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A Metaheuristic and LP-Based Approach to Irregular Face Coloring in Planar Graphs

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Abstract. In irregular coloring, each vertex is labeled with a unique color code, a tuple consisting of its assigned color and the number of neighbors in each color class. This work proposes a local search algorithm as a metaheuristic approach to the irregular face coloring problem in planar graphs, with a particular focus on fullerene molecular structures. Additionally, a linear programming model is utilized to validate the performance of the proposed algorithm. The methodology demonstrates efficient solutions for irregular coloring in fullerene graphs, bridging combinatorial optimization with practical applications in chemistry and materials science.

Keywords. Irregular coloring, Face coloring, Linear programming, Metaheuristic algorithm, Fullerene graphs, Planar graphs

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1 Background and Motivation

Graph coloring is a central topic in graph theory and combinatorics, with wide-ranging applications in scheduling, resource allocation, frequency assignment, and molecular chemistry. The idea was first formally introduced by Francis Guthrie in 1852, which spurred the development of diverse coloring techniques, including equitable coloring, list coloring, and irregular coloring, each designed for particular practical needs [3].

For a graph G, the degree of a vertex $v \in V$, denoted deg(v), is the number of edges incident to v. A proper coloring assigns colors to vertices such that adjacent vertices receive different colors, thereby preventing conflicts or overlaps in various contexts.

1.1 Notations and Definitions

A function f is called a *proper coloring* of a graph G if $f(u) \neq f(v)$ for each $uv \in E(G)$.

Let f be a proper coloring of graph G. For a vertex v of G, the *color code* of vertex v, denoted by $c(v)$, is the vector

$$c(v) = (x_1, x_2, \ldots, x_k),$$

where x_i represents the number of neighbors of v colored with color i.

A proper coloring f of G with the property that $c(u) \neq c(v)$ for each pair of distinct vertices $u, v \in V(G)$ is called an *irregular coloring* of G.

This concept was first introduced by Radcliffe et al. in [10], motivated by a graph-theoretic problem concerning methods to distinguish all the vertices of a connected graph. A few years later, Anderson et al. [1] explored irregular colorings of regular graphs. The irregular chromatic number for derived graphs, such as the flower graph, middle graph, and total graph, was investigated Rohini et al. in [11]. Recently, graph labeling has emerged as a significant area of study in graph theory, involving the assignment of integers to vertices, edges, or both, typically under specific rules or constraints.

An irregular coloring assigns a distinct color code to each vertex. The minimum k of colors that yields unique codes for all vertices is the *irregular chromatic number* $\chi_{ir}(G)$ [1].

Driven by the wide variety of real- world problems, several extensions of vertex coloring have been introduced. For instance, in [7], a face-distance coloring of graphs was recently proposed to partition atoms in Fullerenes. The same study also discussed applications of face colorings within mathematical chemistry. Inspired by this idea, we introduce the notion of irregular face coloring in the present work.

A *fullerene graph* is a planar, 3-regular (cubic) graph that models fullerene molecules, carbon structures arranged in spherical, tubular, or ellipsoidal forms. These graphs are connected, planar, and cubic, implying that each vertex has degree 3 [2, 12]. Throughout, we denote by F_n a fullerene with n vertices.

Exploring irregular coloring in fullerenes yields insights into the structural and functional properties of these molecules, with meaningful implications for chemistry and materials science. The concept of irregular face coloring assigns unique color codes for molecular faces, enabling topological distinction between carbon pentagons and hexagons, an essential feature for isomer identification in chemical graph models.

2 Local Search Algorithm for Irregular Coloring

Since determining the irregular chromatic number is an NP-hard problem, metaheuristic algorithms constitute a practical and effective strategy for tackling this problem. This paper adopted a local search algorithm as the principal metaheuristic framework, and its performance is further supported through linear programming formulations.

A local search algorithm is a heuristic optimization technique that initiates from an initial solution and iteratively makes small, incremental changes to obtain superior solutions within a constrained neighborhood.

In this section, a practical heuristic scheme is introduced to address the irregular coloring problem. The algorithm starts with a proper coloring and iteratively refines it by minimizing conflicts until an irregular coloring is produced or a predefined computational bound is reached. This iterative improvement mechanism demonstrates an efficient way to explore the solution space in this complex optimization problem [5, 8].

2.1 Local Search Algorithms for Irregular Coloring

The irregular coloring problem is NP-hard, so this section presents two practical, modular algorithms: a Local Search Algorithm for Irregular Coloring (LSA-IC) and a Supporting Routine for Random Proper Coloring and Conflict Counting (PRC-CC). The Python implementation offers a workable approach that ensures proper coloring and unique vertex color codes.

Local Search Algorithm Overview

1. Initialize with a random proper coloring.

2. Iteratively attempt to decrease the number of conflicts (vertices with identical color codes or adjacent vertices assigned the same color) by recoloring selected vertices.

3. Terminate when an irregular coloring is obtained or when the algorithm reaches the maximum allowed number of iterations.

In Table 1, the notation and definitions relevant to the LSA-IC is presented. For ease of reference, the table below provides each symbol and its meaning with an appropriate caption. Specifically, the entries and definitions for G, k, MaxIter, v, C_0, C_i, C^*, c, c', and the function conf(C) are described.

The Python implementation of this algorithm offers a practical local search approach for irregular graph coloring, ensuring both proper coloring and unique color codes for all vertices.

Algorithm 6 Local Search Algorithm for Irregular Coloring (LSA-IC)

Input: Graph G, number of colors k, maximum iterations *MaxIter*.

Output: An irregular vertex coloring C' of G or a failure signal.

Generate a random proper coloring C_0 for G with k colors (via Algorithm 7).

for $i = 0$ to *MaxIter* **do**

  Compute number of conflicts in C_i.

  if the number of conflicts is 0 **then**

    return C_i as a valid irregular coloring.

  else

    Randomly select a vertex v.

    Let the current color of v be c.

    for each alternative color $c' \in \{1, \ldots, k\} \setminus \{c\}$ **do**

      Temporarily assign c' to v.

      if the new coloring is proper and reduces conflicts **then**

        Update the best coloring and conflict count.

      end if

    end for

    Update C_{i+1}.

  end if

end for

return failure.

2.2 Irregular Coloring of Some Fullerenes

TheWe adapt a local search algorithm to compute $\chi_{ir}(G)$ for certain Fullerenes including an isomer under the isolated-pentagon-rule (IPR) with 80 vertices, denoted by F_{80}^{IPR}, as well as F_{100}^{IPR}, and F_{120}^{IPR} (IPR with 100 and 120 vertices, respectively) (see [12]).

2.3 Irregular Coloring of Some Hypercubes

A hypercube graph (Q_n) represents the vertices and edges of an n-dimensional hypercube. These graphs have 2^n vertices and are n-regular, meaning every vertex has degree n.

Table 1: Notation used in Algorithms

Symbol	Meaning	Description
G	Input graph	The graph on which the irregular coloring problem is defined.
k	Maximum number of colors	The upper bound on the color set $\{1, \ldots, k\}$.
MaxIter	Maximum iterations	Upper limit on the number of iterations of the algorithm.
v	A vertex of the input graph	A generic vertex in G.
C_0	Initial random proper coloring	The starting coloring of G with k colors.
C_i	Coloring at iteration i	The coloring obtained in iteration i.
C^*	Irregular coloring of the graph	A coloring in which all vertices have distinct color codes.
c	Current color of vertex v	The color currently assigned to vertex v.
c'	New color of vertex v	A candidate color for v in a recoloring step.
conf(C)	Conflict function	Computes conflicts for coloring C. It produces a matrix with n rows and $k+1$ columns, where n is the number of vertices. Each row encodes the color code of a vertex. If the rows are pairwise distinct, there is no conflict under the first condition. The second condition enforces that adjacent vertices do not share the same color. The total conflict count is the sum of conflicts under both conditions.

Algorithm 7 Proper Random Coloring and Conflict Counting (PRC-CC)

Input: Graph G, coloring C, number of colors k.

Output: Number of conflicts in C.

Assign each vertex a color from $\{1, \ldots, k\}$ such that adjacent vertices have different colors.

For each vertex, compute its color code.

Pairwise compare all vertices' codes:

  If two vertices share same code, increment conflict count.

  If two adjacent vertices share the same color, increment improper-conflict count.

return the sum of conflicts.

For example, the 5-dimensional hypercube (Q_5) has 32 vertices and is 5-regular.

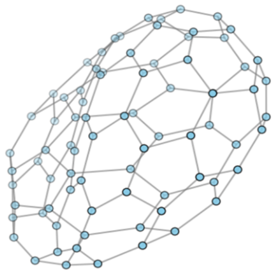
2.4 Computational Results

Using the local search algorithm, we computed results for Fullerenes and hypercubes with various numbers of vertices.

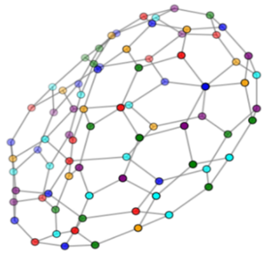
Refer to [1], Theorem 1.3, if c is an irregular k-coloring of a non-trivial connected graph G, then G contains at most

$$k \times \binom{r+k-2}{r},$$

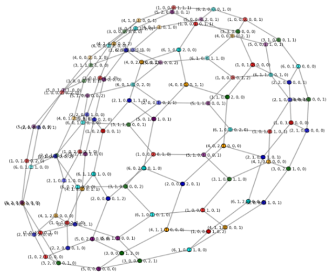
vertices of degree r.



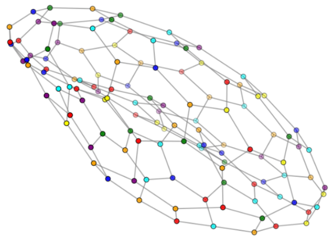
(a) Structure of Fullerene F_{80}



(b) Irregular coloring of F_{80} with $k = 6$

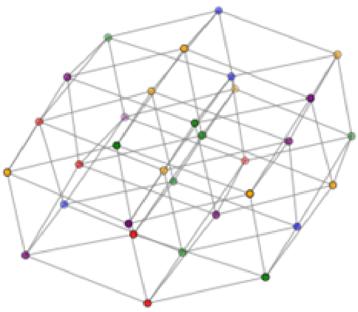


(c) Irregular colored F_{100} with $k = 6$

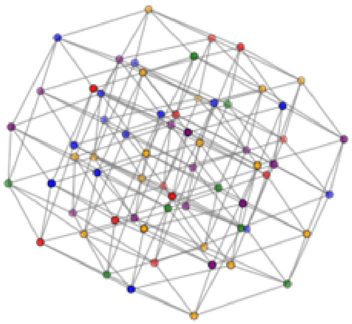


(d) Irregular colored F_{120} with $k = 7$

Figure 1: n denotes the number of vertices and k denotes the number of colors.



(a) Q_5



(b) Q_6

Figure 2: Q_5 $(n = 32)$ and Q_6 $(n = 64)$ irregular colored with $k = 5$.

Fullerenes are 3-regular, while hypercubes are 5- and 6-regular. Consequently, to find an irregular coloring of the target graph using Algorithm 6, it suffices to determine the minimum k that satisfies the mentioned theorem. This observation indicates that the proposed approximate algorithm achieves high performance with a small margin of error, validating its practical applicability and robustness.

Table 2: Results obtained using the local search algorithm.

Number of vertices (n)	By Theorem	By Algorithm	Runtime (s)	Number of iterations
80	5	6	0.0791	194
100	5	6	0.1107	246
120	6	7	0.1024	75
32	4	5	0.0151	5
64	4	5	0.1261	314

3 Integer Linear Programming Model of Irregular Coloring

This section describes an exact computational model for irregular coloring based on integer linear programming (ILP). The objective is to minimize the total number of used colors, subject to coloring feasibility and irregularity constraints.

$$\begin{aligned}
&Min \quad \sum_{i=1}^{n} x_i \\
s.t:& \\
&\sum_{i=1}^{n} y_{v,i} = 1, && v \in V, \\
&y_{v,i} \le x_i, && v \in V,\ \forall i, \\
&y_{u,i} + y_{v,i} \le 1, && u, v \text{ are adjacent},\ \forall i, \\
&\sum_{i=1}^{n} \big(I_{u,v,i} + N_{u,v,i}\big) > 0, && u, v \text{ with } \deg(u) = \deg(v), \\
&x_i \in \{0,1\}, \quad y_{v,i} \in \{0,1\}, && \forall v, i.
\end{aligned} \tag{1}$$

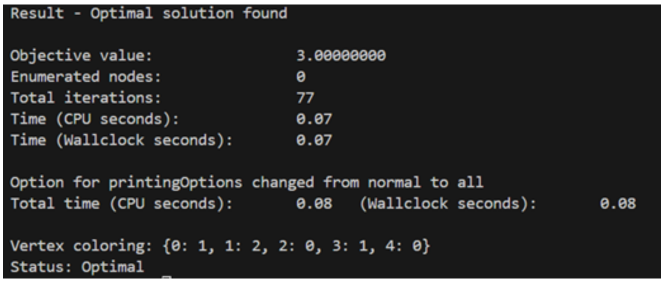
where auxiliary terms are defined as:

$$I_{u,v,i} = \begin{cases} 0, & y_{u,i} = y_{v,i}, \\ 1, & \text{otherwise}, \end{cases} \qquad N_{u,v,i} = \begin{cases} 0, & \sum_{u' \in N(u)} y_{u',i} = \sum_{v' \in N(v)} y_{v',i}, \\ 1, & \text{otherwise}. \end{cases}$$

This ILP enforces a proper coloring and encodes the irregular coloring constraint through neighborhood color-code uniqueness.

Limitations of the ILP Model

Although the ILP model (1) yields exact solutions for the irregular coloring problem, its applicability for all Fullerene graphs is limited by scalability and computational complexity. The model involves a large number of variables and constraints, which grow rapidly with the input size: both the number of vertices (n) and the number of colors directly affect the problem's dimensionality.



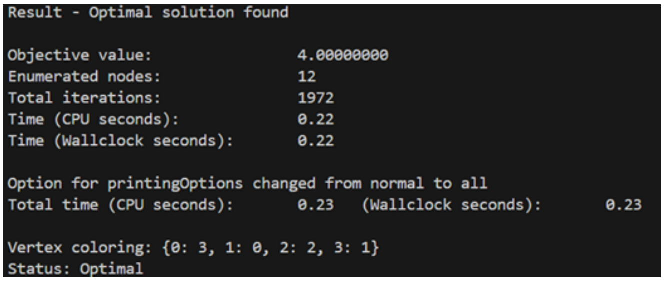
```
Result - Optimal solution found

Objective value:                3.00000000
Enumerated nodes:               0
Total iterations:               77
Time (CPU seconds):             0.07
Time (Wallclock seconds):       0.07

Option for printingOptions changed from normal to all
Total time (CPU seconds):       0.08   (Wallclock seconds):       0.08

Vertex coloring: {0: 1, 1: 2, 2: 0, 3: 1, 4: 0}
Status: Optimal
```

Figure 3: ILP result for path with 5 vertices (path graph, $n = 5$).



```
Result - Optimal solution found

Objective value:                4.00000000
Enumerated nodes:               12
Total iterations:               1972
Time (CPU seconds):             0.22
Time (Wallclock seconds):       0.22

Option for printingOptions changed from normal to all
Total time (CPU seconds):       0.23   (Wallclock seconds):       0.23

Vertex coloring: {0: 3, 1: 0, 2: 2, 3: 1}
Status: Optimal
```

Figure 4: ILP result for cycle with 4 vertices (circle graph, $n = 4$).

Fullerene graphs possess regularity and symmetry, and as the vertex count increases, the size of the ILP grows considerably, often leading to exponential growth in the overall problem size. This imposes substantial computational challenges for ILP solvers.

Exact solving of the ILP for large Fullerene graphs quickly becomes computationally prohibitive, demanding substantial memory and time-resources that are often impractical for routine experimentation. This limitation motivated the application of a metaheuristic local search algorithm, which offers efficient, approximate, yet high-quality solutions.

4 Face Coloring

Face coloring assigns colors to faces of planar graphs so that adjacent faces (sharing an edge) have different colors. Irregular face coloring extends this with unique neighborhood color codes for faces via the dual graph.

Algorithm 8 describes irregular face coloring for planar graphs by constructing the dual graph D and applying the vertex irregular coloring algorithm to D.

Algorithm 8 Irregular Face Coloring Algorithm (IFCA) for planar graphs

Input: A planar graph G, number of colors k, maximum number of iterations *MaxIter*

Output: An irregular face coloring f

Step 1. Check the planarity of graph G.

If G is non-planar, **Then** terminate the algorithm and report an error.

Step 2. Compute a planar embedding of G and extract all faces.

Step 3. Construct the dual graph D, where each vertex represents a face of G, and edges indicate adjacency between faces.

Step 4. Apply Algorithm 1 to the dual graph D to obtain an irregular coloring of its vertices.

Step 5. Map the colors obtained from D back to the corresponding faces of the original graph G.

Step 6. Return the irregular face coloring f.

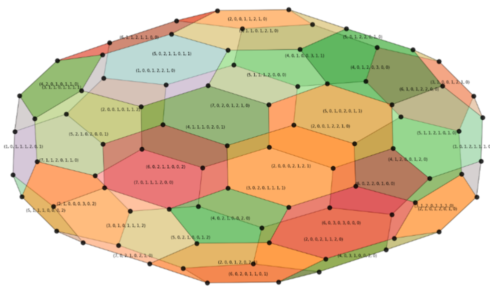


Figure 5: Irregular face coloring of fullerene F_{80} with 7 colors.

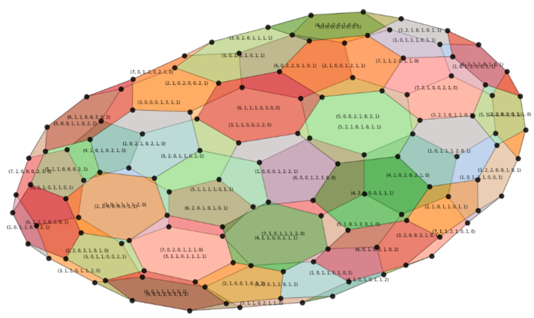


Figure 6: Irregular face coloring of fullerene F_{120} with 7 colors.

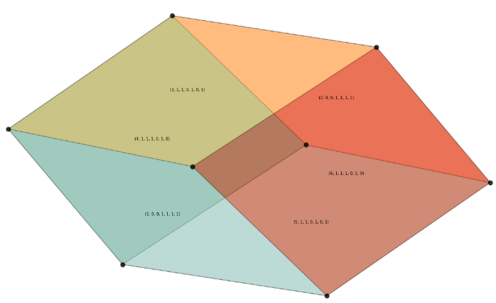


Figure 7: Irregular face coloring of hypercube Q_3 with 6 colors.

5 Conclusion

In this paper, the notion of irregular face coloring of graphs is introduced, and a linear model corresponding to this concept is presented. Furthermore, a local search algorithm for irregular face coloring of graphs is proposed. The comparative results demonstrate the accuracy of the proposed algorithm. For future research, it would be interesting to develop alternative approximation algorithms and compare their performance with that of the proposed approach.

Declarations

Availability of Supporting Data

All data generated or analyzed during this study are included in this published paper.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

Author Contributions

Maedeh Shahabi: Conceptualization; Methodology; Formal analysis; Investigation; Software; Writing – original draft; Visualization. Freydoon Rahbarnia: Methodology; Validation; Resources; Writing – review & editing; Supervision; Theoretical developments; Project administration.

Artificial Intelligence Statement

Artificial intelligence (AI) tools, including large language models, were used solely for language editing and improving readability. AI tools were not used for generating ideas, performing analyses, interpreting results, or writing the scientific content. All scientific conclusions and intellectual contributions were made exclusively by the authors.

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