



Regular integrity in graphs

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Abstract

The integrity is a vulnerability parameter which measures the strength of any communication network. In any chemical reaction, reactants are converted products. Burning fuels, smelting iron, making glass and pottery, brewing beer are the examples of activities incorporating chemical reactions. In this paper, we introduce a new vulnerability parameter known as the regular integrity which is defined as $I_r(G) = \min_{S \subseteq V(G)} \{|S| + m_r(G-S)\}$. After the removal of $S, G-S$ contains regular components with same regularity and $m_r(G-S)$ denotes the regularity of $G-S$. This measure is useful to analyze the stability of a chemical structure after the removal of one or more atoms into the disjoint regular components. The study of this parameter is initiated and find the bigger chemical structures with the given number of atoms and regular integrity number. Also, a method for constructing this type of structures is presented.

Keywords

Integrity, Regular Integrity

AMS Subject Classification : 05C07, 05C12, 05C35, 05C90.

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1. Introduction

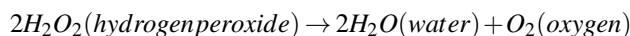
Let $G = (V, E)$ be a finite, non-trivial, undirected and connected graph without loops or multiple edges. $\Delta(G)$, $\delta(G)$, $\alpha(G)$, $\kappa(G)$, $\lambda(G)$ and $\beta(G)$ denote the maximum degree, the minimum degree, the vertex cover number, the connectivity, the edge-connectivity and the independence number of G respectively. A subset S of $V(G)$ is said to be a cut-set if removal of S results a disconnected graph or totally disconnected graph. The open neighbourhood of $v \in V(G)$ denotes $N(v)$, is the set of all vertices that are adjacent to v . $\lceil x \rceil$ denote the smallest integer number that greater than or equals to x with $\lfloor x \rfloor$ to the greatest integer number that smaller than

or equals to x . The complement of G is denoted as \bar{G} , two vertices are adjacent in \bar{G} if and only if they are not adjacent in G .

The network vulnerability is a measure to analyze the stability of the network under a hostile environment. Integrity, Toughness, Tenacity, Rupture degree, Scattering number are some of the network vulnerability parameters. Vertex integrity, introduced by Barefoot et. al. [6]. The integrity $I(G)$ of a graph G is defined as $I(G) = \min\{|S| + m(G-S) : S \subseteq V(G)\}$, where $m(G-S)$ denotes the order of a maximum component of $G-S$. They also studied the concept of the edge integrity of a graph. Bagga et al. [1] introduced the pure edge-integrity, $I_p(G)$ of a graph G is defined as $I_p(G) = \min\{|S| + m_e(G-S) : S \subseteq E(G)\}$, where $m_e(G-S)$ denotes the number of edges in a largest component of $G-S$. The weak integrity was introduced by Kirlangic [7] and is defined as $I_w(G) = \min\{|S| + m_e(G-S) : S \subseteq V(G)\}$.

The formation of bonds between atoms or breaking of bonds by removal atoms from the Chemical structure are known as chemical reaction. Reactants are the substances which go into a chemical reaction and the products are the substances that produced at the end of the reaction. For example, the reaction for breakdown of hydrogen peroxide

(H_2O_2) into water and oxygen can be written as:



In the above example, hydrogen peroxide is our reactant, and it gets broken down into water and oxygen, our products. The chemical reactions can be classified in to oxidation-reduction reactions or non-oxidation-reduction reactions under one scheme. In another scheme, (1) Combination or Synthesis reactions which occur where two or more substances react together to form just one product. (2) Decomposition reactions are one reactant which breaks up to from two or more simpler products, (3) Substitution or Single replacement reactions occur when a more reactive element displaces a less reactive one from a solution its compounds. (4) Metathesis or double displacement reactions involve the exchange of ions between two salts in aqueous solutions. Neutralization and precipitation reactions are types of double displacement reactions are the four major reactions types.

In chemistry, the valence or valency of an element is a measure of its combining power with other atoms when it forms chemical compounds or molecule. The valence is measured as a degree of a vertex in chemical graphs. The nanotechnology is a study of the nanostructures. The carbon nanotubes consists of helical tubes from single or more graphite sheets. These are called as single walled carbon nanotubes and multi-walled carbon nanotubes. These can be imagined as rolled sheets of graphite about different axes. It has some remarkable mechanical properties. It also belongs to the stiffest and elastic known materials.

Loss of carbon atoms from carbon nanotubes TUC_4C_8 by applying chemical reactions and the resulting structure is of the form of the disjoint carbon cycles are not studied much in the literature. The study of these two parts by using the regular integrity parameter is made in this article. We give some of the bounds, regular integrity of standard graphs are obtained in the next section. In the third section, construction of maximum graph with given order and regular integrity number is discussed. Applications of the regular integrity in chemical engineering is presented in the last section.

2. Bounds on Regular Integrity

Definition 2.1. Let $G = (V, E)$ be a simple graph. The regular integrity of G is defined as $I_r(G) = \min_{S \subseteq V(G)} \{|S| + m_r(G - S)\}$.

After the removal of S , $G - S$ contains regular components with same regularity and $m_r(G - S)$ denotes the regularity of $G - S$. A subset S of $V(G)$ is called a regular integrity set if $I_r(G) = \min_{S \subseteq V(G)} \{|S| + m_r(G - S)\}$.

The existence of regular integrity set of G is guaranteed, since every vertex cover of G is a regular integrity set of G .

Theorem 2.2. For any connected graph G , $I_r(G) \leq \alpha(G)$ where $\alpha(G)$ is the vertex cover of G .

Proof. Let S be a vertex cover of G . Then $V - S$ is totally disconnected. Hence $I_r(G) \leq \alpha(G)$. \square

Remark 2.3. For any connected k -regular graph G , $I_r(G) = k, 1 \leq k \leq n - 1$. For : removal of any subset S of vertices from G , $I_r(G) \neq k$.

For example,

1. $I_r(K_n) = n - 1$
2. $I_r(C_n) = 2$
3. $I_r(K_{n,n}) = n$

Theorem 2.4. For any connected graph G , $I_r(G) = 1$ if and only if $G \cong K_{1,n}$.

Proof. Let $G = K_{1,n}$. Then $I_r(G) = 1$. Suppose $I_r(G) = 1$. Then by definition of I_r - set, S contains a single vertex say u and $\langle G - S \rangle$ is a regular graph with regularity 0 on n vertices (since $G - S$ is a totally disconnected graph with vertices v_1, v_2, \dots, v_n). As G is connected, u is adjacent to all $v_i, 1 \leq i \leq n$. Thus $G \cong K_{1,n}$. \square

Theorem 2.5. For any connected graph G , Then $I_r(G) = n - 1$ if and only if $G \cong K_n$.

Proof. Let $G = K_n$. Then $I_r(G) = n - 1$. Let $I_r(G) = n - 1$. Suppose that $G \not\cong K_n$. Then $\beta(G) > 1$. Therefore $I_r(G) \leq n - \beta(G) \leq n - 2$ which is a contradiction. Thus $G \cong K_n$. \square

Corollary 2.6. For any connected graph G , $1 \leq I_r(G) \leq n - 1$.

Theorem 2.7. $I_r(P_n) = \begin{cases} \lfloor \frac{n}{3} \rfloor + 1, n \cong 0, 2 \pmod{3} \\ \lceil \frac{n}{3} \rceil + 1, n \cong 1 \pmod{3} \end{cases}$

where $n \geq 6$

Proof. It is easy to see that $I_r(P_n) = \begin{cases} 1, n = 3 \\ 2, n = 4, 5 \end{cases}$

By the definition of regular integrity,

$$I_r(G) = \min_{S \subseteq V(G)} \{|S| + m_r(G - S)\}.$$

Let $n \geq 6$. It is obvious that the only regular graphs in P_n are K_1 or K_2 . Therefore, $m_r(G - S) = 0$ (or) 1 and hence $I_r(G) \leq |S|$ (or) $|S| + 1$.

Case (i): Suppose $m_r(G - S) = 0$. $\langle G - S \rangle$ is a totally disconnected graph. Therefore, $I_r(G) \leq \alpha(G) = \lfloor \frac{n}{2} \rfloor$.

Case (ii): Suppose $m_r(G - S) = 1$. $\langle G - S \rangle$ contain only K_2 .

Subcase (i): $n \cong 0 \pmod{3}$

To obtain maximum number of disjoint K_2 's, we select atleast $\lfloor \frac{n}{3} \rfloor$ vertices from P_n . Therefore $I_r(P_n) \geq \lfloor \frac{n}{3} \rfloor + 1$. Consider $S = \{v_3, v_6, v_9, \dots, v_n\}$. Clearly, $G - S$ contains disjoint copies of K_2 of regularity 1. Therefore, $I_r(P_n) \geq \lfloor \frac{n}{3} \rfloor + 1$. Thus, $I_r(P_n) = \lfloor \frac{n}{3} \rfloor + 1$.

Subcase (ii): $n \cong 1 \pmod{3}$

To obtain maximum number of disjoint K_2 's, we select atleast $\lceil \frac{n}{3} \rceil$ vertices from P_n . Therefore $I_r(P_n) \geq \lceil \frac{n}{3} \rceil + 1$. Consider $S = \{v_1, v_4, v_7, \dots, v_n\}$. Clearly, $G - S$ contains disjoint copies of K_2 of regularity 1. Therefore, $I_r(P_n) \geq \lceil \frac{n}{3} \rceil + 1$. Thus, $I_r(P_n) = \lceil \frac{n}{3} \rceil + 1$.



Subcase (iii): $n \cong 2(mod\ 3)$

To obtain maximum number of disjoint K_2 's, we select atleast $\lfloor \frac{n}{3} \rfloor$ vertices from P_n . Therefore $I_r(P_n) \geq \lfloor \frac{n}{3} \rfloor + 1$. Consider $S = \{v_3, v_6, v_9, \dots, v_{n-2}\}$. Clearly, $G - S$ contains disjoint copies of K_2 of regularity 1. Therefore, $I_r(P_n) \geq \lfloor \frac{n}{3} \rfloor + 1$. Thus, $I_r(P_n) = \lfloor \frac{n}{3} \rfloor + 1$. \square

Theorem 2.8. $I_r(K_{m,n}) = \min\{m, n\} = \alpha(K_{m,n})$.

Theorem 2.9. $I_r(K_2 \times P_n) = \begin{cases} 2(\lfloor \frac{n}{3} \rfloor + 1), n \cong 0, 2(mod\ 3) \\ 2(\lceil \frac{n}{3} \rceil + 1), n \cong 1(mod\ 3) \end{cases}$

where $n \geq$

Proof. It is easy to see that $I_r(K_2 \times P_n) = \begin{cases} 3, n = 3 \\ 4, n = 4, 5 \\ 6, n = 6 \end{cases}$

Let $V(K_2 \times P_n) = \{u_1, u_2, \dots, u_n\} \cup \{v_1, v_2, \dots, v_n\}$. Let $n \geq$. It is easy to verify that the maximum order regular graphs in $K_2 \times P_n$ is C_4 . Therefore, $m_r(G - S) = 2$. Thus, $I_r(G) \leq |S| + 2$.

Suppose $m_r(G - S) = 2$. $\langle G - S \rangle$ contain only C_4 .

Subcase (i): $n \cong 0(mod\ 3)$

To obtain maximum number of disjoint C_4 's, we select atleast $2(\lfloor \frac{n}{3} \rfloor)$ vertices from $K_2 \times P_n$. Therefore $I_r(K_2 \times P_n) \geq \lfloor \frac{n}{3} \rfloor + 1$. Consider $S = \{u_3, u_6, u_9, \dots, u_n\} \cup \{v_3, v_6, v_9, \dots, v_n\}$. Clearly, $G - S$ contains disjoint copies of C_4 of regularity 2. Therefore, $I_r(K_2 \times P_n) \geq 2(\lfloor \frac{n}{3} \rfloor + 1)$. Thus, $I_r(K_2 \times P_n) = 2(\lfloor \frac{n}{3} \rfloor + 1)$.

Subcase (ii): $n \cong 1(mod\ 3)$

To obtain maximum number of disjoint C_4 's, we select atleast $2(\lceil \frac{n}{3} \rceil)$ vertices from $K_2 \times P_n$. Therefore $I_r(K_2 \times P_n) \geq 2(\lceil \frac{n}{3} \rceil + 1)$. Consider $S = \{u_1, u_4, u_7, \dots, u_n\} \cup \{v_1, v_4, v_7, \dots, v_n\}$. Clearly, $G - S$ contains disjoint copies of C_4 of regularity 2. Therefore, $I_r(K_2 \times P_n) \geq 2(\lceil \frac{n}{3} \rceil + 1)$. Thus, $I_r(K_2 \times P_n) = 2(\lceil \frac{n}{3} \rceil + 1)$.

Subcase (iii): $n \cong 2(mod\ 3)$

To obtain maximum number of disjoint C_4 's, we select atleast $2(\lfloor \frac{n}{3} \rfloor)$ vertices from $K_2 \times P_n$. Therefore $I_r(K_2 \times P_n) \geq 2(\lfloor \frac{n}{3} \rfloor + 1)$. Consider $S = \{u_3, u_6, u_9, \dots, u_{n-2}\} \cup \{v_3, v_6, v_9, \dots, v_{n-2}\}$. Clearly, $G - S$ contains disjoint copies of C_4 of regularity 2. Therefore, $I_r(K_2 \times P_n) \geq 2(\lfloor \frac{n}{3} \rfloor + 1)$. Thus, $I_r(K_2 \times P_n) = 2(\lfloor \frac{n}{3} \rfloor + 1)$. \square

3. Construction of chemical structure with given number of atoms and regular integrity

Theorem 3.1. Let G be a connected chemical structure with n , number of atoms and regular integrity I_r . Then maximum number of bonds in G is $\frac{I_r(I_r-1)}{2} + I_r(n - I_r)$.

Proof. Let S be an I_r -set of G . Then clearly, $I_r(G) = |S| + m_r(G - S)$. Let G_1, G_2, \dots, G_k be the components of $G - S$ and $|S| = s, m_r(G - S) = r$.

To attain maximum the number of bonds, any chemical structure G has the following properties:

- (1) $G[S]$ is a complete substructure of G
- (2) All $G_i (i = 1, 2, \dots, k)$ are regular components of $G - S$
- (3) All atoms in S must be adjacent to all vertices in $G_i (i = 1, 2, \dots, k)$

To obtain the maximum number of bonds, maximize the following function

$$f(s, r) = \binom{s}{2} + s \sum_{i=1}^k n_i + \frac{(n-s)r}{2} \text{ and } I_r = s + r,$$

Therefore, $f(s, r) = \binom{s}{2} + s(n-s) + \frac{(n-s)(I_r-s)}{2}, 1 \leq s \leq I_r$. Clearly, $f(s, r)$ is independent of r . $f(s, r)$ is a function of s alone. That is, $f(s, r)$ becomes $f(s)$.

Since $f'(s) = -\frac{n}{2} - \frac{s+1}{2} > 0$ and so $f(s)$ is an increasing function in the interval $1 \leq s \leq I_r < n - 2$. Hence the maximum value $f(s, r)$ is achieved when $s = I_r$. In such case, the value $r = 0$. That is, $m_r(G - S) = 0$ ($G - S$ is totally independent).

$$\begin{aligned} \max f(s, r) &= f(I_r, r) = \frac{I_r(I_r-1)}{2} + I_r(n - I_r) + \frac{(n-I_r)(0)}{2} \\ \max f(s, r) &= \frac{I_r(I_r-1)}{2} + I_r(n - I_r) \end{aligned}$$

\square

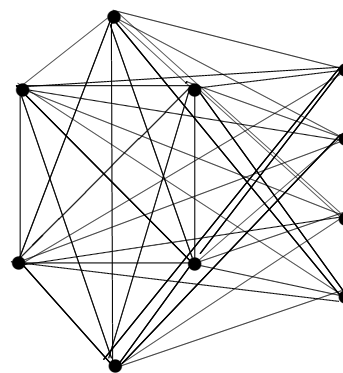
It is easy to see that, if $I_r(G) = n - 1$ then $G \cong K_n$.

Construction:

If $I_r = n - 1$ then construct the complete graph K_n . If $1 \leq I_r \leq n - 2$, then the construction follows three steps:

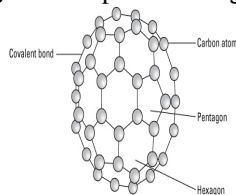
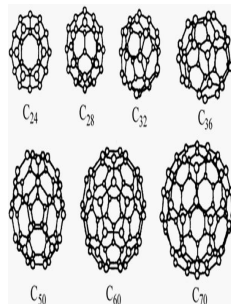
1. Construct K_{I_r}
2. Construct $\overline{K_{n-I_r}}$
3. Join the vertices of K_{I_r} to all the vertices of $\overline{K_{n-I_r}}$.

Illustration 3.2. Let G be a connected graph with number of vertices $n = |V(G)| = 5, I_r(G) = 4$. Then we construct a complete graph K_5 with $\max |E(G)| = 10$. Suppose $n = |V(G)| = 10, I_r(G) = 6$. Then construct a complete graph on six vertices K_6 and a totally disconnected graph $\overline{K_4}$ on the remaining 4 vertices. Join vertices of K_6 to all the vertices of $\overline{K_4}$, as shown in the following figure.



Corollary 3.3. Graph $G = K_2 \times C_n, I_r(G) = 3$, since it is 3-regular graph.



Figure 1. A picture of a gull.**Figure 2.** A picture of a gull.

4. Applications of regular integrity in chemical engineering

Buckyballs are the one of the first nanoparticles were discovered by Richard Smalley, Harry Kroto, and Robert Curl in Rice University, 1985. In the structure of buckyball composes carbon atoms linked to three other carbon atoms by covalent bonds. Also, the carbon atoms are connected in the same pattern of hexagons and pentagons in buckyball. The spherical structure of the buckyball is shown in the Figure:1.

There are 60 carbon atoms in buckyball and is represented as C_{60} . The covalent bonds between carbon atoms provides more strength to buckyballs. Graphite is an assembly of carbon atoms in flat layer of hexagons loosely bound across different layers whereas Diamond is a very solid structure based on the repetitive arrangement of a precise pattern of 8 carbon atoms. In Fullerenes structure, the carbon atoms are disposed as hexagonal and pentagonal rings on the surface of a spherical shell which is shown in the Figure:2.

To analyze chemical structures through graph theory is a well known branch, called chemical graph theory. A molecular (chemical) graph is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure. This is more important to say that the hydrogen atoms are often omitted in any molecular graph. Topological descriptors play a vital role in Quantitative structure-activity (QSAR) and (QSPR) study. A nanostructure is an object of intermediate size between microscopic and molecular structures. It is product derived through engineering at molecular scale. Carbon nanotubes (CNTs) are types of nanostructure which are allotropes of carbon and having a cylindrical shape. $TU_4C_8[p, q]$ is a combination of octagons (any cycle C_8) and quadrangles (any cycle C_4), where p and q denotes number of octagons in a fixed row and column,

respectively, of a 2-dimensional lattice. During a certain type of chemical reaction, loss of carbon atoms from 2D-lattice results disjoint copies of carbon cycles C_n , which are 2-regular graphs. Regular integrity plays a vital role to measure the stability this structure.

5. Conclusion

We have studied a new vulnerability parameter, regular integrity and found basic bounds. We have calculated this parameter for some of the standard graph structure. We showed a maximum network with given order the graph and regular integrity, illustrated such network. At the end, we gave some practical applications of this new parameter in chemical engineering.

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