \leq 3$ and the values of their Randić Indices are shown in Figure 3.1. By easy comparisons, we can check the result of the theorem. The proof is now complete. ∎

Theorem 3.3.3 *The inequality of the conjecture holds for all chemical graphs, i.e., graphs with the maximum degree at most* 4.

Proof. From the the result of Delorme, Favaron and Rautenbach for minimum degree $k = 2$ and the above Theorem 3.3.2 for minimum degree $k = 3$, we know that we only need to check the inequality of the conjecture for 4-regular graphs. It is easy to see that a 4-regular graph of order n has $2n$ edges, and each edge has a weight equal to $\frac{1}{4}$. So, any 4-regular graph G has a Randić index equal to $\frac{n}{2}$. It is then not difficult to check that

$$R(G) = \frac{n}{2} \geq \frac{4(n-4)}{\sqrt{4(n-1)}} + \binom{4}{2}\frac{1}{n-1} = \frac{2(n-4)}{\sqrt{(n-1)}} + \frac{6}{n-1}.$$

The proof is complete. ∎

Remark. The result in this chapter was obtained in July, 2006, which was published in 2008 [65]. Now this conjecture was completely solved by Li, Liu and Liu [63].

Chapter 4

On the Randić Index and the Chromatic Number, the Radius

In this chapter, we will study the relations of the Randić index and the chromatic number, the radius.

4.1 Randić index and the chromatic number

Recall that for a given graph G, a vertex coloring of G is called *proper* if any two adjacent vertices are assigned different colors. The *chromatic number* $\chi(G)$ of G is the minimum number of colors that are needed to color G properly.

Caporossi and Hansen [21] proposed the following conjecture on the relation of the chromatic number and the Randić index, which is also referred in [62]. This section is to give a positive proof to the conjecture.

Conjecture 4.1.1 (Caporossi and Hansen, [21]) *For any connected graph G of order $n \geq 2$ with chromatic number $\chi(G)$ and Randić index $R(G)$,*

$$R(G) \geq \frac{\chi(G)-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{\chi(G)-1} + n - \chi(G)\right).$$

Moreover, the bound is sharp for all n and $2 \leq \chi(G) \leq n$.

At first, we recall some lemmas which will be used in the sequel.

Lemma 4.1.1 (Hansen and Vukicević, [53]) *Let G be a simple graph with Randić index $R(G)$, minimum degree δ and maximum degree Δ. Let v be a vertex of G with degree equal to δ. Then*

$$R(G) - R(G-v) \geq \frac{1}{2}\sqrt{\frac{\delta}{\Delta}}.$$

Lemma 4.1.2 (Li, Liu and Liu, [63]) *Let G be a graph of order n with minimum degree $\delta(G) = k$. Then*

$$R(G) \geq \begin{cases} \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} & \text{if } k \leq \frac{n}{2} \\ \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}} & \text{if } k > \frac{n}{2} \end{cases}$$

where p satisfies that

$$p = \begin{cases} \frac{n}{2} & \text{if } n \equiv 0 (mod\ 4) \\ \lfloor \frac{n}{2} \rfloor \text{ or } \lceil \frac{n}{2} \rceil & \text{if } n \equiv 1 (mod\ 4) \text{ and } k \text{ is even} \\ \lfloor \frac{n}{2} \rfloor & \text{if } n \equiv 1 (mod\ 4) \text{ and } k \text{ is odd} \\ \frac{n-2}{2} \text{ or } \frac{n+2}{2} & \text{if } n \equiv 2 (mod\ 4) \text{ and } k \text{ is even} \\ \frac{n}{2} & \text{if } n \equiv 2 (mod\ 4) \text{ and } k \text{ is odd} \\ \lfloor \frac{n}{2} \rfloor \text{ or } \lceil \frac{n}{2} \rceil & \text{if } n \equiv 3 (mod\ 4) \text{ and } k \text{ is even} \\ \lceil \frac{n}{2} \rceil & \text{if } n \equiv 3 (mod\ 4) \text{ and } k \text{ is odd.} \end{cases}$$

It is easy to see from Lemma 4.1.2 that p is among the numbers $\frac{n-2}{2}, \frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}$ and $\frac{n+2}{2}$.

Lemma 4.1.3 *Let $g(n,k) = -\frac{n^2-4}{8k} + \frac{n^2-4}{4\sqrt{k(n-1)}} - \frac{k-1}{2} - \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}$. Then, for $n \geq 5$, $g(n,k)$ is a decreasing function in k with $\frac{n}{2} < k \leq n-1$.*

Proof. Note that

$$\begin{aligned} \frac{\partial g(n,k)}{\partial k} &= \frac{n^2-4}{8k^2} - \frac{n^2-4}{8k\sqrt{k(n-1)}} + \frac{1}{\sqrt{n-1}} - \frac{1}{2\sqrt{k(n-1)}} - \frac{1}{2} \\ &= \frac{8k^2 + (n^2-4)\sqrt{n-1} - 4k^2\sqrt{n-1}}{8k^2\sqrt{n-1}} - \frac{n^2+4k-4}{8k\sqrt{k(n-1)}} \\ &= \frac{1}{8k^2\sqrt{n-1}}\left(8k^2 + (n^2-4k^2-4)\sqrt{n-1} - (n^2+4k-4)\sqrt{k}\right). \end{aligned}$$

Let

$$h(n,k) = 8k^2 + (n^2 - 4k^2 - 4)\sqrt{n-1} - (n^2 + 4k - 4)\sqrt{k}.$$

We have $\frac{\partial h(n,k)}{\partial k} = 16k - 8k\sqrt{n-1} - 6\sqrt{k} - \frac{n^2-4}{2\sqrt{k}}$ and $\frac{\partial^2 h(n,k)}{\partial k^2} = 16 - 8\sqrt{n-1} - \frac{3}{\sqrt{k}} + \frac{n^2-4}{4k\sqrt{k}}$. For $n \geq 6$,

$$\frac{\partial^2 h(n,k)}{\partial k^2} < 16 - 8\sqrt{n-1} - \frac{3}{\sqrt{n-1}} + \frac{n^2-4}{n\sqrt{2n}} < 0.$$

It is easy to verify that $\frac{\partial^2 h(n,k)}{\partial k^2} \leq 0$ for $n = 5$ and $3 \leq k \leq 4$. Thus, for $n \geq 5$, we have

$$\frac{\partial h(n,k)}{\partial k} < 8n - 4n\sqrt{n-1} - 3\sqrt{2n} - \frac{n^2-4}{\sqrt{2n}} < 0.$$

We then have

$$h(n,k) < h(n, \frac{n}{2}) = 2n^2 - 4\sqrt{n-1} - \frac{(n^2+2n-4)\sqrt{2n}}{2} < 0.$$

Therefore, $\frac{\partial g(n,k)}{\partial k} < 0$ for $n \geq 5$. ∎

Theorem 4.1.2 *For any connected graph G of order $n \geq 2$ with chromatic number $\chi(G)$ and Randić index $R(G)$, we have $R(G) \geq f(\chi(G))$, where the function $f(x) = \frac{x-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{x-1} + n - x\right)$. Moreover, the bound is sharp for all n and $2 \leq \chi(G) \leq n$.*

Proof. Since we only consider connected graphs of order $n \geq 2$, we may assume $\chi(G) \geq 2$ in the following.

By contradiction. We choose G as a minimum counterexample to the assumption $R(G) \geq f(\chi(G))$ with respect to the orders of graphs, i.e.,
(1) $R(G) < f(\chi(G))$;
(2) for any graph H with an order less than that of G, $R(H) \geq f(\chi(H))$.
Denote by $\delta(G) = k$ the minimum degree of G. At first, we prove the following claim:

Claim. $\delta(G) = k \geq \chi(G) - 1$.

Suppose to the contrary that $k < \chi(G) - 1$. Let v be a vertex with minimum degree k. Note that $\chi(G - v) < \chi(G)$, since otherwise $\chi(G - v) = \chi(G)$, by

Lemma 4.1.1,

$$R(G-v) < R(G) < f(\chi(G)) = f(\chi(G-v)),$$

which contradicts to the choice of G. Hence $G-v$ has a proper coloring with $\chi(G)-1$ colors. Since $d(v)=k<\chi(G)-1$, then there exists a vertex u such that the color of u is not appeared in the neighbors of v. Thus v can be colored with that color, which implies that G has a proper coloring with $\chi(G)-1$ colors, a contradiction. The claim is thus proved.

Note that $f(x)$ is an increasing function in $x \geq 2$. Since $f'(x) = \frac{1}{2} + \frac{1}{2\sqrt{(n-1)(x-1)}} - \frac{1}{\sqrt{n-1}}$, $f'(x) > 0$ for all $x \geq 2$ when $n \geq 3$. Then for $n \geq 3$, $f(\chi(G)) \leq f(k+1)$. When $n=2$, $G \cong K_2$, it is easy to verify that $f(\chi(G)) = f(k+1)$ since $\chi(K_2)=2$ and $\delta(K_2)=1$. Thus for $n \geq 2$, we have

$$R(G) < f(\chi(G)) \leq f(k+1) = \frac{k-1}{2} + \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}. \tag{4.1.1}$$

Case 1. $k \leq \frac{n}{2}$.

By Lemma 4.1.2 and the inequality (4.1.1), we have

$$\frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} < \frac{k-1}{2} + \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}.$$

However, since $k \leq \frac{n}{2}$, we have $\frac{\sqrt{k}+1}{2\sqrt{n-1}} \leq \frac{\sqrt{n/2}+1}{2\sqrt{n-1}} \leq 1$. Then,

$$\begin{aligned}
&\frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} - \frac{k-1}{2} - \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}} \\
&= \frac{(n-k-1)(k-\sqrt{k})}{\sqrt{k(n-1)}} - \frac{(k-1)(n-k-1)}{2(n-1)} \\
&= \frac{(n-k-1)(\sqrt{k}-1)}{\sqrt{n-1}}\left(1 - \frac{\sqrt{k}+1}{2\sqrt{n-1}}\right) \geq 0,
\end{aligned}$$

a contradiction.

Case 2. $\frac{n}{2} < k \leq n-1$.

Let

$$q(n,p) = \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}}.$$

By Lemma 4.1.2 and the inequality (4.1.1), we have

$$q(n,p) < \frac{k-1}{2} + \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}. \tag{4.1.2}$$

In the following, we will show that

$$q(n,\frac{n-2}{2}) \geq \frac{k-1}{2} + \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}.$$

By some elementary calculations, we obtain that $q(n,\frac{n-2}{2}) - \frac{k-1}{2} + \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}} \geq 0$ for $2 \leq n \leq 4$ and $\frac{n}{2} < k \leq n-1$, a contradiction. In the following, we assume that $n \geq 5$. Then by Lemma 4.1.3,

$$\begin{aligned}
& q(n,\frac{n-2}{2}) - \frac{k-1}{2} - \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}} \\
= & \frac{n(n+2)}{8(n-1)} + \frac{(n-2)(2k-(n+2))}{8k} + \frac{n^2-4}{4\sqrt{k(n-1)}} \\
& - \frac{k-1}{2} - \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}} \\
= & \frac{n(n+2)}{8(n-1)} + \frac{n-2}{4} + g(n,k) \\
\geq & \frac{n(n+2)}{8(n-1)} + \frac{n-2}{4} + g(n,n-1) \\
= & \frac{n(n+2)}{8(n-1)} + \frac{n-2}{4} - \frac{n^2-4}{8(n-1)} + \frac{n^2-4}{4(n-1)} - \frac{n-2}{2} - 1 = 0.
\end{aligned}$$

In a similar way, we can verify that for each of the cases for $p = \frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}$ or $\frac{n+2}{2}$, $q(n,p) \geq \frac{k-1}{2} + \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}$. The details are omitted. Therefore, we get a contradiction to Inequality (4.1.2), and thus get the require inequality $R(G) \geq f(\chi(G))$.

Note that the bound is sharp for all n and $2 \leq \chi(G) \leq n$. For example, denote by K_n the complete graph on n vertices, then $\chi(K_n) = n$ and $R(K_n) = f(\chi(K_n)) = \frac{n}{2}$. ∎

4.2 Randić index and the radius

The *diameter* $D(G)$ of G is the maximum distance between any pair of vertices of G, i.e., $D(G) = max_{u,v \in V(G)} d(u,v)$. The *eccentricity* of a vertex u, written $\epsilon(u)$, is $\max_{v \in V} d(u, v)$. Note that the diameter equals the maximum of the vertex eccentricities. The *radius* of a graph G is $r(G) = min_{u \in V} \epsilon(u)$.

In [38], Fajtlowicz proposed the following conjecture on the relation of the Randić index and the radius, which is also referred in [62].

Conjecture 4.2.1 (Fajtlowicz, [38]) *For any connected graph G,*

$$R(G) \geq r(G) - 1,$$

where $r(G)$ denotes the radius of G.

Caporossi and Hansen [21] proved that for all trees T, $R(T) \geq r(T) + \sqrt{2} - \frac{3}{2}$, and for trees T except even paths, $R(T) \geq r(T)$. In [76], the conjecture is verified for unicyclic graphs, bicyclic graphs and connected graphs of order $n \leq 9$ with $\delta(G) \geq 2$. Recently, You and Liu [98] proved that the conjecture is true for biregular graphs, tricyclic graphs and connected graphs of order $n \leq 10$.

In this section, we will prove that for any connected graph G of order n with minimum degree $\delta(G)$, the conjecture holds for $\delta(G) \geq \frac{n}{5}$ and $n \geq 25$, furthermore, for any arbitrary real number $0 < \varepsilon < 1$, if $\delta(G) \geq \varepsilon n$, the conjecture holds for sufficiently large n.

Lemma 4.2.1 (Erdös *et al.*, [35]) *Let G be a connected graph with n vertices and with minimum degree $\delta(G) \geq 2$. Then*

$$r(G) \leq \frac{3n - 9}{2\delta(G) + 2} + 5.$$

Theorem 4.2.2 *For any connected graph G of order n with minimum degree $\delta(G)$, $R(G) \geq r(G) - 1$ holds for $\delta(G) \geq \frac{n}{5}$ and $n \geq 25$. Furthermore, for any arbitrary real number ε $(0 < \varepsilon < 1)$, if $\delta(G) \geq \varepsilon n$, $R(G) \geq r(G) - 1$ holds for sufficiently large n.*

Proof. Let G be a connected graph of order n with minimum degree $\delta(G) = k$. By Lemma 4.2.1, we have $r(G) \leq \frac{3n-9}{2k+2} + 5$. We consider the following two cases:

Case 1. $k \leq \frac{n}{2}$.

By Lemma 4.1.2, we only need to consider the following inequality,

$$\frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} \geq \frac{3n-9}{2k+2} + 5 - 1.$$

In fact, let

$$f(n,k) = \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} - \frac{3n-9}{2k+2} - 4.$$

Then,

$$\frac{\partial f(n,k)}{\partial k} = \frac{2k-1}{2(n-1)} + \frac{n-3k}{2\sqrt{k(n-1)}} + \frac{6(n-3)}{(2k+2)^2}.$$

If $n \geq 3k$, we can directly obtain that $\frac{\partial f(n,k)}{\partial k} > 0$. Now we assume that $2k \leq n < 3k$, and then

$$\frac{\partial f(n,k)}{\partial k} = \frac{1}{2\sqrt{n-1}} \left(\frac{2k-1}{\sqrt{n-1}} - \frac{3k-n}{\sqrt{k}} \right) + \frac{6(n-3)}{(2k+2)^2}.$$

Denote by

$$h(n,k) = \frac{2k-1}{\sqrt{n-1}} - \frac{3k-n}{\sqrt{k}} = \frac{2k-1}{\sqrt{n-1}} - 3\sqrt{k} + \frac{n}{\sqrt{k}}.$$

Since

$$\frac{\partial h(n,k)}{\partial k} = \frac{2}{\sqrt{n-1}} - \frac{3}{2\sqrt{k}} - \frac{n}{2k\sqrt{k}} < \frac{2}{\sqrt{n-1}} - \frac{3}{2\sqrt{k}} - \frac{2k}{2k\sqrt{k}} < 0,$$

then for $n \geq 2$,

$$h(n,k) > h(n, \frac{n}{2}) = \sqrt{n-1} - \sqrt{\frac{n}{2}} \geq 0,$$

and thus $\frac{\partial f(n,k)}{\partial k} > 0$.

If $k \geq \frac{n}{5}$ and $n \geq 25$, we have

$$f(n,k) \geq f(n, \frac{n}{5}) = \frac{n(n-5)}{50(n-1)} + \frac{4n^2}{5\sqrt{5n(n-1)}} - \frac{15(n-3)}{2n+10} - 4 > 0.$$

Actually, for any arbitrary real number ε $(0 < \varepsilon < 1)$, if $k \geq \varepsilon n$,

$$f(n,k) > f(n, \varepsilon n) > \frac{\varepsilon(1-\varepsilon)n^2}{\sqrt{\varepsilon n(n-1)}} - \frac{3n-9}{2\varepsilon n+2} - 4 > 0$$

for sufficiently large n.

Case 2. $\frac{n}{2} < k \leq n-1$.

Let

$$q(n,p) = \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}}.$$

In the following, we will show that for every $p \in \{\frac{n-2}{2}, \frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}, \frac{n+2}{2}\}$ and $n \geq 13$,

$$q(n,p) \geq \frac{3n-9}{2k+2} + 5 - 1.$$

In fact, if $p = \frac{n-2}{2}$, denote by

$$\begin{aligned} h(n,k) &= q(n, \frac{n-2}{2}) - \frac{3n-9}{2k+2} - 4 \\ &= \frac{n(n+2)}{8(n-1)} + \frac{(n-2)(2k-(n+2))}{8k} + \frac{n^2-4}{4\sqrt{k(n-1)}} - \frac{3n-9}{2k+2} - 4. \end{aligned}$$

Notice that

$$\frac{\partial h(n,k)}{\partial k} = \frac{n^2-4}{8k^2} - \frac{n^2-4}{8k\sqrt{k(n-1)}} + \frac{6(n-3)}{(2k+2)^2} > 0,$$

since $8k^2 \leq 8k\sqrt{k(n-1)}$, i.e., $\sqrt{k} \leq \sqrt{n-1}$. Thus, for $n \geq 13$, we have

$$h(n,k) > h(n, \frac{n}{2}) = \frac{n(n+2)}{8(n-1)} - \frac{n-2}{2n} + \frac{n^2-4}{2\sqrt{2n(n-1)}} - \frac{3n-9}{n+2} - 4 > 0.$$

In a similar way, we can verify that for each of the cases for $p = \frac{n-1}{2}$, $\frac{n}{2}$, $\frac{n+1}{2}$ or $\frac{n+2}{2}$, $q(n,p) \geq \frac{3n-9}{2k+2} + 5 - 1$. The details are omitted. The proof is now complete. ∎

Chapter 5

The Sharp Bounds of the Zeroth-order General Randić Index of Chemical Graphs

In this chapter, we will consider the zeroth-order general Randić index ${}^0R_\alpha(G)$ of chemical graph G, and give the sharp upper and lower bounds of ${}^0R_\alpha(G)$ by using the order and the size of G.

5.1 Introduction

The *zeroth-order Randić index*, conceived by Kier and Hall [57, 59], is defined as ${}^0R(G) = {}^0R_{-1/2}(G) = \sum_{u\in G} d(u)^{-\frac{1}{2}}$, where the summation goes over all vertices of G. In analogy to the Randić index, Li and Zheng [74] defines the *zeroth-order general Randić index* ${}^0R_\alpha(G)$ of a graph G,

$$ {}^0R_\alpha(G) = \sum_{v\in G} d(u)^\alpha $$

where α is an arbitrary real number.

Pavlović [83] determined the sharp upper bound of the zeroth-order Randić index ${}^0R_\alpha$ of (n,m)-graphs. In [72] Li and Zhao gave the sharp upper and lower bounds of ${}^0R_\alpha$ of trees, with the exponent α equal to m, $-m$, $\frac{1}{m}$ and $-\frac{1}{m}$, where $m \geq 2$ is an integer. Later, Li and Zheng [74] gave an alternative proof for general real number α. Zhang and Zhang [101] determined the sharp upper and lower bounds of ${}^0R_\alpha$ of unicyclic graphs, while Zhang, Wang and Cheng [100] determined the sharp upper and lower bounds of bicyclic graphs. In [55, 66], the authors considered the extremal values of ${}^0R_\alpha$ for the connected (n,m)-graphs. And they gave the sharp lower bound of ${}^0R_\alpha$ for $\alpha < 0$ or $\alpha > 1$, and the sharp upper bound of ${}^0R_\alpha$ for $\alpha < 1$. There are also some gaps.

For chemical trees, Li and Zhao [72] determined the sharp and lower bounds of ${}^0R_\alpha$ for any α. In this chapter, we will investigate the zeroth-order general Randić index for chemical (n,m)-graphs, i.e., connected simple graphs with n vertices, m edges and maximum degree at most 4. We will give the sharp upper and lower bounds of ${}^0R_\alpha$ for any α.

5.2 Main results

Firstly, we need to introduce some notations.

Denote by $\pi(G) = [d_1, d_2, \ldots, d_n]$ the degree sequence of the graph G, where d_i stands the degree of the i-th vertex of G and $d_1 \geq d_2 \geq \cdots \geq d_n$.

If there is a graph, such that $d_i \geq d_j + 2$, let G' be a graph obtained from G by replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$. In other words, if $\pi(G) = [d_1, d_2, \ldots, d_n]$, then $D(G') = [d_1, d_2, \ldots, d_{i-1}, d_i - 1, d_{i+1}, \ldots, d_{j-1}, d_j + 1, d_{j+1}, \ldots, d_n]$.

Note that if $\alpha = 0$ then ${}^0R_\alpha(G) = n$, and if $\alpha = 1$ then ${}^0R_\alpha(G) = 2m$. Therefore, in the following we always assume that $\alpha \neq 0, 1$.

Lemma 5.2.1 *For the two graphs G and G', specified above, we have*

(i). ${}^0R_\alpha(G) > {}^0R_\alpha(G')$ *for* $\alpha < 0$ *or* $\alpha > 1$;

(ii). ${}^0R_\alpha(G) < {}^0R_\alpha(G')$ *for* $0 < \alpha < 1$.

Proof. Since ${}^0R_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha$, we have

$$\begin{aligned}
{}^0R_\alpha(G) - {}^0R_\alpha(G') &= d_i^\alpha + d_j^\alpha - (d_i - 1)^\alpha - (d_j + 1)^\alpha \\
&= [d_i^\alpha - (d_i - 1)^\alpha] - [(d_j + 1)^\alpha - d_j^\alpha] \\
&= \alpha(\xi_1^{\alpha-1} - \xi_2^{\alpha-1}),
\end{aligned}$$

where $\xi_1 \in (d_i - 1, d_i)$, and $\xi_2 \in (d_j, d_j + 1)$. So, by $d_i \geq d_j + 2$, we have $\xi_1 > \xi_2$. Then ${}^0R_\alpha(G) > {}^0R_\alpha(G')$ for $\alpha < 0$ or $\alpha > 1$, whereas ${}^0R_\alpha(G) < {}^0R_\alpha(G')$ for $0 < \alpha < 1$. ∎

Denote by n_i the number of vertices of degree i in a chemical (n, m)-graph G. Then we have

$$ {}^0R_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha = n_1 + 2^\alpha n_2 + 3^\alpha n_3 + 4^\alpha n_4. \tag{5.2.1} $$

Theorem 5.2.1 *Let C^* be a chemical (n, m)-graph with degree sequence $\pi(C^*) = [d_1, d_2, \ldots, d_n]$, such that $|d_i - d_j| \leq 1$ for any $i \neq j$. Then for $\alpha < 0$ or $\alpha > 1$, C^* has the minimum zeroth-order general Randić index among all chemical (n, m)-graphs, whereas for $0 < \alpha < 1$, C^* has the maximum zeroth-order general Randić index among all chemical (n, m)-graphs. Moreover,*

$$ {}^0R_\alpha(C^*) = \begin{cases} 2 + 2^\alpha(n-2) & m = n - 1; \\ 2^\alpha(3n - 2m) + 3^\alpha(2m - 2n) & n \leq m \leq \lfloor \frac{3n}{2} \rfloor; \\ 3^\alpha(4n - 2m) + 4^\alpha(2m - 3n) & \lfloor \frac{3n}{2} \rfloor < m \leq 2n. \end{cases} $$

Proof. We only consider the case $0 < \alpha < 1$, because the proof for the other case is fully analogous. Let G be a chemical graph and $\pi(G) = [d_1, d_2, \ldots, d_n]$. If $G \ncong C^*$, then there must exist a pair (d_i, d_j) such that $d_i \geq d_j + 2$. By Lemma 5.2.1, the graph G', obtained by replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$, has a greater ${}^0R$-value than G. Consequently, G is not a chemical (n, m)-graph with the maximum zeroth-order general Randić index.

To show the existence, we construct the extremal (n, m)-graph C^* (with the minimum ${}^0R$ for $\alpha < 0$ or $\alpha > 1$, and with maximum ${}^0R$ for $0 < \alpha < 1$) by adding edges one by one. First, we start from a tree. There must be at least two 1-degree vertices in a tree. By Lemma 5.2.1, there does not exist any 3-degree vertex, so the extremal tree must be a path P_n. Next we add an edge joining the two leaves of the path. In this way the degrees of all vertices become equal to two, and then we get a cycle. We continue by adding edges one by one, so as to maximize the number of 3-degree vertices, until either there remain no 2-degree vertices, or remains exactly one. If more edges need to be added, then we first connect the 2-degree vertex (if such does exist) with a nonadjacent 3-degree vertex, and continue by connecting pairs of nonadjacent 3-degree vertices. The construction is shown in Figure 5.1. ∎

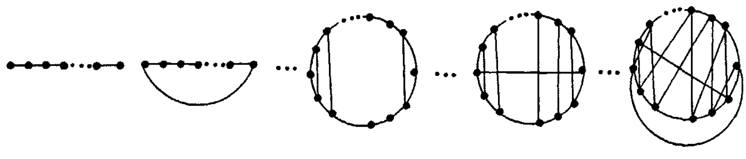

Figure 5.1: Constructing chemical graphs with extremal zeroth-order general Randić index, according to Theorem 5.2.1.

Theorem 5.2.2 *Let G^* be a chemical (n,m)-graph with at most one vertex of degree 2 or 3. If one of the following conditions holds:*

(I) $m = n-1$;

(II) $m \geq n \geq 6$, for $n = 6$, $m \geq 10$, and for $n = 7$, $m \neq 8$,

then for $\alpha < 0$ or $\alpha > 1$, G^* has the maximum zeroth-order general Randić index among all chemical (n,m)-graphs, whereas for $0 < \alpha < 1$, the same graph has the minimum zeroth-order general Randić index among all chemical (n,m)-graphs. Moreover,

$$^0R_\alpha(G^*) = \begin{cases} \frac{4n-2m}{3} + 4^\alpha(\frac{2m-n}{3}) & 2m-n \equiv 0 \ (mod\ 3); \\ \frac{4n-2m-2}{3} + 2^\alpha + 4^\alpha(\frac{2m-n-1}{3}) & 2m-n \equiv 1 \ (mod\ 3); \\ \frac{4n-2m-1}{3} + 3^\alpha + 4^\alpha(\frac{2m-n-2}{3}) & 2m-n \equiv 2 \ (mod\ 3). \end{cases}$$

Proof. Again, we only consider the case $0 < \alpha < 1$, because the proof for the other case is similar. Let G' be a chemical (n,m)-graph and $\pi(G) = [d_1, d_2, \ldots, d_n]$. Let G' possess two vertices of degree 2 or 3, i.e., let there be a pair (d_i, d_j) such that $3 \geq d_i \geq d_j \geq 2$. By Lemma 5.2.1, there is a graph G, obtained by replacing the pair (d_i, d_j) by the pair (d_i+1, d_j-1), that has a smaller ^0R-value than G'. Repeating the above operation until there is no pair (d_i, d_j), such that $3 \geq d_i \geq d_j \geq 2$, we arrive at G^* with the minimum zeroth-order general Randić index. In view of (5.2.1), for G^* we have

$$\begin{cases} n_1 + n_2 + n_3 + n_4 & = & n \\ n_1 + 2n_2 + 3n_3 + 4n_4 & = & 2m \\ n_2 + n_3 & \leq & 1 \end{cases}$$

From the above equations, we have one of the following three options:
(1) $n_2 = n_3 = 0$, implying $n_1 = (4n - 2m)/3$, $n_4 = (2m - n)/3$, if $2m - n \equiv 0 \ (mod\ 3)$;
(2) $n_2 = 1$, $n_3 = 0$, implying $n_1 = (4n - 2m - 2)/3$, $n_4 = (2m - n - 1)/3$, if $2m - n \equiv 1 \ (mod\ 3)$;
(3) $n_2 = 0$, $n_3 = 1$, implying $n_1 = (4n - 2m - 1)/3$, $n_4 = (2m - n - 2)/3$, if $2m - n \equiv 2 \ (mod\ 3)$.

In order to show the existence, we construct G^* by distinguishing the following cases:
(I) if $n = m - 1$.

(I.1) If $2m - n \equiv 0 \ (mod\ 3)$, we first construct a path with n_4 vertices, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

(I.2) If $2m - n \equiv 1 \ (mod\ 3)$, we first construct a path with n_4 vertices, then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4, and finally subdivide an edge by inserting to it a vertex of degree 2.

(I.3) If $2m - n \equiv 2 \ (mod\ 3)$, we first construct a path with $n_4 + 1$ vertices, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

(II) $m \geq n \geq 6$, for $n = 6$, $m \geq 10$, or for $n = 7$, $m \neq 8$.

In Figure 5.2 we show one of the possible graphs G^* for $n_4 \leq 4$, that is $\lfloor (2m - n)/3 \rfloor \leq 4$. For $n_4 \geq 5$, we construct G^* as follows:

(II.1) If $2m - n \equiv 0 \ (mod\ 3)$, we first construct a 4-regular graph on n_4 vertices, then delete $n_1/2$ edges from it, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

(II.2) If $2m - n \equiv 1 \ (mod\ 3)$, we first construct a 4-regular graph on n_4

vertices, then delete $n_1/2$ edges from it, then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4, and finally subdivide an edge inserting to it a vertex of degree 2.

(II.3) If $2m - n \equiv 2 \ (mod\ 3)$, we first construct a 4-regular graph on $n_4 + 1$ vertices, then delete $(n_1 + 1)/2$ edges from it, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

This completes the proof. ∎

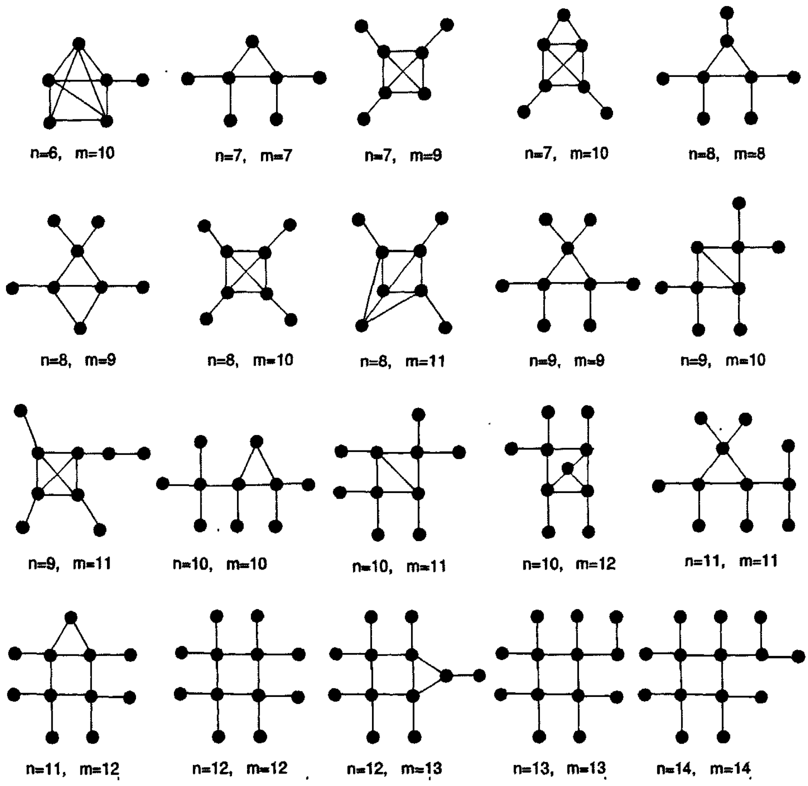

Figure 5.2: Chemical graphs with extremal zeroth-order general Randić index, having four or fewer vertices of degree 4.

Note that Theorem 5.2.2 holds under that conditions $m = n - 1$, or $n = 6$ and $m \geq 10$, or $n = 7$ and $m \neq 8$, or $m \geq n \geq 8$, since for the other pairs of n

and m the extremal degree sequences obtained in Theorem 5.2.2 are not graphic. It is easy to check that for $n = 1, 2, 3$, and for $n \geq 4$ and $m = \binom{n}{2} - 1$ or $m = \binom{n}{2}$ the (n, m)-graph is unique. For $n = 4$ and $m = 4$ or $n = 5$ and $5 \leq m \leq 8$, or $n = 6$ and $6 \leq m \leq 9$, or $n = 7$ and $m = 8$, we can characterize the extremal graphs by examining all possible degree sequences. These extremal graphs are depicted in Figure 5.3 (minimum ones for $0 < \alpha < 1$, maximum ones for $\alpha < 0$ or $\alpha > 1$, except for $n = 5$ $m = 7$, in which (a) is the minimum graph for $0 < \alpha < 1$ and maximum graph for $\alpha < 0$ or $1 < \alpha < 2$, and (b) is the maximum graph for $\alpha \geq 2$).

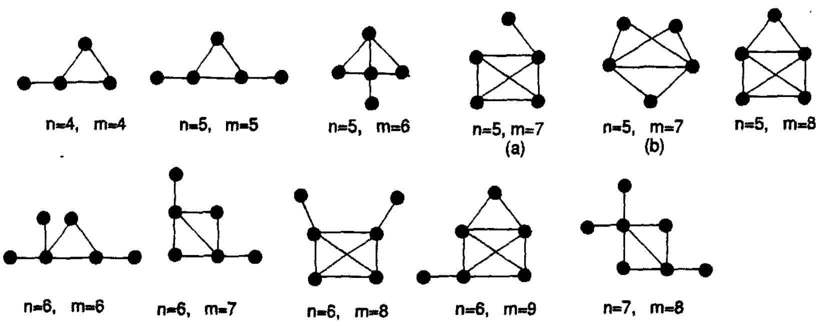

Figure 5.3: Some graphs with extremal zeroth-order general Randić index, for details see text.

Chapter 6

The Diameter and the Inverse Degree

In this chapter, we will investigate the relation between the inverse degree and the diameter.

6.1 Introduction

Given a connected, simple and undirected graph $G = (V, E)$ of order n, let the *inverse degree* $I(G)$ of G be defined by

$$I(G) = {}^0R_{-1}(G) = \sum_{v \in V} \frac{1}{d(v)},$$

where $d(v)$ is the degree of v in G.

The distance between two vertices u and v in G, denoted by $d_G(u, v)$ (or $d(u, v)$ for short), is the length of a shortest path joining u and v in G. The diameter $D(G)$ of G is the maximum distance $d(u, v)$ over all pairs of vertices u and v of G. The *average distance* $\mu(G)$, an interesting graph-theoretical invariant, is defined as the average value of the distances between all pairs of vertices of G, i.e.,

$$\mu(G) = \frac{\sum_{u,v \in V} d(u, v)}{\binom{n}{2}}.$$

A tree is a connected graph of order n and size $n - 1$, while a unicyclic graph is a connected graph of order n and size n.

The concept of the average distance, also called the *mean distance*, was introduced in graph theory by Doyle and Graver [34] as a measure of the "compactness" of a graph. It has already been used in architecture [56] as a tool for the evaluation of floor plans. Since then it has arisen also in the study of molecular structure (see, e.g., [89]), inter-computer connections [60] and telecommunications networks [83]. In a network model, the time delay or signal disgradation for sending a message from one point to another is often proportional to the number of edges a message must travel. The average distance can be used to indicate the average performance of a network, whereas the diameter is related to the worst-case performance.

Graffiti is a program designed to make conjectures about, but not limited to mathematics, in particular graph theory, which was written by Fajtlowicz from the mid-1980's. A numbered, annotated listing of several hundred of Graffiti's conjectures can be found in [39]. Graffiti has correctly conjectured a number of new bounds for several well studied graph invariants. A number of these bounds involve the average distance. For example, the inequality

$$\mu(G) \leq \alpha(G),$$

where $\alpha(G)$ is the independence number of G, which was proved by Chung [24] and improved by Dankelmann [31]. A Graffiti conjecture involving two distance parameters,

$$r(G) \leq \mu(G) + I(G),$$

was disproved by Dankelmann *et al.* [29], where $r(G)$ denotes the radius of G. See [10, 25, 28, 61] for other problems and results.

There is a Graffiti conjecture (see [38, 41])

$$\mu(G) \leq I(G).$$

However, the conjecture was refuted by Erdös, Pach and Spencer in [36]. They proved that, if G is a connected graph of order n and $I(G) \geq 3$, then

$$\left(\frac{2}{3}\lfloor r/3 \rfloor + o(1)\right) \frac{\log n}{\log\log n} \leq \mu(n,r) \leq D(n,r) \leq (6r + o(1)) \frac{\log n}{\log\log n},$$

where $\mu(n,r) = \max\{\mu(G) : I(G) \le r\}$ and $D(n,r) = \max\{D(G) : I(G) \le r\}$. Dankelmann *et al.* [30] improved the the upper bound by a factor of 2,

$$D(G) \le (3I(G) + 2 + o(1))\frac{\log n}{\log\log n},$$

which is also an upper bound on the average distance since $\mu(G) \le D(G)$.

In this chapter, we will give sharp upper bounds for trees and unicyclic graphs. We show that for a tree T of order n. We show that for a tree T of order n

$$D(T) \le \frac{3n - 2I(T) + 1 - \sqrt{4I(T)^2 - (4n-4)I(T) + n^2 - 2n - 7}}{2},$$

while for a unicyclic graph G of order n

$$D(G) \le \frac{3n - 2I(G) - 1 - \sqrt{4I(G)^2 - (4n-12)I(G) + n^2 - 6n + 1}}{2}.$$

6.2 The improved upper bounds

Theorem 6.2.1 *Let T be a tree of order n. Then*

$$D(T) \le \frac{3n - 2I(T) + 1 - \sqrt{4I(T)^2 - (4n-4)I(T) + n^2 - 2n - 7}}{2},$$

with equality if and only if $T \cong T(n, D(T))$, where $T(n, D(T))$ is a tree having a unique vertex with maximum degree $n + 1 - D(T)$ and all other vertices with degree one or two.

Proof. Let T be a tree of order n and $D(T) = d$. If $d = n - 1$, then $T \cong P_n$ and $I(P_n) = \frac{n+2}{2}$. It is easy to check that

$$D(P_n) = \frac{3n - 2I(P_n) + 1 - \sqrt{4I(P_n)^2 - (4n-4)I(P_n) + n^2 - 2n - 7}}{2}.$$

In the following we suppose $T \ncong P_n$. Denote by $T(n,d)$ a tree having a unique vertex with maximum degree $n + 1 - d$ and all other vertices with degree one or two. If $P = u_0u_1 \dots u_d$ is a longest path of T, then the vertices u_0 and u_d must be leaves. Note that there are at most $n - d + 1$ leaves since $D(T) = d$. Suppose the number of leaves in T is k ($k \ge 3$). First, we will show that

$$I(T) \le k + \frac{1}{k} + \frac{n-k-1}{2},$$

with equality if and only if $T \cong T(n, n-k+1)$.

We apply induction on n. It is easy to check that the assertion holds for smaller n. Suppose it holds for $n-1$. It is well-known that every tree has at least two leaves. Let v be a leaf of T and u be the unique neighbor of v.

If $d(u) = 2$, $T - v$ is a tree having $n-1$ vertices and k leaves. Then we have

$$\begin{aligned} I(T) &= \frac{1}{2} + I(T-v) \\ &\leq \frac{1}{2} + k + \frac{1}{k} + \frac{n-1-k-1}{2} = k + \frac{1}{k} + \frac{n-k-1}{2}. \end{aligned}$$

Equality holds if and only if $T - v \cong T(n-1, n-1-k-1)$, i.e., $T \cong T(n, n-k-1)$.

If $d(u) = 3$, $T - v$ is a tree having $n-1$ vertices and $k-1$ leaves. Then for $k \geq 3$ we have

$$\begin{aligned} I(T) &= 1 + \frac{1}{3} - \frac{1}{2} + I(T-v) \\ &\leq \frac{5}{6} + k - 1 + \frac{1}{k-1} + \frac{n-k-1}{2} \leq k + \frac{1}{k} + \frac{n-k-1}{2}, \end{aligned}$$

where equality holds throughout if and only if $T - v \cong T(n-1, n-k-1)$ and $k = 3$. That is to say, in this case, equality holds throughout if and only if $T \cong T(n, n-k-1)$ and $k = 3$. For $k > 3$, $I(T) < I(T(n, n-k-1)) = k + \frac{1}{k} + \frac{n-k-1}{2}$.

If $d(u) \geq 4$, we have $k \geq 4$ and $T - v$ is a tree having $n-1$ vertices and $k-1$ leaves. Then for $k \geq 4$ we have

$$\begin{aligned} I(T) &= 1 + \frac{1}{d(u)} - \frac{1}{d(u)-1} + I(T-v) \\ &\leq 1 - \frac{1}{d(u)(d(u)-1)} + k - 1 + \frac{1}{k-1} + \frac{n-k-1}{2} \\ &\leq k + \frac{1}{k} + \frac{n-k-1}{2}, \end{aligned}$$

where equality holds throughout if and only if $T - v \cong T(n-1, n-k-1)$ and $k = d(u)$. It is easy to check that equality holds throughout if and only if $T \cong T(n, n-k-1)$ in this case.

Considering all the above cases, we have proved the assertion above. Now we will prove the theorem. Notice that $k + \frac{1}{k} + \frac{n-k-1}{2}$ is a strictly increasing function for $k \geq 3$. Thus for a tree with $D(T) = d$, we have

$$\begin{aligned} I(T) &\leq k + \frac{1}{k} + \frac{n-k-1}{2} \\ &\leq n - d + 1 + \frac{1}{n-d+1} + \frac{d-2}{2}. \end{aligned}$$

Now multiplying $2(n-d+1)$ to the two sides of the above inequality, we obtain

$$2(n-d+1)I(T) \leq 2(n-d+1)^2 + 2 + (n-d+1)(d-2).$$

By some simplifications, we obtain a quadratic inequality on d,

$$d^2 - (3n - 2I(T) + 1)d + 2n^2 + 2n + 2 - (2n+2)I(T) \geq 0.$$

We solve the inequality and give the following solution since the diameter $d \leq n-1$,

$$d \leq \frac{3n - 2I(T) + 1 - \sqrt{4I(T)^2 - (4n-4)I(T) + n^2 - 2n - 7}}{2}.$$

The proof is complete. ∎

For a unicyclic graph G, by a similar method to the proof of Theorem 6.2.1, we get

$$I(G) \leq n - d - 1 + \frac{1}{n-d+1} + \frac{d}{2}\,.$$

Then we obtain the following theorem.

Theorem 6.2.2 *Let G be a unicyclic graph of order n. Then*

$$D(G) \leq \frac{3n - 2I(G) - 1 - \sqrt{4I(G)^2 - (4n-12)I(G) + n^2 - 6n + 1}}{2},$$

with equality if and only if $T \cong G(n, D(G))$, where $G(n, D(G))$ is a unicyclic graph having a unique vertex with maximum degree $n + 1 - D(G)$ and all other vertices with degree one or two.

6.3 Comparing of the upper bounds

Our two upper bounds are better than the following one given by Dankelmann *et al.* [30]:

$$D(G) \leq (3I(G) + 2 + o(1))\frac{\log n}{\log\log n}.$$

In fact, we improve the above bound by a factor of approximately $\frac{4}{3} \cdot \frac{\log n}{\log\log n}$ (note that $\frac{\log n}{\log\log n} > 1$). Before proving it, we list the following two results proved by Li and Zhao [72], Zhang and Zhang [101], respectively. Let P_n be the path with n vertices, S_n the star with n vertices, C_n the cycle with n vertices and S_n^+ the graph obtained from S_n by joining two leaves with an edge.

Theorem 6.3.1 (Li and Zhao, [72]) *For a tree T of order n, the inverse degree of T satisfies that*

$$\frac{n+2}{2} \leq I(T) \leq n-1+\frac{1}{n-1},$$

where the left inequality is an equality if and only if $T \cong P_n$, the right inequality is an equality if and only if $T \cong S_n$.

Theorem 6.3.2 (Zhang and Zhang, [101]) *For a unicyclic graph G of order n, the inverse degree of G satisfies that*

$$\frac{n}{2} \leq I(G) \leq n-2+\frac{1}{n-1},$$

where the left inequality is an equality if and only if $T \cong C_n$, the right inequality is an equality if and only if $T \cong S_n^+$.

At first, for a tree T of order n, we will show that the following inequality holds for $\frac{n+2}{2} \leq I(T) \leq n-1+\frac{1}{n-1}$:

$$\frac{3n-2I(T)+1-\sqrt{4I(T)^2-(4n-4)I(T)+n^2-2n-7}}{2} < \frac{3}{4}(3I(T)+2).$$

By some simplifications, we can transform the above inequality into the following one:

$$6n-13I(T)-4 < 2\sqrt{4I(T)^2-(4n-4)I(T)+n^2-2n-7}. \tag{6.3.1}$$

When $\frac{n+2}{2} \leq I(T) \leq n-1+\frac{1}{n-1}$, we have $6n-13I(T)-4<0$ and $4I(T)^2-(4n-4)I(T)+n^2-2n-7>0$. Thus inequality (6.3.1) holds obviously, which implies that our bound is a better one.

By similar discussions as above, for a unicyclic graph G of order n, we can prove that the following inequality holds for $\frac{n}{2} \leq I(G) \leq n - 2 + \frac{1}{n-1}$:

$$\frac{3n - 2I(G) - 1 - \sqrt{4I(G)^2 - (4n - 12)I(G) + n^2 - 6n + 1}}{2} < \frac{3}{4}(3r(G) + 2),$$

which also implies that our bound is a better one.

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在学期间发表的学术论文与研究成果

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