DETERMINING A GRAPH'S CHROMATIC NUMBER FOR PART CONSOLIDATION IN AXIOMATIC DESIGN

A Thesis

Presented to

The Faculty of the Department of Mathematics

San José State University

In Partial Fulfillment
of the Requirements for the Degree
Master of Science

by
Jeffery A. Cavallaro
December 2019

© 2019

Jeffery A. Cavallaro

ALL RIGHTS RESERVED

The Designated Thesis Committee Approves the Thesis Titled

DETERMINING A GRAPH'S CHROMATIC NUMBER FOR PART CONSOLIDATION IN AXIOMATIC DESIGN

by

Jeffery A. Cavallaro

APPROVED FOR THE DEPARTMENT OF MATHEMATICS

SAN JOSÉ STATE UNIVERSITY

December 2019

Sogol Jahanbekam, Ph.D. Department of Mathematics

Wasin So, Ph.D. Department of Mathematics

Jordan Schettler, Ph.D. Department of Mathematics

ABSTRACT

DETERMINING A GRAPH'S CHROMATIC NUMBER FOR PART CONSOLIDATION IN AXIOMATIC DESIGN

by Jeffery A. Cavallaro

Mechanical engineering design practices are increasingly moving towards a framework called *axiomatic design* (AD), which starts with a set of independent *functional requirements* (FRs) for a manufactured product. A key tenet of AD is to decrease the *information content* of a design in order to increase the chance of manufacturing success. One important way to decrease information content is to fulfill multiple FRs by a single part: a process known as *part consolidation*. Thus, an important parameter when comparing two candidate designs is the minimum number of parts needed to satisfy all of the FRs. One possible method for determining the minimum number of parts is to represent the problem by a graph, where the vertices are the FRs and the edges represent the need to separate their endpoint FRs into separate parts. The answer then becomes the solution to a vertex coloring problem: finding the chromatic number of such a graph. Unfortunately, the chromatic number problem is known to be NP-hard. This research investigates a new algorithm that determines the chromatic number for a graph and compares the new algorithm's computer runtime performance to other well-known algorithms using random graph analysis.

ACKNOWLEDGMENTS

This material is based upon work supported by the National Science Foundation–USA under grants #CMMI-1727190 and CMMI-1727743. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the National Science Foundation.

TABLE OF CONTENTS

Lis	st of Tal	bles .		viii
Lis	st of Fig	gures		xi
1	Axion	natic	Design	1
	1.1		ign	1
	1.2		Axiomatic Design Framework	
	1.3		Axioms	5
	1.4		Consolidation	9
2	Graph	Theo	ory	11
	2.1		ple Graphs	11
	2.2		er and Size	13
	2.3		ph Relations	14
	2.3	-	Labels	14
	2.3	3.2	Vertex Color	15
	2.4		graphs	18
	2.5		tators	20
	2.5		Vertex Removal	20
	2.5		Edge Addition	21
	2.5		Edge Removal	
	2.5		Vertex Contraction	22
	2.5		Graph Complement	23
	2.6		ependent Sets	24
	2.7		jues	25
	2.8		nected Graphs	27
	2.8		Walks	27
	2.8		Paths	29
	2.8		Connected	30
	2.8		Components	31
	2.8		Impact on Coloring	
	2.9		tex Degree	33
	2.10		•	35
		зре 10.1	cial Graphs	36
		10.1	Empty Graphs	36
			Paths	
		10.3	Cycles	37
		10.4 10.5	Complete Graphs	37 38
3			eatic Number Problem	40

	3.1	Prob	olems	40
	3.2	Con	nparing Algorithms	41
	3.2	2.1	Runtime Complexity	41
	3.2	2.2	Space Complexity	44
	3.2	2.3	Runtime Duration	44
	3.3	Chr	omatic Number Lower Bound	44
	3.4	Chr	omatic Number Upper Bound	44
	3.5	The	Christofides Algorithm	44
	3.6		ov Algorithms	44
	3.6	5.1	The Chromatic Polynomial	45
	3.6	5.2	An Exhaustive Algorithm	48
	3.6	5.3	Branch and Bound Strategies	49
4	The Pr	opos	ed Algorithm	51
	4.1		er Loop	52
	4.2		ed Subroutine	53
	4.3	Sup	porting Theorems	57
	4.3	3.1	Maximum Edge Threshold	57
	4.3	3.2	Vertex Removal	60
	4.3	3.3	Minimum Common Neighbor Upper Bound	66
	4.3	3.4	Recursive Steps	71
	4.4	An]	Example	74
5	Toaste	r Des	sign Case Study	86
6	Rando	m Gr	raph Analysis	96
Li	terature	Cited	1	97

LIST OF TABLES

Table 1.	Opener Functional Requirements	9
Table 2.	Classifying Vertex <i>u</i> in Graph <i>G</i>	34
Table 3.	Calculating Common Neighbors 1	77
Table 4.	Calculating Common Neighbors 2	78
Table 5.	Toaster Functional Requirements	87

LIST OF FIGURES

Fig. 1.	The axiomatic design framework	3
Fig. 2.	Mapping FRs to DPs.	4
Fig. 3.	An example of an uncoupled design.	6
Fig. 4.	An example of a decoupled design.	6
Fig. 5.	An example of a coupled design	6
Fig. 6.	Decoupling a design by adding DPs.	8
Fig. 7.	A part consolidation example.	9
Fig. 8.	An example graph (labeled and unlabeled)	12
Fig. 9.	A graph with a 4-coloring	16
Fig. 10.	A Graph with a 3-chromatic coloring.	18
Fig. 11.	Subgraph examples.	19
Fig. 12.	An induced subgraph example.	20
Fig. 13.	A vertex removal example.	21
Fig. 14.	An edge addition example.	21
Fig. 15.	An Edge removal example.	22
Fig. 16.	A vertex contraction example.	23
Fig. 17.	A graph complement example.	24
Fig. 18.	The independent sets of an example graph.	25
Fig. 19.	The maximal cliques of an example graph	26
Fig. 20.	Open and closed walks.	28
Fig. 21.	Repeated vertex at end case.	30
Fig. 22.	Repeated vertex inside case.	30

Fig. 23.	Connected and disconnected graphs	31
Fig. 24.	Vertex degrees and the first theorem of graph theory	35
Fig. 25.	Empty graphs.	36
Fig. 26.	Path graphs.	36
Fig. 27.	Cycle graphs.	37
Fig. 28.	Complete graphs.	37
Fig. 29.	A tree organized from root to leaves.	38
Fig. 30.	The runtime complexity classes.	43
Fig. 31.	V.G Vizing (L), A.A. Zykov (C), and V.I. Voloshin (R) in Odessa (2001) [1]	45
Fig. 32.	Same Colors with Vertex Contraction	46
Fig. 33.	Different Colors with Edge Addition	46
Fig. 34.	Zykov Graph Equation	47
Fig. 35.	A Zykov Tree	50
Fig. 36.	Proposed algorithm outer loop.	53
Fig. 37.	Proposed algorithm called subroutine	56
Fig. 38.	Corollary 8 example.	60
Fig. 39.	Lemma 1 example.	61
Fig. 40.	Theorem 14 example.	63
Fig. 41.	Theorem 15 example.	65
Fig. 42.	Lemma 2 example.	67
Fig. 43.	Case $a_i = 1$ contradiction	68
Fig. 44.	Corollary 10 example.	71
Fig. 45.	An example graph.	75

Fig. 46.	Step: $G - \{h\}$.	76
Fig. 47.	Step: $G - g$	77
Fig. 48.	Step: $G \cdot ad$	79
Fig. 49.	Step: $G + ad$.	80
Fig. 50.	Step: $G - \{b, f\}$	82
Fig. 51.	Initial coloring.	83
Fig. 52.	Coloring b and f	83
Fig. 53.	Coloring g	84
Fig. 54.	Final chromatic coloring.	84
Fig. 55.	An example toaster.	86
Fig. 56.	First candidate design.	87
Fig. 57.	Design 1—remove FR ₂ .	88
Fig. 58.	Design 1—Remove FR ₄ and FR ₃ .	89
Fig. 59.	Design 1—chromatic coloring.	90
Fig. 60.	Second candidate design.	91
Fig. 61.	Design 2—remove FR ₆ .	92
Fig. 62.	Design 2—remove FR ₅ .	93
Fig. 63.	Design 2—remove FR ₂ .	93
Fig. 64.	Design 2—remove FR ₄ and FR ₇ .	94
Fig. 65	Design 2 chromatic coloring	05

1 AXIOMATIC DESIGN

The axiomatic design (AD) framework was developed in the late 20th century by Professor Nam P. Suh while at MIT and the NSF [2]. This was in response to concern in the engineering community that *design* was being practiced almost exclusively as an ad-hoc creative endeavor with very little in the way of scientific discipline. In the words of Professor Suh:

It [design] might have preceded the development of natural sciences by scores of centuries. Yet, to this day, design is being done intuitively as an art. It is one of the few technical areas where experience is more important than formal education [2].

Professor Suh was not making these claims in an educational vacuum, but in the shadow of several recent major design failures such as the Union Carbide plant disaster in India, nuclear power plant accidents at Three Mile Island and Chernobyl, and the Challenger space shuttle O-ring failure. Furthermore, Professor Suh asserts that design-related issues resulting in production problems and operating failures were increasingly happening in everything from consumer products to big-ticket items. As a result, AD has been widely adopted by companies to promote efficiency and accuracy in the design process, resulting in more reliable products and reduced manufacturing costs [3].

The following sections provide an overview of axiomatic design as specified in detail by Professor Suh [2], [4], and summarized by Behdad, et al. [5], [6]. Following the overview is a description of how an algorithm like the algorithm proposed by this research can be a helpful tool to a designer using the AD framework.

1.1 Design

Design is defined as the process by which it is determined *what* needs to be achieved and then *how* to achieve it. Thus, the decisions on what to do are just as important as the decisions on how to do it. *Creativity* is the process by which experience and intuition are used to generate solutions to perceived needs. This includes pattern matching to and

adapting existing solutions and synthesizing new solutions. Thus, creativity plays a vital role in design. Different designers may approach the same problem differently, and their varying levels of creativity may lead to very different, yet still plausible, solutions. Therefore, there needs to be a design-agnostic method for comparing different designs with the goal of selecting the best one.

This discussion will sound familiar to mathematicians, since creativity is a very important part of solving math problems, particularly in the writing of proofs. Thus, the field of mathematics has established various tests on what constitutes a good proof. For example:

- Does every conclusion result by proper implication from existing definitions, axioms, and previously proved conclusions?
- Is direct proof, contrapositive proof, proof by contradiction, or proof by induction the best approach for a particular problem?
- Do proofs by induction contain clear basic, assumptive, and inductive steps?
- Are all subset and equality relationships properly proved via membership implication?
- Are all necessary cases included and stated in a mutually exclusive manner?
- Are degenerate cases sufficiently highlighted?
- Are all equivalences proved in a proper circular fashion?
- Are key and reused conclusions highlighted in lemmas?

In short, Professor Suh was looking for a similar framework for the more general concept of design.

1.2 The Axiomatic Design Framework

The *best* design among a set of candidates is the design that exactly satisfies a clearly defined set of needs and has the greatest probability of success in meeting those needs. In a desire not to hinder the creative element needed for design, yet provide some

methodology to distinguish bad designs from good designs from better designs, the diagram in Fig. 1 establishes the overall framework for axiomatic design.



Fig. 1. The axiomatic design framework.

Design starts with the desire to satisfy a set of precisely stated *customer needs*. The term *customer* refers to any entity that expresses needs, and can be as varied as individuals, organizations, or society. In the *problem definition* phase, the designer determines how the customer needs will be met by generating a minimal list of *functional requirements* (FRs) that directly and exclusively fulfill the needs. It is this list of FRs that determines exactly *what* is to be accomplished.

Once the set of FRs has been determined, the designer begins the *creative process* by mapping the FRs into solutions that are embodied in so-called *design parameters* (DPs). The DPs contain all of the information concerning *how* the various FRs are to be satisfied: parts lists, drawings, specifications, etc. The FRs exist in a design-agnostic *functional space* and the DPs exist in a solution-specific *physical space*. It is the designer's job to provide the most efficient mapping between the two spaces. This process is represented by Fig. 2.



Fig. 2. Mapping FRs to DPs.

Simple problems may require only one level of FRs; however, more complicated designs may require a hierarchial structure of FRs from more general to more detailed requirements. This type of design is often referred to as *top-down* design. Each individual FR layer has its own DP mapping. In fact, the mapping process on one level should be completed prior to determining the FRs for the next level. This is because DP choices on one level may affect requirements on the next level. For example, consider a FR related to a moving part in a design. The DP for this FR could specify that the part be moved either manually or automatically. Each choice would result in different FRs for the actual mechanism selected by the DP.

The FR/DP mapping at each level in the design hierarchy is described by the *design equation*, which is shown in Equation 1.

$$[FR] = [A][DP] \tag{1}$$

The design equation is a matrix equation that maps a vector of m FRs to a vector of n DPs via an $m \times n$ design matrix A. As will be shown later in this section, good designs require

m = n. A full discussion of the design matrix element values is well beyond the scope of this research. Instead, the following two summary values are used:

$$A_{ij} = \begin{cases} X, & FR_i \text{ depends on } DP_j \\ 0, & FR_i \text{ does not depend on } DP_j \end{cases}$$

Since the FR/DP mapping is non-unique, there needs to be a method to compare different plausible designs so that the best design can be selected as the final design. Thus, the framework in Fig. 1 includes an *analytical process*, where designs are judged by a set of axioms, corollaries, and theorems that specify the properties common to all good designs. Once the best design, according to this analysis, is selected, it undergoes an *ultimate check* to make sure that it exactly meets all of the customer's needs. If so, then that design is selected as the final design.

1.3 The Axioms

The analytical process is based on two main axioms: the independence axiom and the information axiom. This section describes these axioms and their related corollaries and theorems.

The independence axiom [2] imposes a restriction on the FR/DP mapping:

Axiom 1 (The Independence Axiom). An optimal design always maintains the independence of the FRs. This means that the FRs and DPs are related in such a way that a specific DP can be adjusted to satisfy its corresponding FR without affecting other FRs.

The ideal case is when the design matrix is a diagonal matrix and so each FR is mapped to and is satisfied by exactly one DP. This is referred to as an *uncoupled* design, which is demonstrated in Fig. 3. Uncoupled designs completely adhere to the independence axiom.

$$\begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X & 0 & 0 \\ 0 & X & 0 \\ 0 & 0 & X \end{bmatrix} \begin{bmatrix} DP1 \\ DP2 \\ DP3 \end{bmatrix}$$

Fig. 3. An example of an uncoupled design.

The next best situation is when the design matrix is a lower-triangular matrix. The idea is to finalize the first DPs before moving on to the later DPs. Thus, DP_i can be adjusted without affected FR_1 through FR_{i-1} . This is referred to as a *decoupled* design, which is demonstrated in Fig. 4. Although decoupled designs do not completely adhere to the independence axiom, they may be reasonable compromises in designs that address complex problems.

$$\begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X & 0 & 0 \\ X & X & 0 \\ X & X & X \end{bmatrix} \begin{bmatrix} DP1 \\ DP2 \\ DP3 \end{bmatrix}$$

Fig. 4. An example of a decoupled design.

The worst solution is a non-triangular matrix, where every change in a DP affects multiple FRs in an unconstrained fashion. This is referred to as a *coupled* design, which is demonstrated in Fig. 5. Coupled designs are in complete violation of the independence axiom and generally should be decoupled by reworking the FRs or by adding additional DPs.

$$\begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X & X & X \\ X & X & X \\ X & X & X \end{bmatrix} \begin{bmatrix} DP1 \\ DP2 \\ DP3 \end{bmatrix}$$

Fig. 5. An example of a coupled design.

Unfortunately, adding additional DPs runs counter to the second axiom: the information axiom [2].

Axiom 2 (The Information Axiom). *The best design is a functionally uncoupled design that has the minimum information content.*

The amount of *information* contained in a particular DP is inversely related to the probability that the DP can successfully satisfy its corresponding FR(s) by Equation 2.

$$I = \log_2\left(\frac{1}{p}\right) \tag{2}$$

where p is the probability of success and I is measured in bits. This probability must take into consideration such things as tolerances, ease of manufacture, and failure rates. The information content of a design is then the sum of the information content of its individual DPs.

From these two axioms come the following seven corollaries [2]:

Corollary 1. Decouple or separate parts or aspects of a solution if the FRs are coupled or become interdependent in the designs proposed.

Corollary 2. *Minimize the number of FRs.*

Corollary 3. Integrate design features in a single physical part if FRs can be independently satisfied in the proposed solution.

Corollary 4. Use standardized or interchangeable parts if the use of these parts is consistent with the FRs.

Corollary 5. Use symmetrical shapes and/or arrangements if they are consistent with the FRs.

Corollary 6. *Specify the largest allowable tolerance in stating FRs.*

Corollary 7. Seek an uncoupled design that requires less information than coupled designs in satisfying a set of FRs.

The theorems that arise from these axioms and corollaries are used to prove that an optimal design results from a square design matrix. In other words, the number of FRs should be equal to the number of DPs. First, consider the case where there are more FRs than DPs. This forces a single DP to be mapped to multiple FRs. Otherwise, some FRs cannot be satisfied by the DPs. This result is stated in Theorem 1 [2].

Theorem 1. When the number of DPs is less that the number of FRs, either a coupled design results or the FRs cannot be satisfied.

A possible solution to this problem is given by Theorem 2 [2].

Theorem 2. A coupled design due to more FRs than DPs can be decoupled by adding new DPs if the additional DPs result in a lower triangular design matrix.

An example is show in Fig. 6. Note that the addition of DP3 results in a decoupled design.

$$\begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X & 0 \\ X & X \\ X & X \end{bmatrix} \begin{bmatrix} DP1 \\ DP2 \end{bmatrix} \implies \begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X & 0 & 0 \\ X & X & 0 \\ X & X & X \end{bmatrix} \begin{bmatrix} DP1 \\ DP2 \\ DP3 \end{bmatrix}$$

Fig. 6. Decoupling a design by adding DPs.

Next, consider the case where the number of FRs is less than the number of DPs. Assuming that the design is not coupled, this means that either a DP exists that does not address any FRs or multiple DPs exist that address a single FR and hence can be integrated into a single DP. Such a design is called a *redundant* design. This is addressed by Theorem 3 [2].

Theorem 3. When there are less FRs than DPs then the design is either coupled or redundant.

Finally, the previous three theorems lead to the conclusion in Theorem 4 [2].

Theorem 4. In an ideal design, the number of FRs is equal to the number of DPs.

1.4 Part Consolidation

One particularly important design parameter is the number of parts in a product design. According to Professor Suh:

Poorly designed products often cost more because they use more materials or parts than do well-designed products. They are often difficult to manufacture and maintain [2].

Decreasing the number of parts in a design while maintaining the independence of the FRs is consistent with Corollary 3 and lowers the information content of the design. In fact, Tang, et al. [7] describe how part consolidation reduces the weight and complexity of a final product while boosting reliability and reducing cost.

An informative example of part consolidation is the combination can/bottle opener shown in Fig. 7. The design of this handy utensil has two FRs, shown in Table 1. Both FRs are consolidated into a single part, yet remain independent as long as there is no desire to open a can and a bottle simultaneously (although that would be a popular trick around a campfire).

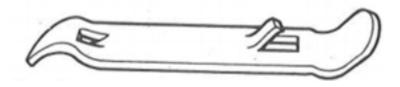


Fig. 7. A part consolidation example.

Table 1
Opener Functional Requirements

FR1	Open beverage cans
FR2	Open beverage bottles

The goal of this research is to provide designers with a tool that they can use to determine the minimum number of parts required to realize a particular design at a particular level in a FR/DP hierarchy. The designer is required to construct a graph whose vertices are the FRs and whose edges indicate that the endpoint FRs need to be realized by separate parts due to various design constraints. How these edges are actually determined is beyond the scope of this research. Adjacent FRs are candidates for part consolidation. The goal is to find the chromatic number of the resulting graph, which corresponds to the minimum number of parts required for the candidate design.

To be a viable tool, a computer program must be able to deliver an answer in a reasonable amount of time. Unfortunately, finding the chromatic number of a graph is known to be an NP-hard problem [8] and so the time required to find a solution grows exponentially with the number of vertices in the graph. Thus, this research proposes an algorithm that can be run on a computer and provides a designer with an answer in a reasonable amount of time that is hopefully shorter than other well-known algorithms. Designs with different minimum part requirements can then be compared during the analytical process phase of the axiomatic design as part of the overall process of selecting the best design.

2 GRAPH THEORY

This section presents the concepts, definitions, and theorems from the field of graph theory that are needed in the development of the proposed algorithm. This material is primarily taken from the undergraduate graph theory text by Chartrand and Zhang (2012) [9] and the graduate graph theory text by West (2001) [10].

2.1 Simple Graphs

The problem of part consolidation is best served by a class of graphs called *simple graphs*. A *simple graph* is a mathematical object represented by an ordered pair G = (V, E) consisting of a finite and non-empty set of *vertices* (also called *nodes*): V(G), and a finite and possibly empty set of edges: E(G). Each edge is represented by a two-element subset of V(G) called the *endpoints* of the edge: $E(G) \subseteq \mathscr{P}_2(V(G))$. For the remainder of this work, the use of the term "graph" implies a "simple graph." Thus, a part consolidation problem can be represented by a graph whose vertices are the functional requirements (FRs) of the design and whose edges indicate which endpoint FRs should never be combined into a single part.

The choice of two-element subsets of V(G) for the edges has certain ramifications that are indeed characteristics that differentiate a simple graph from other classes of graphs:

- 1) Every two vertices of a graph are the endpoints of at most one edge; there are no so-called *multiple* edges between two vertices.
- 2) The two endpoint vertices of an edge are always distinct; there are no so-called *loop* edges on a single vertex.
- 3) The two endpoint vertices are unordered, suggesting that an edge provides a bidirectional connection between its endpoint vertices.

When referring to the edges in a graph, the common notation of juxtaposition of the vertices will be used instead of the set syntax. Thus, edge $\{u,v\}$ is simply referred to as uv or vu.

Graphs are often portrayed visually using labeled or filled circles for the vertices and lines for the edges such that each edge line is drawn between its two endpoint vertices. An example graph is shown in Fig. 8.



Fig. 8. An example graph (labeled and unlabeled).

When two vertices are the endpoints of the same edge, the vertices are said to be *adjacent* or are called *neighbors*, and the edge is said to *join* its two endpoint vertices. Furthermore, an edge is said to be *incident* to its endpoint vertices. In the example graph of Fig. 8, vertex a is adjacent to vertices b, d, and e; however, it is not adjacent to vertex c.

As demonstrated by vertex c in Fig. 8, there is no requirement that every vertex in a graph be an endpoint for some edge. In fact, a vertex that is not incident to any edge is called an *isolated* vertex.

We can also speak of adjacent edges, which are edges that share exactly one endpoint. Note that two edges cannot share both of their endpoints — otherwise they would be multiple edges, which are not allowed in simple graphs. In the example graph of Fig. 8, edge *ab* is adjacent to edges *ad* and *ae* via common vertex *a*, and *be* via common vertex *b*.

2.2 Order and Size

Two of the most important characteristics of a graph are its *order* and its *size*. The *order* of a graph G, denoted by n(G) or just n when G is unambiguous, is the number of vertices in G: n = |V(G)|. The *size* of a graph G, denoted by m(G) or just m when G is unambiguous, is the number of edges in G: m = |E(G)|. In the example graph of Fig. 8: n = 5 and m = 4.

Since every two vertices can have at most one edge between them, the number of edges has an upper bound:

Theorem 5. Let G be a graph of order n and size m:

$$m \le \frac{n(n-1)}{2}$$

Proof. Since each pair of distinct vertices in V(G) can have zero or one edges joining them, the maximum number of possible edges is $\binom{n}{2}$, and so:

$$m \le \binom{n}{2} = \frac{n!}{2!(n-2)!} = \frac{n(n-1)}{2}$$

Some choices of graph order and size lead to certain degenerate cases that serve as important termination cases for the proposed algorithm:

- The *null* graph is the non-graph with no vertices (n = m = 0).
- The *trivial* graph is the graph with exactly one vertex and no edges (n = 1, m = 0). Otherwise (n > 1), a graph is called *non-trivial*.
- An *empty* graph is a graph containing no edges (m = 0).
- A *complete* graph is a graph containing every possible edge $\left(m = \frac{n(n-1)}{2}\right)$. Note that both the null and trivial graphs are empty.

2.3 Graph Relations

In addition to its vertices and edges, a graph may be associated with one or more relations. Each relation has V(G) or E(G) as its domain and is used to associate vertices or edges with problem-specific attributes such as labels or colors. Note that there are no particular limitations on the nature of such relations — everything from a basic relation to a bijective function are possible. Some authors include these relations and their codomains as part of the graph tuple; however, since these extra tuple elements don't affect the structure of a graph, we will not do so.

In practice, when a graph theory problem requires a particular vertex or edge attribute, the presence of some corresponding relation \mathcal{R} is assumed and we say something like, "vertex v has attribute a," instead of the more formal, "vertex v has attribute $\mathcal{R}(v)$."

The following sections describe the two relations used by the proposed algorithm.

2.3.1 *Labels*

One possible relation associated with a graph G is a bijective function $\ell: V(G) \to L$ that assigns to each vertex a unique identifying label. The codomain L is the set of available labels. When such a function is present, the graph is said to be a *labeled* graph and the vertices are considered to be distinct. Otherwise, a graph is said to be *unlabeled* and the vertices are considered to be identical (only the structure of the graph matters).

The vertices in a labeled graph are typically drawn as open circles containing the corresponding labels, whereas the vertices in an unlabeled graph are typically drawn as filled circles. This is demonstrated in the example graph of Fig. 8: the graph on the left is labeled and the graph on the right is unlabeled.

Since the labeling function ℓ is bijective, a vertex $v \in V(G)$ with label "a" can be identified by v or $\ell^{-1}(a)$. In practice, the presence of a labeling function is assumed for a labeled graph and so a vertex is freely identified by its label. This is important to note when a proof includes a phrase such as, "let $v \in V(G)$..." since v may be a reference to

any vertex in V(G) or may call out a specific vertex by its label; the intention is usually clear from the context.

The design graphs that act as the inputs to the proposed algorithm are labeled graphs, where the labels represent the various functional requirements: $FR_1, FR_2, FR_3, \dots, FR_n$.

2.3.2 Vertex Color

Other graph theory problems require that a graph's vertices be distributed into some number of sets based on some problem-specific criteria. Usually, this distribution is a true partition (no empty sets), but this is not required depending on the problem. One popular method of performing this distribution on a graph G is by using a *coloring* function $c:V(G) \to C$, where C is a set of *colors*. Vertices with the same color are assigned to the same set in the distribution. Although the elements of C are usually actual colors (red, green, blue, etc.), a graph coloring problem is free to select any value type for the color attribute. Note that there is no assumption that c is surjective, so the codomain C may contain unused colors, which correspond to empty sets in the distribution.

A coloring $c:V(G)\to C$ on a graph G is called *proper* when no two adjacent vertices in G are assigned the same color: for all $u,v\in V(G)$, if $uv\in E(G)$ then $c(u)\neq c(v)$. Otherwise, c is called *improper*. A proper coloring with |C|=k is called a k-coloring of G and G is said to be k-colorable, meaning the actual coloring (range of c) uses c0 uses c1 colors.

An example of a 4-coloring is shown in Fig. 9.



$$c(a) =$$
green $c(b) =$ blue

 $C = \{\text{green}, \text{blue}, \text{red}, \text{orange}\}$

$$c(c) = green$$

$$c(d) =$$
orange

$$c(e) = \text{red}$$

Fig. 9. A graph with a 4-coloring.

Since there is no requirement that a coloring c be surjective, the codomain C may contain unused colors. For example, the coloring shown in Fig. 9 is surjective, but we can add an unused color to C:

$$C = \{\text{green}, \text{blue}, \text{red}, \text{orange}, \text{brown}\}$$

Now, c is no longer surjective, and according to the definition, G is 5-colorable — the coloring c uses at most 5 colors (actually only 4), which is the cardinality of the codomain. This fact is generalized by Theorem 6.

Theorem 6. Let G be a graph and let $r \in \mathbb{N}$. If G is k-colorable then G is (k+r)-colorable.

Proof. Although this conclusion is fairly intuitive, it is always best to construct a proper coloring function under the given conditions so that the result is based on the definition. So start by assuming that G is of order n and is k-colorable. This means that there exists a coloring function $c:V(G)\to C$ that is proper with |C|=k. Let $V(G)=\{v_1,\ldots,v_n\}$ and let $C=\{c_1,\cdots,c_k\}$. Now, let $C'=\{c_1,\cdots,c_{k+r}\}$ and define $c':V(G)\to C'$ by:

$$c'(v) = c(v)$$

Assume that u and v are two nonadjacent vertices in G: $uv \notin E(G)$. Since c is proper:

$$c'(u) = c(u) \neq c(v) = c'(v)$$

and so c' is proper with |C'| = k + r.

Therefore, G is k+r-colorable.

Furthermore, for a graph G of order n, if $n \le k$ then we can conclude that G is k-colorable, since there are sufficient colors to assign each vertex its own unique color. This result is stated in Theorem 7, which will turn out to be an important termination case for the proposed algorithm.

Theorem 7. Let G be a graph of order n and let $k \in \mathbb{N}$. If $n \le k$ then G is k-colorable.

Proof. Assume $n \le k$. Let $V(G) = \{v_1, \dots, v_n\}$ and let $C = \{c_1, \dots, c_k\}$. Now, define $c: V(G) \to C$ by:

$$c(v_i) = c_i$$

which is possible since, by assumption, $n \le k$. Finally, assume that v_i and v_j are two nonadjacent vertices in G: $v_i v_j \notin E(G)$. Since the c_i are distinct:

$$c(v_i) = c_i \neq c_j = c(v_j)$$

and so c is proper with |C| = k.

Therefore, *G* is *k*-colorable.

Since $k \in \mathbb{N}$, by the well-ordering principle there exists some minimum k such that a graph G is k-colorable. This minimum k is called the *chromatic number* of G, denoted by $\chi(G)$. A k-coloring for a graph G where $k = \chi(G)$ is called a k-chromatic coloring of G.

Returning to the example 4-coloring of Fig. 9, note that vertex d can be colored blue and then orange can be excluded from the codomain, resulting in a 3-coloring. This is

shown in Fig. 10. Since there is no way to use less than 3 colors to obtain a proper coloring of the graph, the coloring is 3-chromatic. Note that when a coloring is chromatic, there are no unused colors (empty sets) and hence the distribution is a true partition.



Fig. 10. A Graph with a 3-chromatic coloring.

2.4 Subgraphs

The basic strategy of the proposed algorithm is to arrive at a solution by mutating an input graph into simpler graphs such that a solution is more easily determined. The algorithm utilizes three particular mutators: vertex deletion, edge addition, and vertex contraction. Before describing these mutators, it will be helpful to describe what is meant by graph equality and a *subgraph* of a graph.

To say that graph G is equal to graph H, denoted by G = H, means that the exact same graph is given two names: G and H. It is specifically not a comparison between two different graphs. Two different graphs that have the same structure, meaning there exists an adjacency-preserving bijection between the vertices of the two graphs, are referred to as being isomorphic, denoted by $G \cong H$, and are not considered to be equal. Of course, if G = H then $G \cong H$; however, the converse is usually not true. In fact, G = H if and only if V(G) = V(H) and E(G) = E(H).

To say that H is a subgraph of a graph G, denoted by $H \subseteq G$, means that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. Thus, H can be achieved by removing zero or more vertices and/or edges from G, and G can be achieved by adding zero or more vertices and/or edges to H. Once again, H is not a different graph. If H is a different graph then one can say that it is isomorphic to a subgraph of G, but not a subgraph of G itself. By definition, $G \subseteq G$ and the null graph is a subgraph of every graph.

When G and H differ by at least one vertex or edge then H is called a *proper* subgraph of G, denoted by $H \subset G$. In fact, $H \subset G$ if and only if $H \subseteq G$ but $H \neq G$, meaning $V(H) \subset V(G)$ or $E(H) \subset E(G)$. When H and G differ by edges only: V(H) = V(G) and $E(H) \subseteq E(G)$, then H is called a $spanning \ subgraph$ of G.

The concept of subgraphs is demonstrated by graphs G, H, and F in Fig. 11. H is a proper subgraph of G by removing vertices c and d and edges ad and be. F is a proper spanning subgraph of G because F contains all of the vertices in G but is missing edges ab and be.



Fig. 11. Subgraph examples.

An *induced* subgraph is a special type of subgraph. Let G be a graph and let $S \subseteq V(G)$. The subgraph of G induced by S, denoted by G[S], is a subgraph H such that V(H) = S and for every $u, v \in S$, if u and v are adjacent in G then they are also adjacent in G. Such a subgraph G is called an *induced subgraph* of G.

In the examples of Fig. 11, H is not an induced subgraph of G because it is missing edge be. Likewise, a proper spanning subgraph like F can never be induced due to missing edges. In fact, the only induced spanning subgraph of a graph is the graph itself. Fig. 12 adds edge be so that H is now an induced subgraph of G.



Fig. 12. An induced subgraph example.

2.5 Mutators

The following sections describe the graph mutators used by the proposed algorithm.

2.5.1 Vertex Removal

Let G be a graph and let $S \subseteq V(G)$. The induced subgraph obtained by removing all of the vertices in S (and their incident edges) is denoted by:

$$G - S = G[V(G) - S]$$

If $S \neq \emptyset$ then G - S is a proper subgraph of G. If S = V(G) then the result is the null graph.

Fig. 13 shows an example of vertex removal: vertices c and e are removed, along with their incident edges ae and be.



Fig. 13. A vertex removal example.

If S consists of a single vertex v then the alternate syntax G - v is used instead of $G - \{v\}$.

The proposed algorithm uses vertex removal to simplify a graph that is assumed to be *k*-colorable into a smaller graph that is also *k*-colorable.

2.5.2 Edge Addition

Let G be a graph and let $u, v \in V(G)$ such that $uv \notin E(G)$. The graph G + uv is the graph with the same vertices as G and with edge set $E(G) \cup \{uv\}$. Note that G is a proper spanning subgraph of G + uv.

Fig. 14 shows an example of edge addition: edge cd is added.



Fig. 14. An edge addition example.

The proposed algorithm uses edge addition to prevent two non-adjacent FRs from being consolidated into the same part.

2.5.3 Edge Removal

The proposed algorithm does not use edge removal; however, a number of related algorithms do rely on this mutator so it is presented here. Let G be a graph and let $X \subseteq E(G)$. The spanning subgraph obtained by removing all of the edges in X is denoted by:

$$G - X = H(V(G), E(G) - X)$$

Thus, only edges are removed — no vertices are removed. If $X \neq \emptyset$ then G - X is a proper subgraph of G. If X = E(G) then the result is an empty graph.

Fig. 15 shows an example of edge removal: edges ae and be are removed.



Fig. 15. An Edge removal example.

If X consists of a single edge e then the alternate syntax G - e is used instead of $G - \{e\}$.

2.5.4 Vertex Contraction

Vertex contraction is a bit different because it does not involve subgraphs. Let G be a graph and let $u, v \in V(G)$. The graph $G \cdot uv$ is constructed by identifying u and v as one vertex (i.e., merging them). Any edge between the two vertices is discarded. Any other edges that were incident to the two vertices become incident to the new single vertex. Note that this may require supression of multiple edges to preserve the nature of a simple graph.

Fig. 16 shows an example of vertex contraction: vertices a and b are contracted into a single vertex. Since edges ae and be would result in multiple edges between a and e, one of the edges is discarded. Edges bc and bd also become incident to the single vertex.



Fig. 16. A vertex contraction example.

For the operation $G \cdot uv$, if $uv \in E(G)$ then the operation is also referred to as *edge* contraction. If $uv \notin E(G)$ then the operation is also referred to as *vertex identification*. The proposed algorithm uses vertex identification to consolidate two non-adjacent FRs into the same part.

2.5.5 Graph Complement

One final important graph mutator is the *complement* of a graph. For a graph G, the *complement* of G, denoted by \bar{G} , is the graph with the same vertex set as G:

 $V(G)=V(\bar{G}),$ and with edge set $E(\bar{G})=\mathscr{P}_2(V(G))-E(G);$ if $u,v\in G$ are adjacent in G $(uv\in E(G))$ then they are not adjacent in \bar{G} $(uv\notin E(\bar{G})).$

An example of a graph complement operation is shown in Fig. 17.



Fig. 17. A graph complement example.

Some important properties of the complement of a graph are stated in Proposition 1.

Proposition 1. Let G be a graph of order n and size m:

- 1) $\bar{\bar{G}} = G$
- 2) G is empty if and only if \bar{G} is complete.
- 3) $n(\bar{G}) = n$
- 4) $m(\bar{G}) = \frac{n(n-1)}{2} m$

For example, in Fig. 17, since n(G) = 4 and m(G) = 3, it is the case that $n(\bar{G}) = 4$ and:

$$m(\bar{G}) = \frac{4(4-1)}{2} - 3 = 6 - 3 = 3$$

2.6 Independent Sets

The primary purpose of a k-coloring of a graph G is to distribute the vertices of G into k so-called *independent* (some possibly empty) sets. For a graph G, an *independent* set $S \subseteq V(G)$, sometimes called a *stable* set, is a set of pairwise non-adjacent vertices in G: for all $u, v \in S$, $uv \notin E(G)$. By definition, the empty set is an independent set of every graph G. A *maximal* independent set of a graph G, sometimes referred to as a MIS of G, is an independent set of G that cannot be extended by an additional vertex in G. MISs of G are never proper subsets of other independent sets in G. The cardinality of the largest possible MIS in a graph G, denoted by G, is called the *independence number* for G.

Consider the example in Fig. 18. Although the graph contains independent sets of sizes 1 and 2, none of these are maximal. All of the maximal independent sets are of sizes 3 and 4, and so $\alpha(G) = 4$.

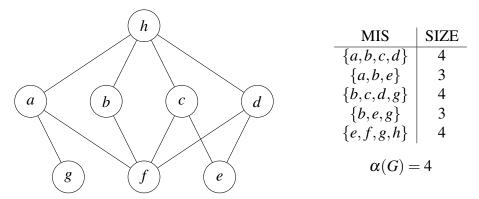


Fig. 18. The independent sets of an example graph.

Since a k-chromatic coloring of a graph G is surjective, there are no unused colors (empty sets) and so the coloring partitions the vertices of G into exactly k non-empty independent sets. The goal of the proposed algorithm is to find a chromatic coloring of a design graph so that the resulting independent sets indicate how to consolidate the FRs into a minimum number of parts: one part per independent set.

2.7 Cliques

A *clique* is a complete subgraph of a graph. A clique of order k in a graph G is called a k-clique of G. A *maximal* clique in a graph G is a clique in G that cannot be extended by an additional vertex in V(G); maximal cliques in G are never proper subgraphs of other cliques in G. The order of the largest possible maximal clique in a graph G, denoted by $\omega(G)$, is called the *clique number* for G.

Consider the example in Fig. 19. Although the graph contains cliques of orders 1 and 2, none of these are maximal. All of the maximal cliques are of orders 3 and 4, and so $\omega(G) = 4$.



Fig. 19. The maximal cliques of an example graph.

Since it is true that two nonadjacent vertices in a graph must be adjacent in the graph's complement, there is an important relationship between the independent sets of a graph and the cliques in the graph's complement. This relationship is stated in Theorem 8.

Theorem 8. Let G be a graph and let $S \subseteq V(G)$. S is an independent set in G if and only if $\bar{G}[S]$ is a clique in \bar{G} . Furthermore, S is maximal in G if and only if $\bar{G}[S]$ is maximal in \bar{G} and so $\alpha(G) = \omega(\bar{G})$.

Proof. By definition, for all $u, v \in V(G)$, u is not adjacent to v in G if and only if u and v are adjacent in \bar{G} , and so G[S] is empty if and only if $\bar{G}[S]$ is complete. Therefore, S is an independent set in G if and only if $\bar{G}[S]$ is a clique in \bar{G} .

Furthermore, assume that S is maximal in G but assume by way of contradiction that $\bar{G}[S]$ is not maximal. Then there exists $v \in V(\bar{G})$ such that $v \notin S$ and $\bar{G}[S \cup \{v\}]$ is a clique in \bar{G} , and thus $S \cup \{v\}$ is an independent set in G. But $S \subset S \cup \{v\}$, violating the maximality of S. Therefore $\bar{G}[S]$ is maximal in \bar{G} .

Similarly, assume that $\bar{G}[S]$ is maximal in \bar{G} but assume by way of contradiction that S is not maximal in G. Then there exists $v \in V(G)$ such that $v \notin S$ and $S \cup \{v\}$ is an independent set in G, and thus $\bar{G}[S \cup \{v\}]$ is a clique in \bar{G} . But $\bar{G}[S] \subset \bar{G}[S \cup \{v\}]$, violating the maximality of $\bar{G}[S]$. Therefore S is maximal in G.

Indeed, the graphs in Fig. 18 and Fig. 19 are complements and, as expected, every MIS in Fig. 18 is a maximal clique in Fig. 19.

Since a k-clique of a graph G needs at least k colors in any proper coloring of G, the clique number of G provides a nice lower bound for the chromatic number of G. Unfortunately, the clique number problem is known to be NP-hard as well [11]. Thus, there are many attempts in the literature to find a good lower bound for the clique number of a graph G, usually denoted by $\omega'(G)$. If such a lower bound is known then the conclusion of Proposition 2 holds:

Proposition 2. Let G be a graph with clique number lower bound $\omega'(G)$:

$$\omega'(G) \leq \omega(G) \leq \chi(G)$$

2.8 Connected Graphs

The edges of a graph suggest the ability to "walk" from one vertex to another along the edges. A graph where this is possible for any two vertices is called a *connected* graph. The concept of connectedness is an important topic in graph theory; however, an ideal coloring algorithm should work regardless of the connected nature of an input graph. The concept of connectedness and how it impacts coloring is described in this section.

2.8.1 Walks

The undirected edges in a simple graph suggest bidirectional connectivity between their endpoint vertices. This leads to the idea of "traveling" between two vertices in a graph by following the edges joining intermediate adjacent vertices. Such a journey is referred to as a *walk*.

A u-v walk W in a graph G is a finite sequence of vertices $w_i \in V(G)$ starting with $u=w_0$ and ending with $v=w_k$:

$$W = (u = w_0, w_1, \dots, w_k = v)$$

such that $w_i w_{i+1} \in E(G)$ for $0 \le i < k$. To say that W is *open* means that $u \ne v$. To say that W is *closed* means that u = v. The *length* k of W is the number of edges traversed: k = |W|. A *trivial* walk is a walk of zero length — i.e, a single vertex: W = (u).

The bidirectional nature of the edges in a simple graph suggests the following proposition:

Proposition 3. Let G be a graph and let u - v be a walk of length k in G. G contains a v - u walk of length k in G by traversing u - v in the opposite direction.

An example of two walks of length 4 is shown in Fig. 20. W_1 is an open walk because it starts and ends on distinct vertices, whereas W_2 is a closed walk because it starts and ends on the same vertex.



Fig. 20. Open and closed walks.

Vertices and edges are allowed to be repeated during a walk. Certain special walks can be defined by restricting such repeats:

trail An open walk with no repeating edges (a,b,c,a,e)path A trail with no repeating vertices (a,e,b,c)circuit A closed trail (a,b,e,a,c,d,a)cycle A closed path (a,e,b,c,a)

The example special walks stated above refer to the graph in Fig. 20.

2.8.2 *Paths*

When discussing the connectedness of a graph, the main concern is the existence of paths between vertices. Let G be a graph and let $u, v \in V(G)$. To say that u and v are connected means that G contains a u-v path.

But if there exists a u-v walk in a graph G, does this also mean that there exists a u-v path in G — i.e. a walk with no repeating edges or vertices? The answer is yes, as shown by the following theorem:

Theorem 9. Let G be a graph and let $u, v \in V(G)$. If G contains a u - v walk of length k then G contains a u - v path of length $\ell \le k$.

Proof. Assume that G contains at least one u-v walk of length k and consider the set of all possible u-v walks in G; their lengths form a non-empty set of positive integers. By the well-ordering principle, there exists a u-v walk P of minimum length $\ell \le k$:

$$P = (u = w_0, \dots, w_\ell = v)$$

We claim that *P* is a path.

Assume by way of contradiction that P is not a path, and thus P has at least one repeating vertex. Let $w_i = w_j$ for some $0 \le i < j \le \ell$ be such a repeating vertex. There are two possibilities:

Case 1: The walk ends on a repeated vertex $(j = \ell)$. This is demonstrated in Fig. 21.



Fig. 21. Repeated vertex at end case.

Let $P' = (u = w_0, w_1, \dots, w_i = v)$ be the walk shown in green in Fig. 21. P' is a u - v walk of length $i < \ell$ in G.

Case 2: A repeated vertex occurs inside the walk $(j < \ell)$. This is demonstrated in Fig. 22.



Fig. 22. Repeated vertex inside case.

Let $P' = (u = w_0, w_1, \dots, w_i, w_{j+1}, \dots, w_\ell = v)$ be the walk shown in green in the Fig. 22. P' is a u - v walk of length $\ell - (j - i) < \ell$ in G.

Both cases contradict the minimality of the length of *P*.

$$\therefore P \text{ is a } u - v \text{ path of length } \ell \leq k \text{ in } G.$$

2.8.3 Connected

A connected graph G is a graph whose vertices are all connected: for all $u, v \in V(G)$ there exists a u - v path. Otherwise, G is said to be disconnected. Examples of connected and disconnected graphs are shown in figure 23.



COLVICECTER

Fig. 23. Connected and disconnected graphs.

By definition, the trivial graph is connected since the single vertex is connected to itself by a trivial path (of length 0).

2.8.4 Components

It would seem that a disconnected graph is composed of some number of connected subgraphs that partition the graph's vertex set under a connected equivalence relation.

Each such subgraph is called a *component* of the graph.

Let G be a graph and let $\mathscr G$ be the set of all connected subgraphs of G. To say that a graph $H \in \mathscr G$ is a *component* of a G means that H is not a subgraph of any other connected subgraph of $\mathscr G$: for every $F \in \mathscr G - \{H\}$ it is the case that $H \not\subset F$. The number of distinct components in G is denoted by k(G), or just k if G is unambiguous. For a connected graph: k(G) = 1.

Each component of a graph G is denoted by G_i where $1 \le i \le k(G)$. We also use union notation to denote that G is composed of its component parts:

$$G = \bigcup_{0 \le i \le k(G)} G_i$$

Furthermore the G_i are induced by the vertex equivalence classes of the connectedness relation:

Theorem 10. Let G be a graph with component G_i . G_i is an induced subgraph of G.

Proof. By definition, G_i is a maximal connected subgraph of G. So assume by way of contradiction that G_i is not an induced subgraph of G. Thus, G_i is missing some edges that when added would result in a connected induced subgraph H of G. But then $G_i \subset H$, contradicting the maximality of G_i .

$$\therefore G_i$$
 is an induced subgraph of G .

2.8.5 Impact on Coloring

The impact of disconnectedness on coloring depends on the selected algorithm. One might assume that the selected algorithm should be run on each component individually in order to determine each $\chi(G_i)$ and then, as pointed out by Zykov (1949) [12], conclude that the maximum such value is sufficient for $\chi(G)$:

$$\chi(G) = \max_{1 \leq i \leq k(G)} \chi(G_i)$$

For example, consider the disconnected graph in Fig. 23. The graph contains two components, so number the components from left-to-right:

$$\chi(G_1)=3$$

$$\chi(G_2)=2$$

$$\chi(G) = \max\{3, 2\} = 3$$

Using this technique requires application of an initial algorithm to partition the graph into components. Such an algorithm is well-known and is described by Hopcroft and Tarjan (1973) [13]. The algorithm is recursive. It starts by pushing a randomly selected

vertex on the stack and walking the vertex's incident edges, removing each edge as it is traversed. As each unmarked vertex is encountered, it is assigned to the current component. Vertices with incident edges are pushed onto the stack and newly isolated vertices are popped off the stack. Once the stack is empty, any previously unmarked vertex is selected to start the next component and the process continues until all vertices are marked. Given a graph G of order n and size m, this algorithm runs in $\max(n, m)$ steps.

Alternatively, an ideal coloring algorithm could be run on the entire graph at once regardless of the number of components in the graph. The proposed algorithm is such a solution, and therefore saves the needless work of partitioning the graph into components first.

2.9 Vertex Degree

Besides a graph's order and size, the next most important parameter is the so-called *degree* of each vertex. In order to define the degree of a vertex, we need to define what is meant by a vertex's *neighborhood* first. Let G be a graph and let $u \in V(G)$. If $v \in V(G)$ is adjacent to u then u and v are called *neighbors*. Note that for simple graphs, a vertex is never a neighbor of itself. The *neighborhood* of u, denoted by N(u), is the set of all the neighbors of u in G:

$$N(u) = \{ v \in V(G) \, | \, uv \in E(G) \}$$

The *degree* of u, denoted by $\deg_G(u)$ or just $\deg(u)$ if G is unambiguous, is then defined to be the cardinality of its neighborhood: $\deg(u) = |N(u)|$. Thus, the degree of a vertex can be viewed as the number of neighbor vertices or the number of incident edges.

When considering the degrees of all the vertices in a graph, the following limits are helpful:

$$\delta(G) = \min_{v \in V(G)} \deg(v)$$

$$\Delta(G) = \max_{v \in V(G)} \deg(v)$$

Therefore, we can state the conclusion of Proposition 4:

Proposition 4. Let G be a graph of order n. For every vertex $v \in G$:

$$0 \le \delta(G) \le \deg(v) \le \Delta(G) \le n - 1$$

Intuitively, as $\delta(G)$ increases, a graph becomes denser (more edges) resulting in more adjacencies, making it harder to find a proper coloring at lower values of k.

Vertices can be classified based on their degree, as shown in Table 2.

Table 2 Classifying Vertex u in Graph G

deg(u)	TYPE
0	isolated
1	pendant, end, leaf
n-1	universal
even	even
odd	odd

Isolated vertices have degree 0; they are not adjacent to any other vertex in G.

Pendant (also called end or leaf) vertices have degree 1; they are adjacent to exactly one other vertex in G. Universal vertices are adjacent to every other vertex in G. Even vertices are adjacent to an even number of vertices in G and odd vertices are adjacent to an odd number of vertices in G. Note that if G has a universal vertex then it cannot have an isolated vertex, and vice-versa.

The degrees of the vertices in a graph and the number of edges in the graph are related by the so-called First Theorem of Graph Theory:

Theorem 11 (First Theorem of Graph Theory). Let G be a graph of size m:

$$\sum_{v \in V(G)} \deg(v) = 2m$$

Proof. When summing all the degrees, each edge is counted twice: once for each endpoint.

These concepts are demonstrated by the graph in Fig. 24.



Fig. 24. Vertex degrees and the first theorem of graph theory.

2.10 Special Graphs

The following sections described some special classes of graphs that are important to the execution of the proposed algorithm.

2.10.1 Empty Graphs

An *empty* graph of order n, denoted by E_n , is a graph with one or more vertices (n > 1) and no edges (m = 0). An empty graph is connected if and only if n = 1. Examples of empty graphs are shown in Fig. 25.



Fig. 25. Empty graphs.

The null graph (n = 0) is denoted by E_0 and is defined to be 0-chromatic. All other empty graphs are 1-chromatic and thus are important termination conditions for the proposed algorithm.

2.10.2 Paths

A path graph of order n and length n-1, denoted by P_n , is a connected graph consisting of a single open path. Examples of path graphs are shown in Fig. 26.



Fig. 26. Path graphs.

Note that $P_1 = E_1$ is 1-chromatic, whereas $P_{n>1}$ is 2-chromatic.

Paths are not particularly important to the proposed algorithm; however, they are used in the definition of cycles.

2.10.3 Cycles

A *cycle* graph of order n and length n for $n \ge 3$, denoted by C_n , is a connected graph consisting of a single closed path. When n is odd then C_n is called an *odd* cycle and when n is even then n is called an *even* cycle.

Examples of cycle graphs are shown in Fig. 27.



Fig. 27. Cycle graphs.

Note that even cycles are 2-chromatic; however, odd cycles are 3-chromatic.

Cycles are not particularly important to the proposed algorithm; however, they are used in the definition of trees, which are important to the later analysis of coloring algorithms.

2.10.4 Complete Graphs

A *complete* graph of order n and size $\frac{n(n-1)}{2}$, denoted by K_n , is a connected graph that contains every possible edge: $E(G) = \mathcal{P}_2(V(G))$. Thus, all of the vertices in a complete graph are universal.

Examples of complete graphs are shown in Fig. 28.



Fig. 28. Complete graphs.

Note that $K_1 = P_1 = E_1$.

Since all of the vertices in a complete graph are adjacent to each other, each vertex requires a separate color in order to achieve a proper coloring. Thus, K_n is n-chromatic and is also an important termination condition for the proposed algorithm.

2.10.5 Trees

A *tree* is a connected graph that contains no cycles as subgraphs. Typically, one vertex of the tree is selected as the *root* vertex and then the tree is depicted in layers that contain vertices that are equidistant from the root vertex. Thus, the bottom layer is composed entirely of pendant vertices, but pendant vertices can exist in the other layers as well. Such pendant vertices are usually referred to as *leaves* in this context.

An example tree is shown in Fig. 29. The root vertex r is shown in red and the leaf vertices b, e, g, h, i, j, k are shown in green.



Fig. 29. A tree organized from root to leaves.

Trees are important because they can be used to track so-called "branch-and-bound" algorithms; each vertex represents a branch choice of the algorithm and thus a particular

state of the problem. All such states can be visited using a so-called *depth-first* walk. In the example in Fig. 29, such a depth-first walk would be:

$$(r,a,d,i,d,a,e,a,f,j,f,k,f,a,r,b,r,c,g,c,h,c,r)$$

Note that this walk guarantees that each vertex is visited at least once.

When such a tree is applied to the problem of exhaustively finding the chromatic number of a graph via a sequence of vertex contraction and edge addition choices, the tree is called a *Zykov* tree and the algorithm is called a *Zykov* algorithm [8]. Zykov algorithms are described in detail in the following sections. In fact, the proposed algorithm is a variation of a standard Zykov algorithm.

3 THE CHROMATIC NUMBER PROBLEM

The chromatic number problem is *inherently intractable*. Informally, this means that finding a solution for a given input graph, regardless of the means, can take a very, very long time in the worst cases. Thus, trying to find an efficient but exact method of solution that satisfies all cases is a fool's errand; about the best that can be done is to perform better than existing well-known methods in most cases. This section begins with a brief overview of inherent intractability and describes why the chromatic number problem is of this type. Most of this material is based on the early yet still very influential text by Garey and Johnson (1979) [14] with some help from Spiser (2013) [15]. Following the overview is an examination of some of the well-known algorithms for finding the chromatic number of a graph.

3.1 Problems

A problem consists of three parts:

- 1) A specific question to be answered.
- 2) A description of zero or more input parameters.
- 3) A statement of the properties that the *solution* is required to satisfy.

An *instance* of a problem is constructed by specifying particular values for each input parameter. The step-by-step procedure that translates the input parameters to a corresponding well-defined solution is called an *algorithm*. To say that an algorithm *solves* a problem Π means that the algorithm produces a valid solution for every possible instance I of the problem Π .

The chromatic number problem accepts a graph G and uses an algorithm to obtain a number $k \in \mathbb{N}$ where k is the minimum value such that G is k-colorable. The proposed algorithm is one such algorithm that can be used to solve the problem. Other examples are the Christofides (1971) [16] and the Corneil/Graham (1973) [11] algorithms, which are

introduced later in this section and will be compared to the proposed algorithm using random graph analysis.

3.2 Comparing Algorithms

Computation theory is the branch of computer science that is concerned with determining and comparing the runtime performance of algorithms. The history and specifics of computation theory, although interesting, are beyond the scope of this research. This section presents a brief overview of what is needed from the field of computation theory in order to characterize the chromatic number problem.

Algorithms are typically compared using three parameters:

- 1) Runtime complexity
- 2) Space complexity
- 3) Runtime duration

These parameters are discussed in the following sections.

3.2.1 Runtime Complexity

Runtime complexity measures the number of steps required to obtain a solution for the worst possible input parameter and is a function of some *length* parameter of the problem. For graph algorithms, the length parameter is usually the order of the graph, although size and structure can also affect the worst case scenario.

The runtime complexity of an algorithm is stated using the so-called big- \mathcal{O} notation: to say that an algorithm has $\mathcal{O}(f(n))$ runtime complexity means that the maximum number of steps required to obtain a solution for a given length parameter n is asymptotic to the function f(n) as $n \to \infty$. Roughly speaking, tractable problems are those problems with polynomial $\mathcal{O}(n^c)$ or better runtime complexity for some real number constant $c \ge 0$, and intractable problems are those problems with exponential $\mathcal{O}(c^{f(n)})$ or worse runtime complexity for some real number constant c > 1. Exponential problems are usually

associated with so-called *brute force* algorithms that must try all possibilities from an exponentially increasing set of candidate solutions in order to find the desired solution.

What constitutes a *step* in an algorithm is relative to the overall runtime complexity of the algorithm: any process that has significantly less runtime complexity than the runtime complexity of the whole algorithm can be called a step. For example, a process that has polynomial runtime complexity can be called a step of an algorithm that has exponential runtime complexity.

Runtime complexity is used in two different ways to compare algorithms:

- 1) What is the runtime complexity for finding a solution to a problem given a particular input parameter?
- 2) What is the runtime complexity for verifying that a given solution is in fact a solution for a given input parameter?

The two comparisons can be very different. For example, finding a k-clique in a graph G for a particular value of k has exponential runtime complexity; however, determining whether or not a given subgraph of a graph is a k-clique has polynomial runtime complexity.

These two methods of comparison are used to classify the runtime complexity of algorithms as follows:

- **P** Algorithms with polynomial or better runtime complexity to find or verify a solution.
- **NP** A superset of P with varying runtime complexity to find a solution but polynomial runtime complexity to verify a solution.
- **NP-complete** A subset of NP problems that have been proven to have the same runtime complexity to find a solution. It is an open question as to whether P = NP; however, it is conjectured that they are not equal.

NP-hard Algorithms that have been proved to have the same runtime complexity as the NP-complete problems to find a solution but varying runtime complexity to verify a solution.

The relationships between these runtime complexity classes, assuming $P \neq NP$, is shown in Fig. 30.

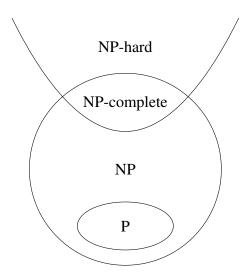


Fig. 30. The runtime complexity classes.

For the purposes of this research, the NP-complete problems are assumed to have exponential runtime complexity to find a solution and polynomial runtime complexity to verify a solution, and the NP-hard problems are assumed to have exponential runtime for both finding and verifying solutions.

The chromatic number problem is NP-hard: it requires exponential time to exhaustively generate and check all possible independent set partitions to find a partition with the smallest number of independent sets k, and the same basic procedure must be used to verify that given a supposed k-chromatic coloring, there does not exist a proper coloring for smaller k.

3.2.2 Space Complexity

Space complexity measures the maximum amount of memory required at any point in time when an algorithm is run on a computer program. The limited memory and CPU power in early computers forced algorithm designers and programmers to make careful tradeoffs between CPU cycles and the storage of intermediate results. With today's fast CPUs and practically unlimited virtual memory systems, such concerns are not as important. Thus, space complexity will not be considered when comparing the selected well-known algorithms to the proposed algorithm.

3.2.3 Runtime Duration

Runtime duration is an empirical measurement of how long an algorithm runs on a given computer, usually on best, average, and worst-case input parameter values. Determining the runtime complexity for some algorithms can be very complicated when the number of possible steps is dependent on the peculiarities of the input parameters. In the case of graph algorithms, such things as order, size, and edge density can all affect the number of steps. Furthermore, runtime complexity is geared towards theoretical comparisons between algorithms, not actual runtime of an algorithm implementation on a given computer. Thus, an important part of this research is a random graph analysis of several well-known algorithms and the proposed algorithm.

3.3 Estimating the Chromatic Number of a Graph

Since the chromatic number problem is NP-hard, an alternative to finding an exact answer is to find lower and upper bounds for the actual value. If these bounds happen to match then they provide the actual chromatic number. The following sections describe well-known methods for finding the upper and lower bounds for the chromatic number of a graph.

3.3.1 Chromatic Number Lower Bound

3.3.2 Chromatic Number Upper Bound

3.4 The Christofides Algorithm

3.5 Zykov Algorithms

An exhaustive, exponential-time algorithm for determining the chromatic number of a graph is derived from a nondeterministic Turing machine technique attributed to Ukranian graph theorist Alexandre A. Zykov (1922–2013) [17].



Fig. 31. V.G Vizing (L), A.A. Zykov (C), and V.I. Voloshin (R) in Odessa (2001) [1]

3.5.1 The Chromatic Polynomial

In his 1949 paper (translated by the AMS in 1952) [12], Zykov addresses the question: given a graph G and a number $k \in \mathbb{N}$, how many ways are there to properly color G using at most k colors? In fact, he is not particularly concerned about the chromatic number,

which he calls the *rank*, of a graph. To solve this problem, Zykov notes that in any proper coloring of a graph:

- 1) Nonadjacent vertices have either the same color or different colors.
- 2) Adjacent vertices always have different colors.

If nonadjacent vertices have the same color then they can be contracted and the resulting graph retains the same k-coloring as the original graph. This is demonstrated in Figure 3.6.1.

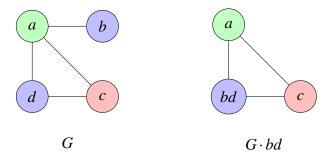


Fig. 32. Same Colors with Vertex Contraction

If nonadjacent vertices have different colors then they can be joined by an edge and the resulting graph retains the same k-coloring as the original graph. This is demonstrated in Figure 3.6.1.

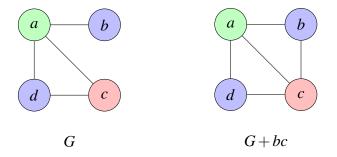


Fig. 33. Different Colors with Edge Addition

By applying these steps recursively, all of the possible distributions of the nonadjacent nodes to independent sets are generated. The termination condition for each recursive path is a complete graph of some varying order k. Each node in the complete graph represents an independent set of nonadjacent nodes in the original graph that have been combined via vertex contraction. Thus, each complete graph of order k represents a possible k-coloring of the original graph. The complete graphs of smallest order represent chromatic colorings and their order is the chromatic number of the original graph.

Zykov uses a graph equation syntax to record the recursive processing of a graph, where each line in the equation represents the next recursive layer. Isomorphic graphs are combined with a frequency multiplier at each layer. This is demonstrated in Figure 3.6.1.

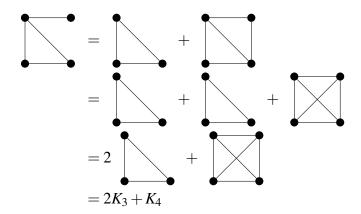


Fig. 34. Zykov Graph Equation

Determining whether two graphs are isomorphic is hard, so combining isomorphic graphs in all but the very simple cases should be skipped; the complete graphs resulting from the further processing of two isomorphic graphs will eventually be combined anyway by the end.

Zykov was trying to determine the number of k-colorings of a graph without color indifference: each permutation of colors for a particular distribution is considered unique. Thus, Zykov multiplied each complete graph coefficient in the final line of a graph equation by the number of permutations from selecting the order n of the particular

complete graph from *k* colors:

$$k^{(n)} = k(k-1)(k-2)\cdots(k-n+1)$$

Thus, the total number of unique colorings from the example shown in Figure 3.6.1 using k colors would be:

$$M(G,k) = 2k^{(3)} + k^{(4)}$$

This is known as the factorial form of the *chromatic polynomial* for the graph. The corresponding *expanded form* is:

$$M(G,k) = k^4 - 4k^3 + 5k^2 - 2k$$

Read (1968) [18] expands on the construction of the factorial form of the chromatic polynomial for a graph and proves several theorems regarding the expanded form. Some examples are:

- 1) $M(G,k) = M(G \cdot uv) + M(G + uv)$, where u and v are any two nonadjacent vertices in the current recursive step.
- 2) The degree of M(G,k) is the order of G.
- 3) The highest order coefficient is 1.
- 4) There is no constant term.
- 5) The terms alternate in sign.

In fact, Read shows that the expanded form is actually an inclusion-exclusion equation resulting from starting with all possible proper and improper colorings k^n and then subtracting the improper colorings.

3.5.2 An Exhaustive Algorithm

Corneil and Graham extend Zykov's work with the following theorem [11]:

Theorem 12 (Corneil and Graham, 1973). Let G be a graph and let u and v be two nonadjacent vertices in G:

$$\chi(G) = \min\{\chi(G \cdot uv), \chi(G + uv)\}\$$

Zykov's method combined with Theorem 12 can be used to construct an exhaustive algorithm for finding the chromatic number and a chromatic coloring for a graph G. We define S to be a first-in-first out (FIFO) stack of graphs and X to be the last found complete graph of the smallest order. Each vertex in X represents a set of contracted vertices.

- 1) Construct a graph G' that is isomorphic to G and where each vertex in G' is a list of contracted vertices initialized to a one element list containing the corresponding vertex in G.
- 2) Push G' onto S.
- 3) If S is empty then return n(X) and X.
- 4) If the graph on the top of *S* is complete:
 - a) Pop the graph off of the top of S and save it as H.
 - b) If X is not set or n(H) < n(X) then let X = H. Otherwise, discard H.
 - c) Go to step 3.
- 5) The graph on the top of S is not complete. Pop the graph off of S and save it as H.
- 6) Pick any two nonadjacent vertices u and v in H.
- 7) Push H + uv onto S.
- 8) Construct $H' = H \cdot uv$, where the contracted vertex list for the new contracted vertex is a concatenation of the lists for u and v.
- 9) Push H' onto S.
- 10) Go to step 4.

The steps of this algorithm can be tracked via a so-called *Zykov tree* [11]. The Zykov tree for the example in Figure 3.6.1 is shown in Figure 3.6.2. Note that the exhaustive algorithm corresponds to a depth-first walk of the tree.

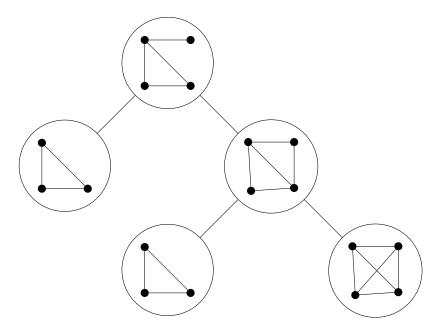


Fig. 35. A Zykov Tree

3.5.3 Branch and Bound Strategies

Using a Zykov tree suggests that the exhaustive algorithm is a candidate for a branch-and-bound solution, where the branching is accomplished via vertex contraction and edge addition and the bounding is some method to prematurely terminate a branch. Corneil and Graham suggest such a bounding technique through the determination of so-called α -clusters; however, the algorithm for finding such clusters has $\mathscr{O}(n^3)$ runtime complexity.

4 THE PROPOSED ALGORITHM

The major advantages of the Zykov and Christofides algorithms described in the previous section are that they don't depend on the connectedness of a graph, an example of a chromatic coloring is readily available, and the fact that the algorithms can be coded rather easily to run on a computer. Their major disadvantage is its their high runtime complexity, which as was shown is inherent to the chromatic number problem.

Thus, the goals of the proposed algorithm are as follows:

- 1) It should not depend on whether the graph is connected or not.
- 2) An example of a chromatic coloring should be available.
- 3) It can be easily coded for execution on a computer.
- 4) It has better runtime performance than the existing algorithms.

To accomplish these goals, the proposed algorithm loops on successively higher values of k. For each candidate k value, a graph is assumed to be k-colorable and a modified version of a Zykov algorithm is executed to either prove or disprove this assumption. Since a candidate k value is known, certain reversible steps can be applied to mutate G into simpler graphs with equivalent colorability and test for early termination of the current Zykov tree. The first k for which G (or one of its simplifications) is found to be k-colorable is the chromatic number of G.

One slight disadvantage of the proposed algorithm is that whereas the other algorithms readily provide examples of actual chromatic colorings, the proposed algorithm requires a reverse traversal of its reversible steps in order to construct such a coloring. However, as was stated earlier, it is more important during the axiomatic design analytical process to know the minimum number of parts as opposed to an actual FR allocation to those parts.

This algorithm was first proposed by the author and his advisor in collaboration with a team of mechanical engineering researchers from SUNY Buffalo [5]. It accepts a graph G as input, provides $\chi(G)$ as output, and is composed of an outer loop on values of k and a

subroutine called by the outer loop to determine if G is k-colorable. The outer loop and called subroutine are summarized in the following sections. A complete description of the theorems that support the various steps in algorithm and the application of the algorithm to a sample graph then follow.

4.1 Outer Loop

The outer loop accepts a graph G as input and returns $\chi(G)$. It initially checks for some degenerate cases and then loops on increasing values of k. For each value of k, the called subroutine executes a modified Zykov algorithm to determine if G is k-colorable. The first such successful return identifies $\chi(G)$.

The steps of the outer loop are as follows:

- 1) If n = 0 then return 0, thus handling the degenerate case of a null graph.
- 2) If m = 0 then return 1, thus handling the degenerate case of an empty graph.
- 3) Initialize *k* to 2.
- 4) Call the subroutine to determine if G is k-colorable. The subroutine returns a possibly simplified G called G' and a boolean value R that reports the result of the test.
- 5) If G is k-colorable (R = true) then return k.
- 6) Replace G with G'. As will be seen, doing this avoids needless reapplication of certain steps in the called subroutine.
- 7) Increment *k*.
- 8) Go to step 4.

A flowchart of these steps is shown in Fig. 36.

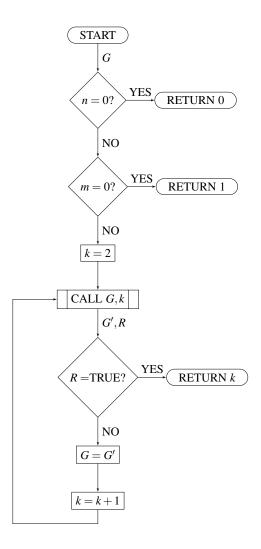


Fig. 36. Proposed algorithm outer loop.

The outer loop is guaranteed to terminate because k will eventually be greater than or equal to n. Thus, by Theorem 7, the current state of G is k-colorable, causing the called subroutine to return true.

4.2 Called Subroutine

The called subroutine executes a modified version of a Zykov algorithm that determines whether a graph is k-colorable. It accepts the current state of G of order n and size m and the current value of $k \ge 2$ as inputs. It returns a possibly simplified version of

G and a boolean value indicating whether or not G is k-colorable. Internally, various tests are applied to trim the corresponding Zykov tree or abandon it all together based on the current value of k.

The steps of the called subroutine and references to their associated theorems are as follows:

- 1) If $n \le k$ then return true (Theorem 7).
- 2) Calculate a maximum edge threshold:

$$a = \frac{n^2(k-1)}{2k}$$

- 3) If m > a then return false (Corollary 8).
- 4) Construct the set *X* of all vertices with degree less than *k*:

$$X = \{ v \in V(G) | \deg(v) < k \}$$

- 5) If $X \neq \emptyset$ then replace G with G X and go to step 1 (Corollary 9).
- 6) Calculate the common number of neighbors between each pair of vertices in *G*, stopping if one vertex's neighborhood is found to be a subset of another.
- 7) If G has vertices u and v such that $N(u) \subseteq N(v)$ then replace G with G u and go to step 1 (Theorem 15).
- 8) Let b be the smallest number of common neighbors between any pair of vertices in G as found in step 6:

$$b = \min_{u,v \in V(G)} |N(u) \cap N(v)|$$

9) Calculate an upper bound for the minimum number of common neighbors between any pair of vertices in *G*:

$$c = n - 2 - \frac{n-2}{k-1}$$

10) If b > c then return false (Corollary 10).

- 11) Select two non-adjacent vertices $u, v \in V(G)$ with the smallest number of common neighbors as found in step 6. It will be shown below that such a pair of vertices is guaranteed to exist in the current state of G.
- 12) Assume that u and v are assigned the same color by letting $G' = G \cdot uv$. Recursively call this routine to see if G' is k-colorable. If so, then return true (Theorem 17).
- 13) Assume that u and v are assigned different colors by letting G' = G + uv. Recursively call this subroutine to see if G' is k-colorable. If so, then return true (Theorem 17).
- 14) Since neither of the assumptions in steps 12 nor 13 hold, conclude that *G* is not *k*-colorable and return false.

A flowchart of these steps is shown in Fig. 37.



Fig. 37. Proposed algorithm called subroutine.

Step 1 is the success termination condition. Success occurs when G is simplified by removing sufficent vertices (steps 4–7) or when the outer loop has sufficiently incremented k (step 7) such that $n \le k$.

Steps 4–7 attempt to remove vertices to achieve a simpler graph that is equivalently k-colorable. Each time a vertex is removed, the Zykov branches associated with that vertex are skipped. Since these same steps would just be repeated for k+1, the subroutine returns the current state of the possibly simplified G to the outer loop as a starting point for the next candidate value of k.

Steps 2–3 and 8–10 apply tests that attempt to disprove that the current state of G is k-colorable for the current value of k. If so, then the current Zykov tree is abandoned and the subroutine returns false. This allows the outer loop to continue with k+1.

The remaining steps of the called subroutine, steps 11-14, constitute the recursive portion of the modified Zykov algorithm. The recursive calls are guaranteed to terminate because either there will be sufficient vertex contractions such that $n \le k$, resulting in a true return, or sufficient edge additions such that the graph becomes complete and (as will be shown) is rejected by step 3, resulting in a false return. Note that in the event of a false return, any modifications to the current state of G resulting from the recursive calls are not returned to the outer loop.

4.3 Supporting Theorems

This section contains the theorems that support the steps in the called subroutine. Remember that the success check of step 1 is already supported by Theorem 7.

4.3.1 Maximum Edge Threshold

The maximum edge threshold test of steps 2 and 3 is supported by Theorem 13.

Theorem 13 (Maximum Edge Threshold). *Let G be a graph of order n and size m and let k* $\in \mathbb{N}$. *If G is k-colorable then:*

$$m \le \frac{n^2(k-1)}{2k}$$

Proof. Assume that G is k-colorable. This means that V(G) can be distributed into k independent (some possibly empty) subsets. Call these subsets $A_1, \ldots A_k$ and let $a_i = |A_i|$. Thus, each $v \in A_i$ can be adjacent to at most $n - a_i$ other vertices in G, and hence the maximum number of edges incident to vertices in A_i is given by: $a_i(n - a_i) = na_i - a_i^2$. Now, using Theorem 11, the maximum number of edges in G is given by:

$$m \le \frac{1}{2} \sum_{i=1}^k (na_i - a_i^2)$$

with the constraint:

$$\sum_{i=1}^{k} a_i = n$$

This problem can be solved using the Lagrange multiplier technique. We start by defining:

$$F(a_1, ..., a_k) = f(a_1, ..., a_k) - \lambda g(a_1, ..., a_k)$$

$$= \frac{1}{2} \sum_{i=1}^k (na_i - a_i^2) - \lambda \sum_{i=1}^k a_i$$

$$= \sum_{i=1}^k \left(\frac{1}{2} na_i - \frac{1}{2} a_i^2 - \lambda a_i \right)$$

Now, optimize by taking the gradient and setting the resulting vector equation equal to the zero vector:

$$\nabla F = \sum_{i=1}^{k} \left(\frac{n}{2} - a_i - \lambda\right) \hat{a}_i = \mathbf{0}$$

This results in a system of *k* equations of the form:

$$\frac{n}{2} - a_i - \lambda = 0$$

And so:

$$a_i = \frac{n}{2} - \lambda$$

Plugging this result back into the contraint:

$$\sum_{i=1}^{k} a_i = \sum_{i=1}^{k} \left(\frac{n}{2} - \lambda \right) = k \left(\frac{n}{2} - \lambda \right) = n$$

Solving for λ yields:

$$\lambda = \frac{n}{2} - \frac{n}{k}$$

And finally, to get a_i in terms of n and k:

$$a_i = \frac{n}{2} - \left(\frac{n}{2} - \frac{n}{k}\right) = \frac{n}{k}$$

Therefore:

$$m \le \frac{1}{2} \sum_{i=1}^{k} \left[n \left(\frac{n}{k} \right) - \left(\frac{n}{k} \right)^2 \right] = \frac{k}{2} \left(\frac{n^2 k - n^2}{k^2} \right) = \frac{n^2 (k-1)}{2k}$$

The called subroutine actually uses the contrapositive of this result, as stated in Corollary 8.

Corollary 8. *Let* G *be a graph of order n and size m and let* $k \in \mathbb{N}$ *. If:*

$$m > \frac{n^2(k-1)}{2k}$$

then G is not k-colorable.

Corollary 8 is demonstrated by Fig. 38. The shown graph G has n=4, m=5, and $\chi(G)=3$. Testing for k=2:

$$a = \frac{4^2(2-1)}{2 \cdot 2} = 4$$

But m = 5 > 4 = a and so we can conclude that G is not 2-colorable. However, testing for k = 3;

$$a = \frac{4^2(3-1)}{2 \cdot 3} = 5.3$$

So $m = 5 \ge 5.3 = a$ and thus *G may* be 3-colorable, since this test only provides a necessary and not a sufficient condition.

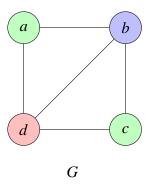


Fig. 38. Corollary 8 example.

In fact, the test of Corollary 8 will always fail for a complete graph when k < n. Since k, n > 0:

$$\frac{n(n-1)}{2} - \frac{n^2(k-1)}{2k} = \frac{kn(n-1) - n^2(k-1)}{2k}$$

$$= \frac{kn^2 - kn - kn^2 + n^2}{2k}$$

$$= \frac{n^2 - kn}{2k}$$

$$= \frac{n(n-k)}{2k}$$

$$> 0 \qquad (n > k)$$

4.3.2 Vertex Removal

The theorems that support vertex removal make use of Lemma 1.

Lemma 1. Let G be a graph and let $v \in V(G)$. If G is k-colorable then G - v is also k-colorable.

Proof. Assume that G is k-colorable. Let $c:V(G)\to C$ be such a coloring, and so |C|=k. Intuitively, removing v from G should not affect the proper coloring of the remaining vertices. Thus, we should be able to construct a proper coloring for G-v based upon c. So consider the restricted coloring function $c'=c|_{V(G-v)}$ and assume $uw\in E(G-v)$. Since c is proper:

$$c'(u) = c(u) \neq c(w) = c'(w)$$

Thus, c' is a proper coloring of G - v using at most k colors.

Therefore
$$G - v$$
 is k -colorable.

Lemma 1 is demonstrated in Fig. 39. No matter which vertex is removed, the resulting subgraph is still properly colored using at most four (in fact, three) colors.

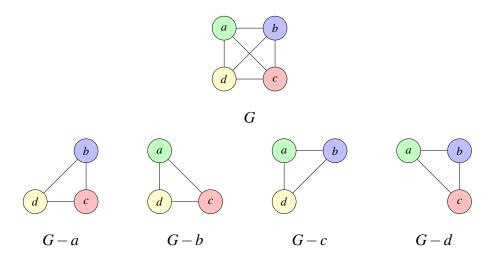


Fig. 39. Lemma 1 example.

Steps 4 and 5 remove vertices with degrees less than *k*. This is supported by Theorem 14.

Theorem 14. Let G be a graph and let $v \in V(G)$ such that $\deg(v) < k$ for some $k \in \mathbb{N}$. G is k-colorable if and only if G - v is k-colorable.

Proof. Assume that G is k-colorable. Therefore, by Lemma 1, G - v is also k-colorable.

For the converse, assume that G - v is k-colorable. Let $c: V(G - v) \to C$ be such a coloring, and so |C| = k. By assumption, $\deg(v) < k$, so v has at most k - 1 neighbors in G, using at most k - 1 colors. This means that there should be an additional color that can be assigned to v in G such that the coloring remains proper. So let

 $N(v) = \{v_1, \dots, v_r\} \subseteq V(G - v)$ for some r < k, and let $c[N(v)] = \{c_1, \dots, c_s\} \subset C$ for some $s \le r < k$. Since c[N(v)] is a proper subset of C, select $c_k \in C - c[N(v)]$ and define $c' : V(G) \to C$ as follows:

$$c'(u) = \begin{cases} c(u), & u \neq v \\ c_k, & u = v \end{cases}$$

Now, assume that $uw \in E(G)$ and consider the following two cases:

Case 1: $v \notin uw$

Since *c* is proper:

$$c'(u) = c(u) \neq c(w) = c'(w)$$

Case 2: $v \in uw$

Assume without loss of generality (AWLOG) that u = v. This means that $c'(v) = c_k$ and $c'(w) = c(w) \in c[N(v)]$. But $c_k \notin c[N(v)]$ and so $c'(v) \neq c'(w)$.

Thus, c' is a proper coloring of G using at most k colors.

Therefore G is k-colorable. \square

Theorem 14 is demonstrated in Fig. 40 for k = 4 and deg(v) = 3.

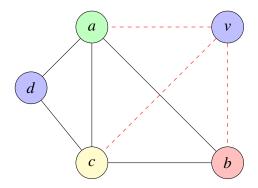


Fig. 40. Theorem 14 example.

The called subroutine actually removes all such vertices at once, which is supported by the inductive proof in Corollary 9.

Corollary 9. Let G be a graph of order n and let $X = \{v \in V(G) | \deg(v) < k\}$ for some $k \in \mathbb{N}$. G is k-colorable if and only if G - X is k-colorable.

Proof. (by induction on |X|)

Base Case: Let |X| = 0.

But G - X = G (trivial case).

Inductive Assumption: Let |X| = r.

Assume that G is k-colorable if and only if G - X is k-colorable.

Inductive Step: Consider |X| = r + 1.

Since |X| = r + 1 > 0, there exists $v \in X$ such that $\deg(v) < k$. Let $Y = X - \{v\}$ and note that |Y| = |X| - 1 = (r + 1) - 1 = r. So, G is k-colorable if and only if G - v is k-colorable (Theorem 14) if and only if (G - v) - Y is k-colorable (inductive assumption).

Therefore, by the principle of induction, G is k-colorable if and only if G - X is k-colorable.

Returning to the example in Fig. 40, note that $X = \{v, b\}$ is the set of all vertices with degree less than 4 and so both could be removed at once in accordance with Corollary 9. Furthermore, after these vertices are removed, the remaining vertices a, b, and c will all have degree 2. Since 2 < 4, the remaining vertices are subsequently removed, leaving n = 0 < 4, indicating that the graph is indeed 4-colorable. This iterative collapsing of a graph is an ideal situation.

Step 7 removes vertices whose neighborhoods are subsets of other vertices. This is supported by Theorem 15.

Theorem 15. Let G be a graph and let $u, v \in V(G)$ such that $N(u) \subseteq N(v)$. G is k-colorable if and only if G - u is k-colorable.

Proof. Assume that G is k-colorable. Therefore, by Lemma 1, G - u is also k-colorable.

For the converse, assume that G - u is k-colorable. Let $c : V(G - u) \to C$ be such a coloring, and so |C| = k. By definition, $u \notin N(u)$, and since, by assumption, $N(u) \subseteq N(v)$, it is also the case that $u \notin N(v)$. Hence, u is not adjacent to v in G. But everything that is adjacent to u in G is also adjacent to v in both G - u and G. Since everything adjacent to v has a different color than v, we should be able to assign u the same color as v in G in order to get a proper coloring of G.

Let $S = N(u) \cap N(v) = \{w_1, \dots w_r\} \subset V(G - u)$ for some $r = \deg(u) \leq \deg(v)$. For all $w \in S$, $w \in N(v)$ meaning $vw \in E(G - u)$. And, because c is proper, it must be the case that $c(w) \neq c(v)$. So define $c' : V(G) \to C$ as follows:

$$c'(w) = \begin{cases} c(w), & w \neq u \\ c(v), & w = u \end{cases}$$

Now, assume that $wz \in E(G)$ and consider the following two cases:

Case 1: $u \notin wz$

Since *c* is proper:

$$c'(w) = c(w) \neq c(z) = c'(z)$$

Case 2: $u \in wz$

Assume without loss of generality (AWLOG) that u = w. Since $vz \in E(G)$ and c is proper:

$$c'(u) = c(v) \neq c(z) = c'(z)$$

Thus, c' is a proper coloring of G using at most k colors.

Therefore *G* is *k*-colorable.

Theorem 15 is demonstrated in Fig. 41. Since $N(u) \subseteq N(v)$, G and G-u are equivalently colorable. Futhermore, once u is removed, the degrees of vertices a and c will have degree 2. So if k=3, those two vertices are subsequently removed by step 5. The remaining graph is of order 2, which then passes the success check of step 1 because 2 < 3, so indeed the graph is 3-colorable. Once again, this iterative removal of vertices is very powerful.

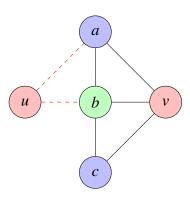


Fig. 41. Theorem 15 example.

4.3.3 Minimum Common Neighbor Upper Bound

Steps 8–10 establish an upper bound for the minimum common neighbor count between any two vertices in a graph that is assumed to be k-colorable. This limit is dependent on the following facts that are guaranteed by previous steps:

- 1) $2 \le k < n$
- 2) There are no $u, v \in V(G)$ such that $N(u) \subseteq N(v)$

The supporting theorem uses these facts along with Lemma 2 in its proof.

Lemma 2. Let G be a graph and let S be a non-empty independent subset of V(G). If there exists a vertex $v \in S$ such that v is adjacent to all vertices in V(G) - S (i.e., N(v) = V(G) - S) then for all vertices $u \in S$ it is the case that $N(u) \subseteq N(v)$.

Proof. Assume that such a v exists and then assume that $u \in S$. If u = v then (trivially) N(v) = N(v), so assume $u \neq v$. Furthermore, since $u, v \in S$ and S is independent (by assumption), it must be the case that u and v are not neighbors.

Case 1: $N(u) = \emptyset$.

Therefore, by definition, $N(u) = \emptyset \subseteq N(v)$.

Case 2: $N(u) \neq \emptyset$.

Assume that $w \in N(u)$. This means that w is adjacent to u and hence $w \notin S$, since S is an independent set. So $w \in V(G) - S$ and thus, by assumption, v is adjacent to w and we can conclude that $w \in N(v)$. Therefore $N(u) \subseteq N(v)$.

Therefore, for all $u \in S$, $N(u) \subseteq N(v)$.

Lemma 2 is demonstrated in Fig. 42. Note that since $v \in S$ is adjacent to every vertex in V(G) - S, vertex $u \in S$ can't help but be adjacent to some subset of N(v).

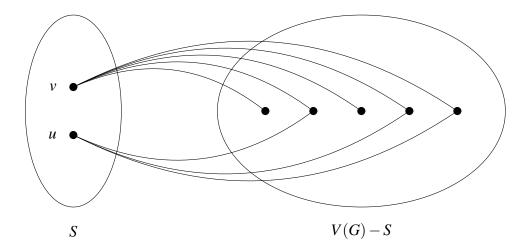


Fig. 42. Lemma 2 example.

Theorem 16 establishes the desired upper bound.

Theorem 16. Let G be a graph of order n and size m such that there are no $u, v \in V(G)$ where $N(u) \subseteq N(v)$, and let $k \in \mathbb{N}$ such that $2 \le k < n$. If G is k-colorable then there exists two vertices $w, z \in V(G)$ such that:

$$|N(w) \cap N(z)| \le n - 2 - \frac{n-2}{k-1}$$

Proof. Assume that G is k-colorable. This means that V(G) can be distributed into k independent (some possibly empty) subsets A_1, \ldots, A_k such that $a_i = |A_i|$ and $a_1 \ge a_2 \ge \cdots \ge a_k$. Since n > k, by the pigeonhole principle, it must be the case that $a_1 \ge 2$. Assume that $v \in A_1$.

First, assume by way of contradiction (ABC) that v is adjacent to all other vertices in $V(G)-A_1$. Since $a_1 \geq 2$, there exists $u \in A_1$ such that $u \neq v$ and u is not adjacent to v. Thus, by Lemma 2, $N(u) \subseteq N(v)$, contradicting the assumption. Note that this contradiction also eliminates the degenerate case where $A_1 = V(G)$; however, this case does not occur here because the graph would be an empty graph and would have been

eliminated by previous steps. Therefore, there exists some $v' \in V(G) - A_1$ such that v is not adjacent to v'. Assume that $v' \in A_i$ for some i such that $1 < i \le k$:

Case 1: $a_i = 1$

By the pigeonhole principle:

$$a_1 \ge \left\lceil \frac{n-1}{k-1} \right\rceil \ge \frac{n-1}{k-1}$$

Now, assume by way of contradiction (ABC) that v' is adjacent to all vertices in $V(G) - A_1 - A_i$ and assume $u \in N(v)$. Then it must be the case that $u \in V(G) - A_1 - A_i$, and so u is adjacent to v', and thus $u \in N(v')$. Therefore $N(v) \subseteq N(v')$, which contradicts the assumption. This situation is demonstrated by Fig. 43.

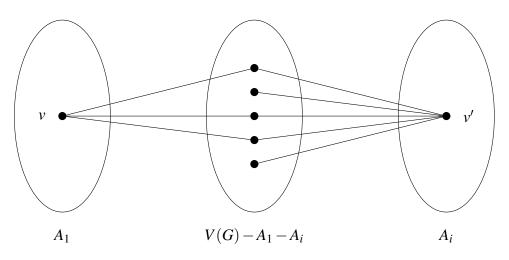


Fig. 43. Case $a_i = 1$ contradiction.

So there must exist some $u \in V(G) - A_1 - A_i$ such that u is not adjacent to v'. This results in the upper bound:

$$|N(v) \cap N(v')| \le n - |\{u, v'\}| - a_1 \le n - 2 - \frac{n-1}{k-1}$$

Note that since $v \in A_1$, it is already counted in a_1 . Comparing this bound to the desired bound:

$$\left(n-2-\frac{n-2}{k-1}\right) - \left(n-2-\frac{n-1}{k-1}\right) = \frac{(n-1)-(n-2)}{k-1} = \frac{1}{k-1} > 0$$

for $k \ge 2$. Thus the new bound is tighter and so:

$$|N(v) \cap N(v')| \le n - 2 - \frac{n-1}{k-1} \le n - 2 - \frac{n-2}{k-1}$$

Case 2: $a_i = 2$

By the pigeonhole principle:

$$a_1 \ge \left\lceil \frac{n-2}{k-1} \right\rceil \ge \frac{n-2}{k-1}$$

This results in the upper bound:

$$|N(v) \cap N(v')| \le n - a_i - a_1 \le n - 2 - \frac{n-2}{k-1}$$

Case 3: $a_i \ge 3$

By the pigeonhole principle:

$$a_1 \ge \left\lceil \frac{n-3}{k-1} \right\rceil \ge \frac{n-3}{k-1}$$

This results in the upper bound:

$$|N(v) \cap N(v')| \le n - a_i - a_1 \le n - 3 - \frac{n - 3}{k - 1}$$

Comparing this to the desired bound:

$$\left(n-2-\frac{n-2}{k-1}\right)-\left(n-3-\frac{n-3}{k-1}\right)=1-\frac{(n-3)-(n-2)}{k-1}=1-\frac{1}{k-1}>0$$

for $k \ge 2$. Thus the new bound is tighter and so:

$$|N(v) \cap N(v')| \le n - 3 - \frac{n-3}{k-1} \le n - 2 - \frac{n-2}{k-1}$$

Therefore, there exists $w, v \in V(G)$ such that:

$$|N(w) \cap N(z)| \le n - 2 - \frac{n-2}{k-1}$$

The called subroutine actually uses the contrapositive of this result, as stated in Corollary 10.

Corollary 10. Let G be a graph of order n and size m such that there are no $u, v \in V(G)$ where $N(u) \subseteq N(v)$, and let $k \in \mathbb{N}$ such that $2 \le k < n$. If for all $w, z \in V(G)$ it is the case that:

$$|N(w) \cap N(z)| > n - 2 - \frac{n-2}{k-1}$$

then G is not k-colorable.

Corollary 10 is demonstrated in Fig. 44. The shown graph has n = 5, is 3-chromatic, and has:

$$\min_{u,v\in V(G)} |N(u)\cap N(v)| = 1$$

Testing for k = 2:

$$5 - 2 - \frac{5 - 2}{2 - 1} = 0$$

But 1 > 0 and so we can conclude that G is not 2-colorable. However, testing for k = 3:

$$5 - 2 - \frac{5 - 2}{3 - 1} = \frac{3}{2}$$

So $1 \ge \frac{3}{2}$ and thus *G* may be 3-colorable, since this test only provides a necessary and not a sufficient condition.



Fig. 44. Corollary 10 example.

4.3.4 Recursive Steps

If nothing more can be done in the preceding steps then steps 11-14 revert to branching. Step 11 selects two non-adjacent vertices with the smallest number of common neighbors. Such a pair must exist. Otherwise, the current state of G is complete, which would have been eliminated by step 3. The first recursive call (step 12) assumes that the two selected vertices have the same color, so they are contracted. The second recursive call (step 13) assumes that the two selected vertices have different colors, so they are joined by an added edge. Each call starts a new branch of the Zykov tree corresponding to the current value of k. If either call returns true then it can be concluded that the input graph was indeed k-colorable. Otherwise, it can be concluded that the input graph is not k-colorable and the called subroutine returns the state of G prior to the recursive calls to the outer loop.

These steps are supported by Theorem 17.

Theorem 17. Let G be a graph of order $n \ge 2$ and let $u, v \in G$ such that u and v are not adjacent. G is k-colorable if and only if $G \cdot uv$ or G + uv is k-colorable.

Proof. Assume that G is k-colorable. Let $c:V(G)\to C$ be such a coloring, and so |C|=k. There are two possibilities, corresponding to the two recursive choices:

Case 1: u and v have the same color: c(u) = c(v).

Let $c_{uv} = c(u) = c(v) \in C$. For all $w \in N(u) \cup N(v)$, since w is adjacent to u and v and because c is proper, it must be the case that w is a different color than the color of u and v: $c(w) \neq c_{uv}$. Let v' be the contracted vertex, so that $N(v') = N(u) \cup N(v)$ and assign color c_{uv} to v'. Define $c' : V(G \cdot uv) \to C$ as follows:

$$c'(w) = \begin{cases} c(w), & w \neq v' \\ c_{uv}, & w = v' \end{cases}$$

Now, assume that $wz \in E(G \cdot uv)$ and consider the following two cases:

Case a: $v' \notin wz$

Since c is proper:

$$c'(w) = c(w) \neq c(z) = c'(z)$$

Case b: $v' \in wz$

Assume without loss of generality that v' = w. Since $z \in N(v')$:

$$c'(v') = c_{uv} \neq c(z) = c'(z)$$

Thus, c' is a proper coloring of $G \cdot uv$ using at most k colors.

Therefore $G \cdot uv$ is k-colorable.

Case 2: u and v have the different colors: $c(u) \neq c(v)$.

By adding edge uv, u and v become adjacent and thus must have different colors.

Thus, u and v can retain their same colors. So define $c':V(G+uv)\to C$ as follows:

$$c'(w) = c(w)$$

Now, assume $wz \in E(G)$. Since c is proper:

$$c'(w) = c(w) \neq c(z) = c'(z)$$

Thus, c' is a proper coloring of G + uv using at most k colors.

Therefore G + uv is k-colorable.

Therefore $G \cdot uv$ or G + uv is k-colorable.

For the converse, assume $G \cdot uv$ or G + uv is k-colorable. Again, there are two cases:

Case 1: $G \cdot uv$ is k-colorable.

Let $c: V(G \cdot uv) \to C$ be such a coloring, and so |C| = k. Let v' be the contracted vertex, and so $N(v') = N(u) \cup N(v)$. Let $c(v') = c_{uv} \in C$. For all $w \in N(v')$ in $G \cdot uv$, since w and v' are adjacent, they must have different colors: $c(w) \neq c_{uv}$.

Consider u and v in G. Since they are not adjacent, they can be assigned the same color. So, defined $c': V(G) \to C$ as follows:

$$c'(w) = \begin{cases} c(w), & w \neq u, v \\ c_{uv}, & w = u \\ c_{uv}, & w = v \end{cases}$$

Now, assume $wz \in E(G)$ and consider the following cases:

Case a: uv = wz

This is not possible since, by assumption, u is not adjacent to v.

Case b: $u \in wz$ and $v \notin wz$

Assume without loss of generality (AWLOG) that u = w. Since $z \in N(u)$ in G, it must be the case that $z \in N(v')$ in $G \cdot uv$. And so:

$$c'(u) = c_{uv} \neq c(w) = c'(w)$$

Case c: $u \notin wz$ and $v \in wz$

Assume without loss of generality (AWLOG) that v = w. Since $z \in N(v)$ in G, it must be the case that $z \in N(v')$ in $G \cdot uv$. And so:

$$c'(v) = c_{uv} \neq c(w) = c'(w)$$

Case d: $u, v \notin wz$

Since c is proper:

$$c'(w) = c(w) \neq c(z) = c'(z)$$

Thus, c' is a proper coloring of G using at most k colors.

Case 2: G + uv is k-colorable.

Let $c: V(G+uv) \to C$ be such a coloring, and so |C| = k. Since u and v are adjacent in G+uv, they must have different colors. Once uv is removed in G, u and v are no longer adjacent and so there are no requirements on their colors. Thus, they can retain their original colors from G+uv. So define $c': V(G) \to C$ as follows:

$$c'(w) = c(w)$$

Now assume $wz \in E(G)$. Since c is proper:

$$c'(w) = c(w) \neq c(z) = c'(z)$$

Thus, c' is a proper coloring of G using at most k colors.

Therefore *G* is *k*-colorable.

4.4 An Example

In this section, the proposed algorithm will be applied to the example graph G of order n = 8 and size m = 12 shown in Fig. 45 in order to determine $\chi(G)$. The steps of the algorithm are then traversed in reverse order to determine a chromatic coloring.

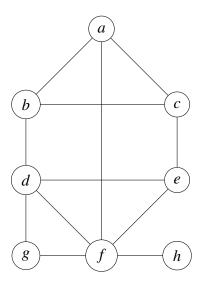


Fig. 45. An example graph.

The algorithm steps are as follows. Outer loop steps are marked by "O#" and called subroutine steps are marked by "I#.". Recursive subroutine calls add a call level: "I#_#."

- 1) (O1) Since n = 8 > 0, G is not the null graph, so continue.
- 2) (O2) Since n = 8 > 1, G is not an empty graph, so continue.
- 3) (O3) Initialize k to 2.
- 4) (O4) Call the subroutine with G and k = 2.
- 5) (I1) $n = 8 \nleq k = 2$, so continue.
- 6) (I2) Calculate the maximum edge threshold for n = 8 and k = 2:

$$a = \frac{n^2(k-1)}{2k} = \frac{8^2(2-1)}{2 \cdot 2} = \frac{64}{4} = 16$$

- 7) (I3) Since m = 12 > 16 = a, continue.
- 8) (I4) Since deg(h) = 1 < 2, set $X = \{h\}$.
- 9) (I5) Since $X \neq \emptyset$, replace G with G X. The result is shown in Fig. 46. Now n = 7 and m = 11.

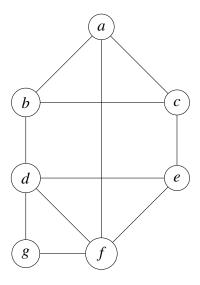


Fig. 46. Step: $G - \{h\}$.

- 10) (I1) $n = 7 \nleq k = 2$, so continue.
- 11) (I2) Calculate the maximum edge threshold for n = 7 and k = 2:

$$a = \frac{n^2(k-1)}{2k} = \frac{7^2(2-1)}{2 \cdot 2} = \frac{49}{4} \approx 12.3$$

- 12) (I3) Since $m = 12 \ge 12.3 = a$, continue.
- 13) (I4) Since $(G) = 2 \ge 2 = k$, set $X = \emptyset$.
- 14) (I5) Since $X = \emptyset$, continue.
- 15) (I6) Calculate the number of common neighbors, looking for any subsets. The results are shown in Table 3.

Table 3
Calculating Common Neighbors 1

		NT	1 49	1' 49
и	v	$ N(u)\cap N(v) $	subset?	adjacent?
а	b	1	N	Y
a	c	1	N	Y
а	d	2	N	N
а	e	2	N	N
а	f	0	N	Y
а	g	1	N	N
b	С	1	N	Y
b	d	0	N	Y
b	e	2	N	N
b	f	2	N	N
b	g	1	N	N
С	d	2	N	N
С	e	0	N	Y
С	f	2	N	N
С	g	0	N	N
d	e	1	N	Y
d	f	2	N	Y
d	g	1	N	Y
e	f	1	N	Y
e	g	2	Y	N
f	g	1	N	Y

16) (I7) Note that $N(g) = \{d, f\}$ and $N(e) = \{c, d, f\}$. Since $N(g) \subseteq N(e)$, replace G with G - g. The result is shown in Fig. 47. Now n = 6 and m = 9.

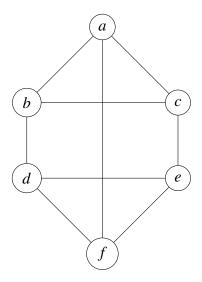


Fig. 47. Step: G - g.

- 17) (I1) $n = 6 \nleq k = 2$, so continue.
- 18) (I2) Calculate the maximum edge threshold for n = 6 and k = 2:

$$a = \frac{n^2(k-1)}{2k} = \frac{6^2(2-1)}{2 \cdot 2} = \frac{36}{4} = 9$$

- 19) (I3) Since $m = 9 \geqslant 9 = a$, continue.
- 20) (I4) Since $(G) = 2 \ge 2 = k$, set $X = \emptyset$.
- 21) (I5) Since $X = \emptyset$, continue.
- 22) (I6) Calculate the number of common neighbors, looking for any subsets. The results are shown in Table 4.

Table 4
Calculating Common Neighbors 2

и	v	$ N(u) \cap N(v) $	subset?	adjacent?
a	b	1	N	Y
a	С	1	N	Y
a	d	2	N	N
a	e	2	N	N
a	f	0	N	Y
b	С	1	N	Y
b	d	0	N	Y
b	e	2	N	N
b	f	2	N	N
c	d	2	N	N
c	e	0	N	Y
c	f	2	N	N
d	e	1	N	Y
d	f	1	N	Y
e	f	1	N	Y

- 23) (I7) Since there are no $u, v \in V(G)$ such that $N(u) \subseteq N(v)$, continue.
- 24) (I8) From Table 4, the minimum number of common neighbors is 0 (e.g., a and f). So set b = 0.
- 25) (I9) Calculate the upper bound for minimum number of common neighbors for n = 6 and k = 2:

$$c = n - 2 - \frac{n-2}{k-1} = 6 - 2 - \frac{6-2}{2-1} = 4 - 4 = 0$$

- 26) (I10) Since b = 0 > 0 = c, conclude that G may be 2-colorable and continue.
- 27) (I11) Based on the results in Table 4, all of the nonadjacent vertices share two common neighbors, so select *a* and *d*.
- 28) (I12) Recursively call the subroutine with $G \cdot ad$, as shown in Fig. 48. Now, n = 5 and m = 7.

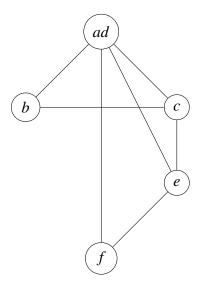


Fig. 48. Step: $G \cdot ad$.

- 29) (I1-1) $n = 5 \nleq k = 2$, so continue.
- 30) (I2-1) Calculate the maximum edge threshold for n = 5 and k = 2:

$$a = \frac{n^2(k-1)}{2k} = \frac{5^2(2-1)}{2 \cdot 2} = \frac{25}{4} = 6.25$$

- 31) (I3-1) Since m = 7 > 6.25 = a, conclude that G is not 2-colorable and return false.
- 32) (I13) Returning to the G of Fig. 47, recursively call the subroutine with G + ad, as shown in Fig. 49. Now, n = 6 and m = 10.

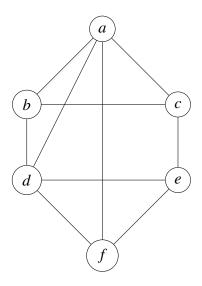


Fig. 49. Step: G + ad.

- 33) (I1-1) $n = 6 \nleq k = 2$, so continue.
- 34) (I2-1) Calculate the maximum edge threshold for n = 6 and k = 2:

$$a = \frac{n^2(k-1)}{2k} = \frac{6^2(2-1)}{2 \cdot 2} = \frac{36}{4} = 9$$

- 35) (I3-1) Since m = 10 > 9 = a, conclude that G is not 2-colorable and return false.
- 36) (I14) Conclude that the G of Fig. 47 is not 2-colorable and return false with this G.
- 37) (O5) Since the called subroutine returned false, G is not 2-colorable, so continue.
- 38) (O6) Replace G with the graph returned by the previous call (Fig. 47).
- 39) (O7) Increment *k* to 3.
- 40) (O4) Call the subroutine with the new G and k = 3.
- 41) (I1) $n = 6 \nleq k = 3$, so continue.
- 42) (I2) Calculate the maximum edge threshold for n = 6 and k = 3:

$$a = \frac{n^2(k-1)}{2k} = \frac{6^2(3-1)}{2 \cdot 3} = \frac{72}{6} = 12$$

43) (I3) Since $m = 9 \ge 11 = a$, continue.

- 44) (I4) Since $\delta(G) = 3 \ge 3 = k$, set $X = \emptyset$.
- 45) (I5) Since $X = \emptyset$, continue.
- 46) (I6) Calculate the number of common neighbors, looking for any subsets. Note that the results are the same as those shown in Table 4.
- 47) (I7) Since there are no $u, v \in V(G)$ such that $N(u) \subseteq N(v)$, continue.
- 48) (I8) From Table 4, the minimum number of common neighbors is 0 (e.g., a and f). So set b = 0.
- 49) (I9) Calculate the upper bound for minimum number of common neighbors for n = 6 and k = 3:

$$c = n - 2 - \frac{n-2}{k-1} = 6 - 3 - \frac{6-2}{3-1} = 3 - 2 = 1$$

- 50) (I10) Since $b = 0 \ge 1 = c$, conclude that G may be 3-colorable and continue.
- 51) (I11) Based on the results in Table 4, all of the nonadjacent vertices share two common neighbors, so select *a* and *d*.
- 52) (I12) Recursively call the subroutine with $G \cdot ad$, as shown in Fig. 48. Now, n = 5 and m = 7.
- 53) (I1-1) $n = 5 \nleq k = 2$, so continue.
- 54) (I2-1) Calculate the maximum edge threshold for n = 5 and k = 3:

$$a = \frac{n^2(k-1)}{2k} = \frac{5^2(3-1)}{2 \cdot 3} = \frac{25}{3} = 8.3$$

- 55) (I3-1) Since $m = 7 \ge 8.3 = a$, conclude that G may be 3-colorable and continue.
- 56) (I4-1) Since $\deg(b) = \deg(f) = 2 < 3 = k$, set $X = \{b, f\}$.
- 57) (I1-5-1) Since $X \neq \emptyset$, replace G with G X. The result is shown in Figure 50. Now n = 3 and m = 3.



Fig. 50. Step: $G - \{b, f\}$

- 58) (I1-1) $n = 3 \le k = 3$, so conclude that the G of Fig. 50 is 3-colorable and return true and this G.
- 59) (I12) The recursive call returned true, so conclude that the returned *G* of Fig. 50 is 3-colorable and return true with this *G*.
- 60) (O4) The called subroutine returned true, so conclude that the returned G of Fig. ?? is 3-chromatic and return $\chi(G) = 3$.

Thus, the algorithm determines that the example G of Figure 45 is 3-chromatic. In order to determine a 3-chromatic coloring for G, first construct a set C of three colors:

$$C = \{\text{green}, \text{blue}, \text{red}\}$$

Next, follow the algorithm's modification steps in reverse order and color the corresponding vertices accordingly. The steps are as follows:

First, color the vertices that are present in the final simplified graph. Assign each
vertex its own color, except assign contracted vertices the same color. This is shown
in Fig. 51.

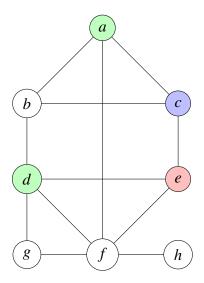


Fig. 51. Initial coloring.

2) The last modification was the removal of vertices *b* and *f*. Note that color selection needs to honor the vertices already colored. This is shown in Fig. 52.



Fig. 52. Coloring b and f.

3) The contracted vertices have already been colored, so the next simplification to address is the removal of g due to the neighborhood subset test. Since $N(g) \subseteq N(e)$,

color g and e the same color. Since e has already been assign a color, use it for g. The result is shown in Fig. 53.

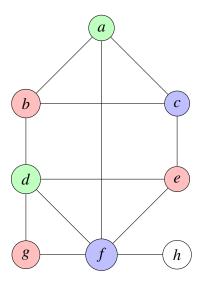


Fig. 53. Coloring g.

4) Finally, color the first removed vertex *h* with any appropriate color. The final result is shown in Fig. 54.

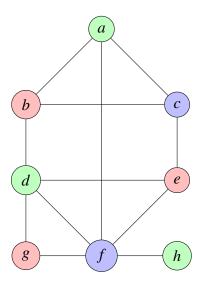


Fig. 54. Final chromatic coloring.

At first glance, one might wonder what advantage this method of coloring has over other sequential methods. The difference is that the other sequential methods only have knowledge about what has already been colored, whereas this method uses assumptions that are made during the simplifications and recursive calls on the entire graph. Thus, the sequential algorithms are heuristic, but this method selects a particular workable coloring path through the resulting Zykov tree.

5 TOASTER DESIGN CASE STUDY

This section contains a simplistic case study of how the proposed algorithm could be used to compare the FR graphs resulting from two slightly different designs of the basic kitchen toaster shown in Fig. 55.



Fig. 55. An example toaster.

The FRs are shown in Table 5. It is assumed that the design is either uncoupled or decoupled and hence the independence of the FRs is as strong as possible.

Table 5
Toaster Functional Requirements

FR ₁	Body contains all parts		
FR ₂	Can be safely moved while hot		
FR ₃	Can hold two slices of bread		
FR ₄	Heats each slice of bread on both sides		
FR ₅	Toasting is manually started		
FR ₆	Toasting is automatically or can be manually stopped		
FR ₇	Heat level can be controlled		

The graph G_1 for the first candidate design with n = 7 and m = 13 is shown in Fig. 56.



Fig. 56. First candidate design.

For k = 2, the maximum edge threshold test fails:

$$\frac{n^2(k-1)}{2k} = \frac{7^2(2-1)}{2 \cdot 2} = \frac{49}{4} \approx 12.3 < 13 = m$$

so G_1 is not 2-colorable.

For k = 3, the maximum edge threshold test passes:

$$\frac{n^2(k-1)}{2k} = \frac{7^2(3-1)}{2 \cdot 3} = \frac{98}{6} \approx 16.3 > 13 = m$$

There are no vertices with degrees less than k = 3; however, note that $N(FR_2) \subseteq N(FR_1)$, so remove vertex FR_2 . The result is shown in Fig. 57.

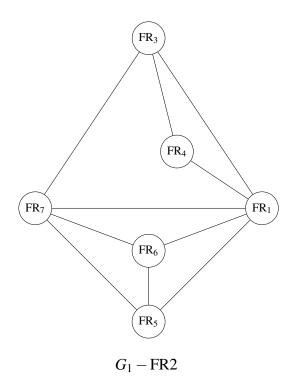
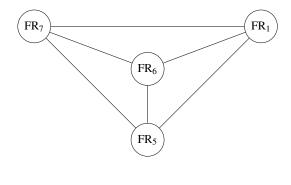


Fig. 57. Design 1—remove FR₂.

Next, since $deg(FR_4) = 2 < 3 = k$, remove FR_4 . As a result of removing FR_4 , $deg(FR_3) = 2 < 3 = k$, so remove FR_3 as well. The result is show in Fig. 58.



$$G_1 - FR_4 - FR_3$$

Fig. 58. Design 1—Remove FR₄ and FR₃.

At this point, $G_1 = K_4$, so it is guaranteed to fail the maximum edge threshold check for k = 3 and thus not be 3-colorable. At k = 4 we have $n = 4 \le 4 = k$. Thus, we can conclude that G_1 is 4-chromatic. An example chromatic coloring with:

$$C = \{\text{green}, \text{blue}, \text{red}, \text{orange}\}$$

is show in Fig. 59.

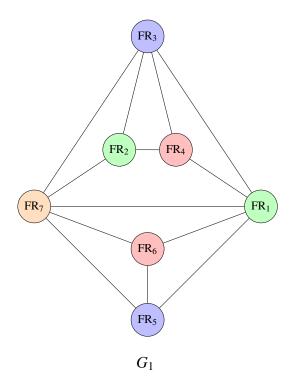


Fig. 59. Design 1—chromatic coloring.

Notice in the design that FR_5 (start toasting) and FR_6 (stop toasting) have been forced into separate parts, conceivably to accommodate the separate "cancel" button shown in Fig. 55. But what if the designer decides to eliminate the cancel button and allow manual cancellation via the lever? Thus, FR_5 and FR_6 no longer need to be separated, so the edge between their vertices can be eliminated. The result is shown in Fig. 60.



Fig. 60. Second candidate design.

Rerun the algorithm on G_2 for n = 7 and m = 12. For k = 2, the maximum edge threshold test passes:

$$\frac{n^2(k-1)}{2k} = \frac{7^2(2-1)}{2 \cdot 2} = \frac{49}{4} \approx 12.3 > 12 = m$$

Note that $N(FR_6) \subseteq N(FR_5)$, so remove FR_6 . The result is shown in Fig. 61.

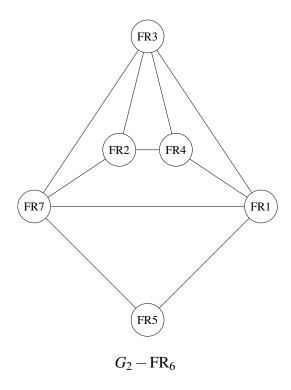


Fig. 61. Design 2—remove FR₆.

Now, with n = 6 and m = 10, G_2 fails the maximum edge threshold test for k = 2:

$$\frac{n^2(k-1)}{2k} = \frac{6^2(2-1)}{2 \cdot 2} = \frac{36}{4} = 9 < 10 = m$$

so G_2 is not 2-colorable.

For k = 3, note that $deg(FR_5) = 2 < 3 = k$, so remove FR₅. The result is shown in Fig. 62.

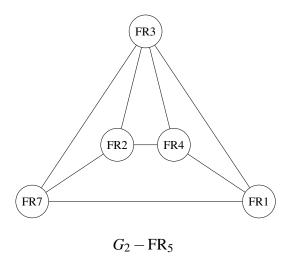


Fig. 62. Design 2—remove FR_5 .

Now, with n = 5 and m = 8, G_2 passes the maximum edge threshold test for k = 3:

$$\frac{n^2(k-1)}{2k} = \frac{5^2(3-1)}{2 \cdot 3} = \frac{50}{6} \approx 8.3 > 8 = m$$

Since $N(FR_2) \subseteq N(FR_1)$, remove FR_2 . The result is shown in Fig. 63.

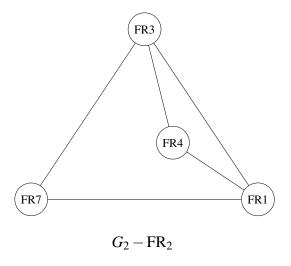


Fig. 63. Design 2—remove FR₂.

Finally, $deg(FR_4) = deg(FR_7) = 2 < 3 = k$, so remove FR₄ and FR₇. The result is shown in Fig. 64.

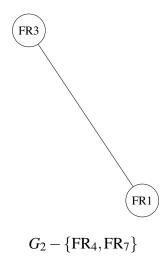


Fig. 64. Design 2—remove FR₄ and FR₇.

This final state of G_2 has $n = 2 \le 3 = k$, so we can conclude that G_2 is 3-chromatic. An example chromatic coloring with:

$$C = \{\text{green}, \text{blue}, \text{red}\}$$

is show in Fig. 65.

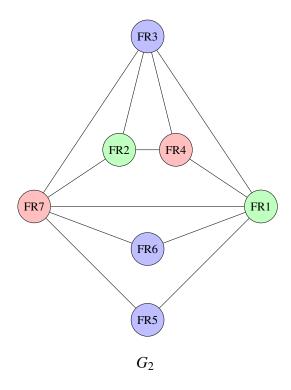


Fig. 65. Design 2—chromatic coloring.

This process gives the designer the feedback that the second design requires only three parts instead of four, and thus has less information content and hence a higher chance of success than the first design. It will be up to the designer to weigh this result against other aspects of the design.

6 RANDOM GRAPH ANALYSIS

Literature Cited

- [1] V. Voloshin, "A tribute to a. a. and t. e. zykovs on the occasion of a. a. zykov's 90th birthday," *Topics in Graph Theory*, November 2013.
- [2] N. P. Suh, *The Principles of Design*. New York: Oxford University Press, 1990.
- [3] R. A. Shirwaiker and G. E. Okudan, "Triz and axiomatic design: A review of case-studies and a proposed synergistic use," *Journal of Intelligent Manufacturing*, vol. 19, pp. 33–47, February 2008.
- [4] N. P. Suh, "Axiomatic design theory for systems," *Research in Engineering Design*, vol. 10, pp. 189–209, 1998.
- [5] S. Behdad, J. Cavallaro, P. K. Gopalakrishnan, and S. Jahanbekam, "A graph coloring technique for identifying the minimum number of parts for physical integration in product design," in *Proceedings of the ASME 2019 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference*, no. DETC2019-98251 in IDETC/CIE 2019, (Anaheim, CA), Aug 18–21 2019.
- [6] S. Behdad, P. K. Gopalakrishnan, S. Jahanbekam, and H. Klein, "Graph partitioning technique to identify physically integrated design concepts," in *Proceedings of the ASME 2018 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference*, no. DETC2018-85646 in IDETC/CIE 2018, (Quebec, Canada), Aug 26–29 2018.
- [7] Y. Tang, S. Yang, and Y. F. Zhao, "Sustainable design for additive manufacturing through functionality integration and part consolidation," in *Handbook of Sustainability in Additive Manufacturing* (S. S. Muthu and M. M. Savalani, eds.), vol. 1, pp. 101–144, Singapore: Springer, 2016.
- [8] C. McDiarmid, "Determining the chromatic number of a graph," *SIAM Journal on Computing*, vol. 8, pp. 1–14, 02 1979.
- [9] G. Chartrand and P. Zhang, *A First Course in Graph Theory*. Mineola, New York: Dover Publications, 2012.
- [10] D. B. West, *Introduction to Graph Theory*. Upper Saddle River, NJ: Prentice Hall, 2^{nd} ed., 2001.

- [11] D. G. Corneil and B. Graham, "An algorithm for determining the chromatic number of a graph," *SIAM Journal on Computing*, vol. 2, pp. 311–318, December 1973.
- [12] A. A. Zykov, *On Some Properties of Linear Complexes*, vol. 7 of *American Mathematical Society Translations Series One*. American Mathematical Society, 1949 (translated 1952).
- [13] J. Hopcroft and R. Tarjan, "Algorithm 447: Efficient algorithms for graph manipulation," *Communications of the ACM*, vol. 16, pp. 372–378, June 1973.
- [14] M. R. Garey and D. S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness*. San Francisco: W.H. Freeman and Company, 1979.
- [15] M. Sipser, *Introduction to the Theory of Computation*. Boston, MA: Cengage Learning, 3rd ed., 2013.
- [16] N. Christofides, "An algorithm for the chromatic number of a graph," *The Computer Journal*, vol. 14, pp. 38–39, January 1971.
- [17] V. Voloshin, "Alexander zykov 1922-2013," January 2014.
- [18] R. C. Read, "An introduction to chromatic polynomials," *Journal of Combinatorial Theory*, vol. 4, pp. 52–71, 1968.