

Decision Trees in Proper Edge k -coloring of Cubic Graphs

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Abstract—This work examines the possibilities of increasing the efficiency of the computation of proper edge k -coloring of cubic graph with the use of machine learning methods. State-of-the-art approaches related to this problem work with time complexity of circa $O(2^{0.427|V(G)|})$, where $|V(G)|$ is number of vertices of given graph G . The main focus of the paper is use of machine learning model of decision trees for the problem of identification of properly edge 3-uncolorable graphs called snarks - well known instance of NP-complete problem. Presented work consists of creation of graph property datasets fitting for the specified machine learning task, building of decision tree models based on the created datasets and identification of properties which are significant in the context of graph edge coloring and are measurable in lower time complexity than the edge coloring itself.

I. INTRODUCTION

Proper edge k -coloring of the cubic graphs is problem, which is frequently computed as the part of scheduling of tasks in the context of large computational systems, register allocation in the compilation of source code into machine code or pattern matching problems [1], [2]. In these problems, algorithm needs to color number of graphs while each edge k -coloring represents NP-complete problem. We are searching for properties and we design methods, which could be used to make coloring of big sets of graphs more effective.

The main objective of this work is the identification of hidden knowledge that affects the proper edge k -colorability of graph. In the process of this search, we used the method of decision trees, where we projected the process of proper coloring with the use of k colors into a classification task while the number of used colors was fixed. In the context of the presented paper, the objective is to correctly classify the input graph described by its properties into one of two classes - properly edge k -colorable graphs or improperly edge k -colorable graphs for fixed k equal to 3 (see Section III for reasoning).

The contributions presented in this paper are:

- Creation of graph property datasets fitting for the specified machine learning task. This type of datasets is very hard to find, therefore we need to use number of datasources in order to create appropriate data.
- Building of decision tree models based on the created datasets in order to classify input graph sets into one of

two considered classes - properly edge k -colorable graphs or improperly edge k -colorable graphs.

- Identification of properties which are significant in the context of graph edge coloring. In the ideal case all of these properties of given graph can be computed in lower time complexity than edge coloring itself, therefore we can make obtaining the information about edge colorability of graph more effective.

The body of the presented paper is structured into three sections. In the section titled Related Works (Section II) we present works from various areas of computer science (data analysis, graph theory, data mining) that are relevant to this paper. In the section III, we give basic information about graphs and the problem of edge k -coloring of graphs, we present the datasets we created, including a description of the properties recorded in them and simple statistical properties of the dataset (centrality, variability and correlation analysis). Section IV of this paper contains the results of the examination of created datasets using decision trees methods and identification of properties that affect the proper edge k -colorability of our sets of graphs.

II. RELATED WORKS

The research presented in this paper is a continuation of our previous work [3], [4]. In these publications, we focused on using permutations of graph adjacency matrices and correct decomposition of datasets to streamline parallel and distributed algorithms of edge 3-coloring of large graph sets. A similar approach was chosen by the authors of the work [5], who analyzed a large set of data while the key concept authors of the work focused on was partitioning of data with a combination of indexing and parallelism.

Our previous work was mostly motivated by the approach of Kowalik in [6], who shows an algorithm for edge-coloring an n -vertex graph using three colors while using polynomial space. Kowalik applies a natural approach of generating inclusion-maximal matchings of the graph. Modern findings in the area of graph theory and improperly edge k -colorable graphs have been published in [7]. Authors of this work determine the value of the chromatic index - number of colors needed for proper edge coloring of a graph - for several basic graph classes including trees, cycles, hypercubes and subdivisions

of complete graphs. Authors also give upper bounds on the chromatic index in terms of other graph parameters, which brings forward the relationship between various graph properties researched in this paper.

In [8], authors use the induction of decision trees and fuzzy decision trees in different applied areas as a relevant problem in Data Mining. Authors of this paper focus on an algorithm for the fuzzy decision tree induction based on Cumulative Mutual Information Estimate. This algorithm is considered in the context of defect detection of blades of gas turbine aircraft engines.

Other applied use of decision trees is described in [9], where authors propose a novel optimization approach to interpretable reinforcement learning that builds decision trees. Proposed approach is based on a two-level optimization scheme that combines the advantages of evolutionary algorithms with the benefits of Q-learning. This method allows decomposing the problem into two sub-problems: the problem of finding a meaningful decomposition of the state space, and the problem of associating an action to each subspace.

III. GRAPHS, GRAPH DATA AND GRAPH PROPERTIES

Graph G is described as pair of sets V (vertices) and E (edges), where [10]

$$G = (V, E), E \subseteq V^2$$

This work considers strictly so called cubic graphs, where number of edges, which are incident to any given vertex is equal to 3. We call this property of vertex the degree of vertex denoted by $deg(V)$ while $max(deg(V))$ is denoted by $\Delta(G)$. Since cubic graphs are smallest non-trivial graphs, they are fitting starting point for making the computation of edge k -coloring of graphs more effective [10].

Proper edge k -coloring of graph is an NP-complete problem [6], which consists of assignment of colors to edges of graphs in such a way, that no adjacent edges are colored with the use of same of the k considered colors (see Fig.1). The Fig. 1 presents improperly colored graph on the left (there is problematic coloring of the edges incident to the A vertex) and same graph colored properly on the right.

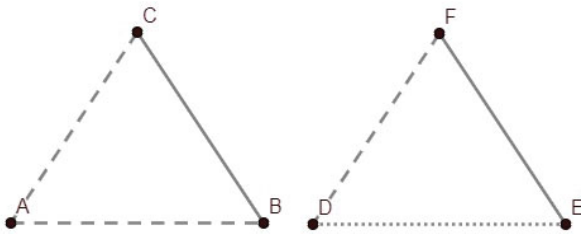


Fig. 1. Example of improperly (left) and properly (right) edge 3-colored graph

Since Vizing's theorem [11] for graph G , formulated as

$$\Delta(G) \leq \chi'(G) \leq \Delta(G) + 1$$

where $\chi'(G)$ is so-called chromatic index (number of colors needed in order to properly edge color the graph G), holds true, we consider two possibilities of edge coloring of cubic graphs - either with the use of 3 or 4 colors. This problem can be solved by edge 3-coloring of graph where:

- In the case the graph is edge 3-colorable, we are talking about a standard cubic graph.
- Otherwise, we talk about the so-called *snark*. However, finding out whether a graph is snark is time-consuming - in the worst case, it is necessary to verify all possible edge 3-colorings of the graph [6].

In this work, we focus on creating a machine learning model that will be able to identify a snark based on properties other than the experimental edge coloring of the graph itself.

A. Graph Datasets for Machine Learning Methods

For the purposes of the aforementioned objective of training a machine learning model of decision trees, which will be able to identify snarks or standard cubic graphs, we need to collect appropriately structured graph datasets. The appropriate structure of the dataset is reflected in the horizontal and vertical aspect of the data:

- it is necessary to create datasets composed of an evenly distributed sample of snarks and cubic graphs,
- it is necessary that we measure a large number of properties about each of the graphs.

Based on these requirements, we created mixed datasets of snarks and standard cubic graphs for 30, 32, 34 and 36 vertex graphs. Each dataset contains 500 graphs in even distribution of 250 snarks and 250 standard cubic graphs. The source of data for the creation of our datasets is the *House of Graphs* portal [12], the *graphFilter* tool [13] and the *SageMath* software [14].

The properties and their description, which were measured for our four datasets are presented in the following list [10]:

- **Average degree** of graph G is arithmetic mean of degrees of all vertices in G .
- Graph G is **bipartite** in the case we can divide the set of vertices of the graph $V(G)$ into two subsets A and B in such a way, that each edge of G connects one or more vertices from A with one or more vertices from B .
- Graph G is **claw-free** in the case it does not contain $K_{1,3}$ (also called *claw*) as an induced subgraph.
- **Clique number** is size of largest complete graph that can be made of the input graph G .
- **Chromatic index** of graph G is minimal number of colors needed in order to color the edges of the graph G properly. Therefore, this property is the key to defining whether the cubic graph is snark (chromatic index of 4) or standard cubic graph (chromatic index of 3). From the point of view of this work, this is the property we want to be able to predict the value for.
- **Chromatic number** of graph G is minimal number of colors needed for proper coloring of vertices of G .
- Graph G is **connected** in the case, that each pair of vertices of G is connected by a path.

TABLE I. BASIC STATISTICAL FEATURES OF RELEVANT (NON-CONSISTENT) PROPERTIES OF GRAPH DATA FOR 30 AND 32 VERTEX GRAPHS

Property of graph	30-vertex graphs				32-vertex graphs			
	min	max	avg	sd	min	max	avg	sd
Bipartite	0	0	0	0	0	1	0,002	0,045
Claw-free	0	0	0	0	0	0	0	0
Clique number	2	3	2,188	0,391	2	3	2,026	0,159
Density	0,103	0,103	0,103	0,0002	0,0967	0,0970	0,0969	0,0001
Diameter	4	10	6,41	1,3196	5	11	6,657	1,031
Edge connectivity	1	3	2,722	0,487	1	3	2,846	0,427
Eulerian	0	0	0	0	0	0	0	0
Matching number	14	15	14,982	0,133	15	16	15,974	0,159
Number of triangles	0	0	0	0	0	0	0	0
Planar	0	0	0	0	0	0	0	0
Radius	3	8	4,748	1,089	4	7	4,922	0,498
Regular	1	1	1	0	1	1	1	0
Vertex connectivity	2	3	2,998	0,0447	1	3	2,846	0,427
Largest L-eigenvalue	5,361	6	5,627	0,136	5,478	6	5,729	0,108
AS Second largest Eigenvalue	2,181	2,961	2,649	0,094	2,236	2,961	2,754	0,094
AS smallest Eigenvalue	-3	-2	-2,626	0,139	-3	-2,478	-2,729	0,108
Laplacian spectrum	0,043	0,819	0,351	0,228	0,039	0,764	0,245	0,094
Chromatic number	3	3	3	0	2	4	3	0,063
Girth	3	7	4,74	1,389	3	6	4,279	0,508
Domination number	8	10	8,474	0,504	8	10	9,008	0,167
Independence number	10	15	12,764	0,559	13	16	13,844	0,433
Chromatic index	3	4	3,5	0,5005	3	4	3,497	0,5004

TABLE II. BASIC STATISTICAL FEATURES OF RELEVANT (NON-CONSISTENT) PROPERTIES OF GRAPH DATA FOR 34 AND 36 VERTEX GRAPHS

Property of graph	34-vertex graphs				36-vertex graphs			
	min	max	avg	sd	min	max	avg	sd
Bipartite	0	0	0	0	0	0	0	0
Claw-free	0	0	0	0	0	0	0	0
Clique number	2	2	2	0	2	2	2	0
Density	0,0909	0,091	0,09095	0,00005	0,0857	0,086	0,0858	0,0001
Diameter	4	11	6,315	1,554	5	8	5,788	0,762
Edge connectivity	2	4	0,489	0,489	3	3	3	0
Eulerian	0	0	0	0	0	0	0	0
Matching number	17	17	17	0	18	18	18	0
Number of triangles	0	0	0	0	0	0	0	0
Planar	0	1	0,002	0,045	0	0	0	0
Radius	4	8	4,711	0,814	4	6	4,746	0,445
Regular	1	1	1	0	1	1	1	0
Vertex connectivity	2	3	2,621	0,486	3	3	3	0
Largest L-eigenvalue	5,416	5,97	5,664	0,079	5,414	5,841	5,677	0,075
AS Second largest Eigenvalue	2,2	2,946	2,611	0,251	2,272	2,912	2,574	0,147
AS smallest Eigenvalue	-2,858	-2,416	-2,663	0,0778	-2,841	-2,414	-2,676	0,075
Laplacian spectrum	0,054	0,799	0,388	0,251	0,196	0,614	0,425	0,145
Chromatic number	3	3	3	0	3	3	3	0
Girth	4	7	5,776	1,272	5	7	6	1,001
Domination number	9	10	9,667	0,472	10	11	10,002	0,0447
Independence number	14	16	14,497	0,504	15	17	15,456	0,503
Chromatic index	3	4	3,501	0,50447894	3	4	3,5	0,501

- **Density** of graph G is ratio between the edges present in G and the maximum number of edges that the G can contain.
- **Diameter** of graph G is length of longest path in the graph G .
- **Domination number** of graph G with the value of n is smallest set of vertices such that every vertex not in the set is adjacent to at least n vertices of the set.
- Graph G is **eulerian** in the case it contains eulerian cycle (graph cycle which uses each edge of G exactly once).
- **Girth** of graph G is length of shortest cycle (in the case there is a cycle in the graph) in G .
- **Group size** of graph G is size of automorphism class for G .
- **Independence number** of graph G is number of an independent set of vertices in G . Vertices are independent when there is no edge between them.
- **Laplacian largest eigenvalue** is largest eigenvalue of Laplacian matrix L of the graph G , while $L = D - A$, where A is adjacency matrix of G and D is diagonal

matrix containing degree of the vertex i on each position $D_{i,i}$.

- **Laplacian spectrum** or algebraic connectivity of graph G is second smallest eigenvalue of Laplacian matrix L for the graph G .
- **Matching number** of graph G is a number of edges that do not have a set of common vertices.
- **Number of components** of graph G is number of connected subgraphs contained in the graph G .
- **Number of edges** of the graph G is the number of connections between the vertices in G .
- **Number of triangles** of the graph G is number of triangles (3 vertex, 3 edge) subgraphs in G . For example of triangle see Fig. 1.
- **Number of vertices** of the graph G .
- Graph G is **planar** in the case, we can draw the graph on plane without any edge crossing.
- **Radius** of the graph G is the minimum graph eccentricity of any graph vertex in a graph. Eccentricity of graph vertex is maximal number of edges between the vertex and any other vertex of G .
- **Regularity** of graph G is graph property which is *true* in the case all of the vertices of the graph are of the same degree.
- **Second largest eigenvalue** of graph G is second largest eigenvalue of adjacency matrix of G .
- **Smallest eigenvalue** of graph G is smallest eigenvalue of adjacency matrix of G .
- **Vertex connectivity** of graph G is smallest number of vertices, whose deletion causes G to be cut into several disconnected components.

B. Properties of Collected Graph Datasets

For each of the graph properties in the datasets we created, we measured the minimum (*min*), maximum (*max*), average value (*avg*) and standard deviation (*sd*) of the property. The values we measured on the given datasets are presented in the Table I for the 30 and 32 vertex datasets and in Table II for the 34 and 36 vertex datasets.

We also measured Pearson correlation and Spearman rank correlation coefficients as a metric for determining the predictive potential of the graph data. The values of correlation coefficient measured for individual graph datasets are visualized on the Figs. 2 and 3.

The Fig. 2 contains the visualization of correlation matrices of the Pearson type which is used for measuring of linear correlation between the values of input and output variables. In the Fig. 3 we offer a visualization of Spearman rank correlation matrices. This correlation coefficient is used for measuring the monotonicity of the relationship between the values of input and output variables.

As evident from the visualization of the correlation matrices for our datasets, there are clear relationships between the properties of the graph structures. The most significant of these relations for all created datasets are those pairs of properties between which we measured one of the computed

types of correlation coefficients in the conventional range of $< 0.8, 1 >$ or $< -1, -0.8 >$. In the list below, we present strongest Pearson correlation coefficient measurements for created datasets:

- For the 30-vertex graph dataset the most significant relationships measured by correlation analysis are: Second largest Eigenvalue and Diameter = 0,932; Laplacian spectrum and Diameter = -0,932; Girth and Diameter = -0,881; Domination number and Diameter = -0,880; Smallest Eigenvalue and Largest Eigenvalue = -0,992; Laplacian spectrum and Second largest Eigenvalue = -0,999; Girth and Second largest Eigenvalue = -0,903; Domination number and Second largest Eigenvalue = -0,902; Girth and Laplacian spectrum = 0,904; Domination number and Laplacian spectrum = 0,903; Domination number and Girth = 0,999.
- 32-vertex graph dataset contains following correlations: Matching number and Clique number = -1; Second largest Eigenvalue and Diameter = 0,889; Laplacian spectrum and Diameter = -0,877; Vertex connectivity and Edge connectivity = 1; Smallest Eigenvalue and Largest Eigenvalue = -0,998; Laplacian spectrum and Second largest Eigenvalue = -0,987.
- The number of significant correlations in the 34-vertex graph dataset is highest of created datasets: Diameter and Density = 0,881; Second largest Eigenvalue and Density = 0,866; Laplacian spectrum and Density = -0,859; Girth and Density = -0,941; Group size and Density = 0,897; Chromatic index and Density = 0,999; Edge connectivity and Diameter = -0,874; Vertex connectivity and Diameter = -0,880; Second largest Eigenvalue and Diameter = 0,890; Laplacian spectrum and Diameter = -0,883; Girth and Diameter = -0,910; Group size and Diameter = 0,872; Chromatic index and Diameter = 0,876; Vertex connectivity and Edge connectivity = 0,989; Second largest Eigenvalue and Edge connectivity = -0,835; Laplacian spectrum and Edge connectivity = 0,829; Girth and Edge connectivity = 0,829; Group size and Edge connectivity = -0,868; Second largest Eigenvalue and Vertex connectivity = -0,840; Laplacian spectrum and Vertex connectivity = 0,835; Girth and Vertex connectivity = 0,841; Group size and Vertex connectivity = -0,875; Smallest Eigenvalue and Largest Eigenvalue = -0,992; Laplacian spectrum and Second largest Eigenvalue = -0,992; Girth and Second largest Eigenvalue = -0,864; Group size and Second largest Eigenvalue = 0,852; Chromatic Index and Second largest Eigenvalue = 0,863; Girth and Laplacian spectrum = 0,857; Group size and Laplacian spectrum = -0,847; Chromatic index and Laplacian spectrum = -0,857; Group size and Girth = -0,889; Chromatic index and Girth = -0,939; Chromatic index and Group size = 0,894.
- For the 36-vertex graph dataset the most significant correlations are the following: Smallest Eigenvalue and Largest Eigenvalue = -0,989; Laplacian spectrum and

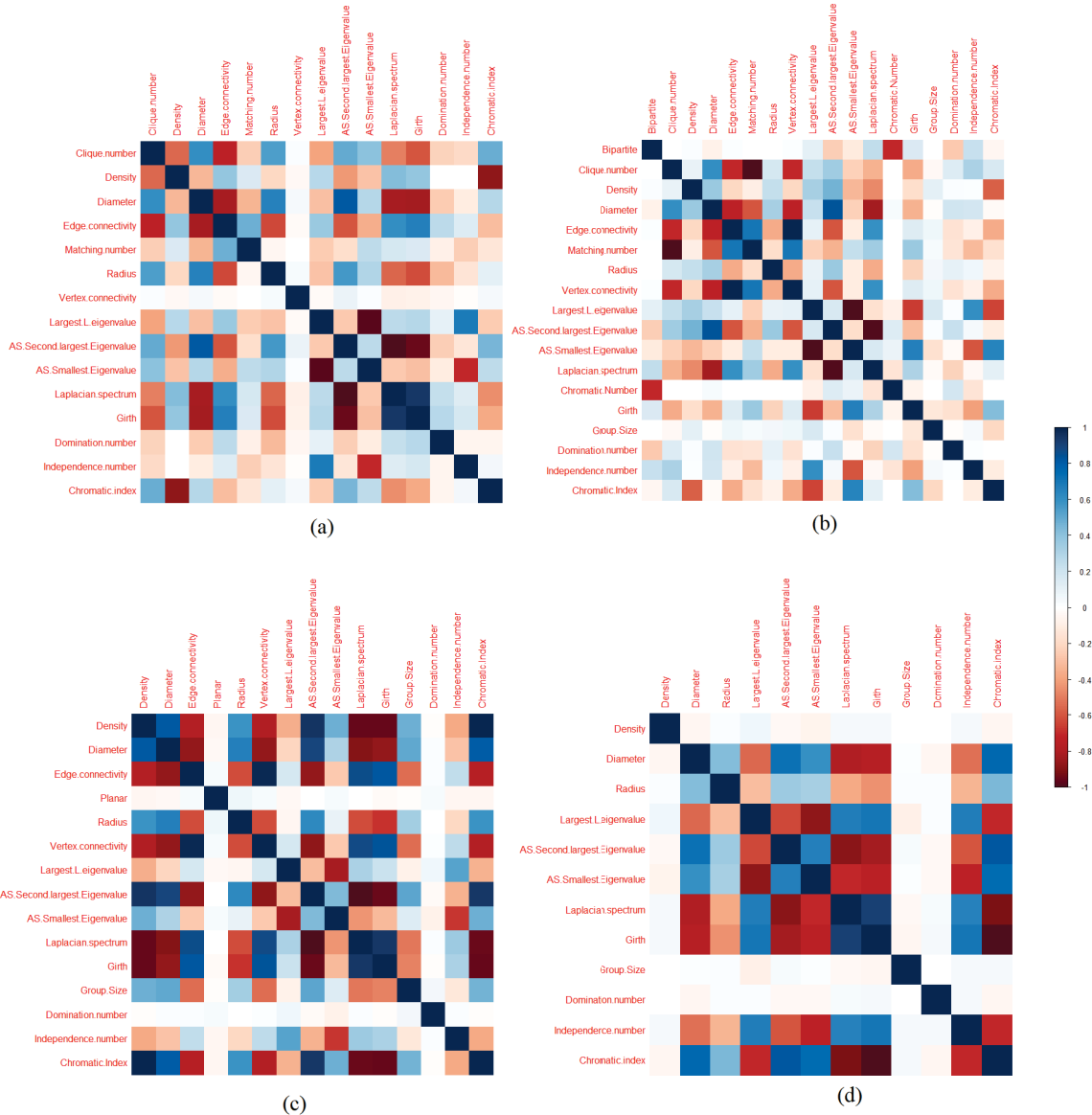


Fig. 2. Correlation matrices for Pearson correlation coefficient for (a) 30 vertex graph dataset, (b) 32 vertex graph dataset, (c) 34 vertex graph dataset and (d) 36 vertex graph dataset

Second largest Eigenvalue = -0,981; Girth and Second largest Eigenvalue = -0,855; Chromatic index and Second largest Eigenvalue = 0,855; Girth and Laplacian spectrum = 0,855; Chromatic index and Laplacian spectrum = -0,855; Chromatic index and Girth = -1.

Based on these relationships found in the data, we should be able to create decision trees that will be suitable for predicting the values of graph properties - especially the chromatic index of the graph.

IV. DECISION TREES FOR GRAPH DATA

In this paper, we use the method of decision trees, where we projected the process of proper edge coloring with the use of

three colors into a classification task. For each of the created datasets of cubic graphs, we assembled a separate decision tree (Figs. 4 - 7), by which we classify the input set of graphs into two groups:

- improperly edge 3-colorable cubic graphs - snarks,
- properly edge 3-colorable cubic graphs.

We reflected this task in the created decision trees into the question "Is input graph G a snark?". Therefore, the value "yes" or "no" is indicated in the decision trees as the answer to this question. On the figs. 4 - 7 answer "yes" is denoted by dark gray, the answer "no" by light gray.

To build decision trees, we used 80% of graphs for training and 20% of graphs as testing sets from each dataset.

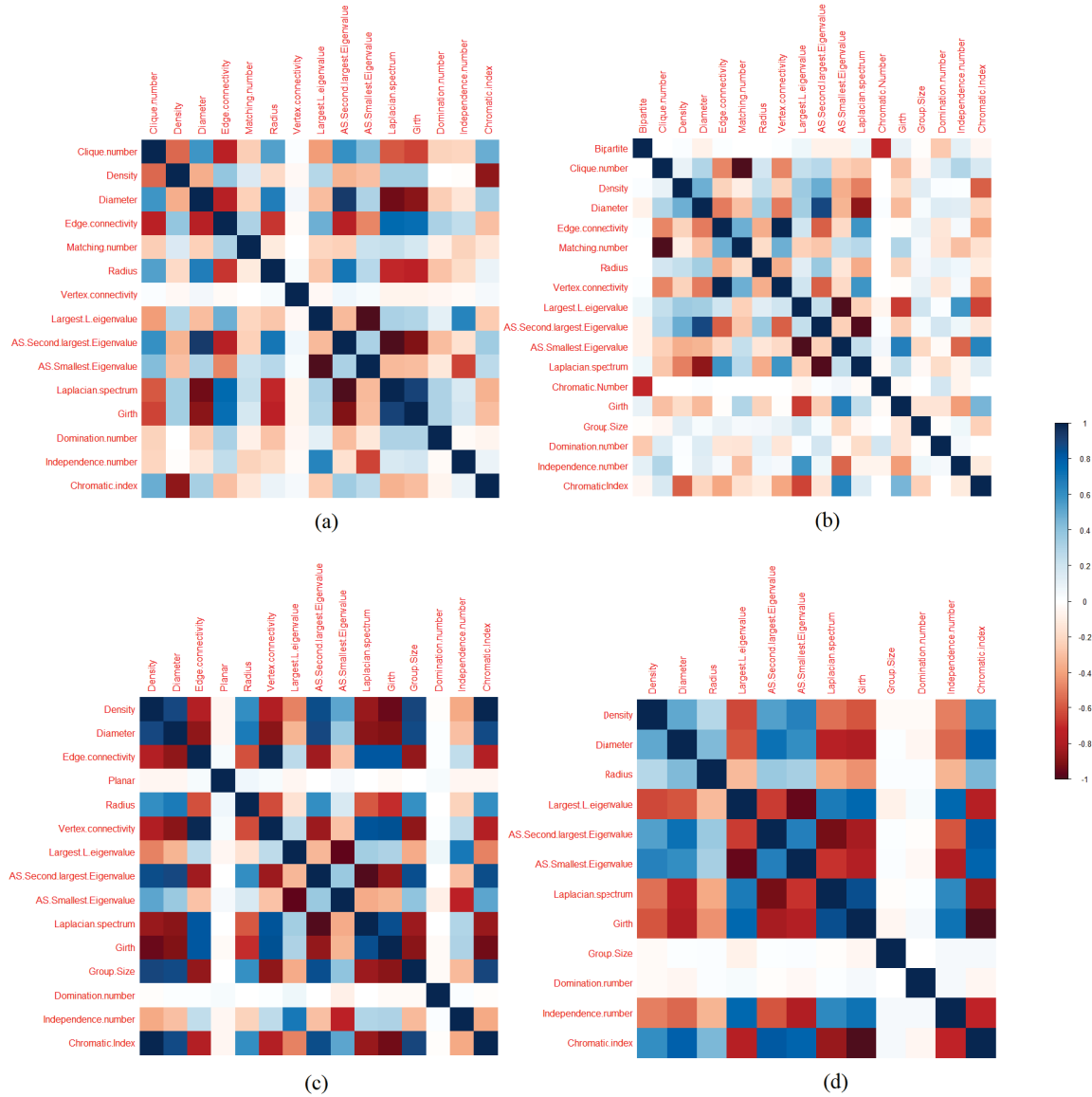


Fig. 3. Correlation matrices for Spearman rank correlation coefficient for (a) 30 vertex graph dataset, (b) 32 vertex graph dataset, (c) 34 vertex graph dataset and (d) 36 vertex graph dataset

In the figs. 4 - 7 we present decision trees constructed on the created datasets. Each node of the decision tree contains property used in decision process with the p -value. Each edge incident with the node contains border for value of this property. Leaves of created decision trees contain the classification of graph data into properly edge 3-colorable cubic graphs and improperly edge 3-colorable cubic graphs.

When studying the decision trees closely, we can see, that in each of the datasets, property of edge 3-colorability of a graph depends on similar set of graph properties, specifically density, second largest eigenvalue, girth, diameter, smallest eigenvalue, radius, group size, vertex connectivity, independence number and largest eigenvalue. It is critical to note, that all of these

properties are computable in lower time complexity compared to proper edge coloring of graph [6], [15], [16]. For the comparison of time complexities of computations see Table III.

The results of the classification of graph data by decision trees are presented in the confusion matrix in the Table IV. Accuracy of the classification into the two chosen groups is computed based on standard accuracy metric [8]:

$$accuracy_S = \frac{t_n + t_p}{t_n + t_p + f_p + f_n}$$

where S is number of vertices of input graphs, t_n is number of true negative samples, t_p is number true positive samples,

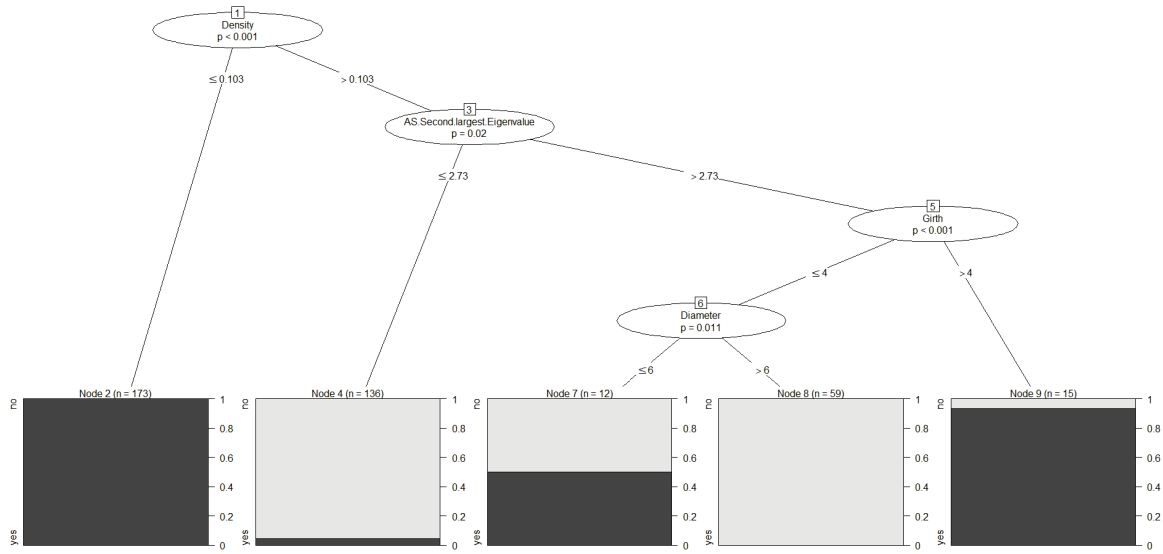


Fig. 4. Decision tree for identification of properly/improperly edge 3-colorable graphs for the dataset of 30 vertex cubic graphs

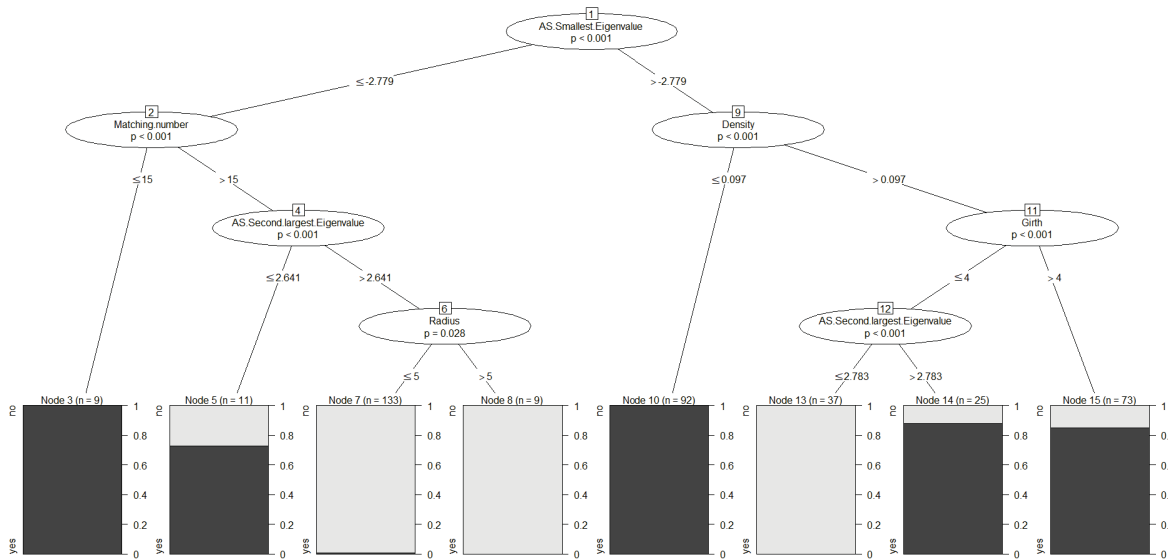


Fig. 5. Decision tree for identification of properly/improperly edge 3-colorable graphs for the dataset of 32 vertex cubic graphs

f_p is number of falsely positive samples and f_n is number of falsely negative samples.

Therefore accuracy of graph classification with the use of created decision trees is:

$$accuracy_{30} = 93.269\%$$

$$accuracy_{32} = 92.857\%$$

$$accuracy_{34} = 96.825\%$$

$$accuracy_{36} = 92.857\%$$

with average accuracy of correct identification of snark in the mixed set of standard cubic graphs and snarks equal to 93.702%.

V. CONCLUSION

With the use of the methods of statistical and predictive analysis, we have shown that within the data set of graph structures, it is possible to measure the predictive potential between individual properties of given graphs. Since most of

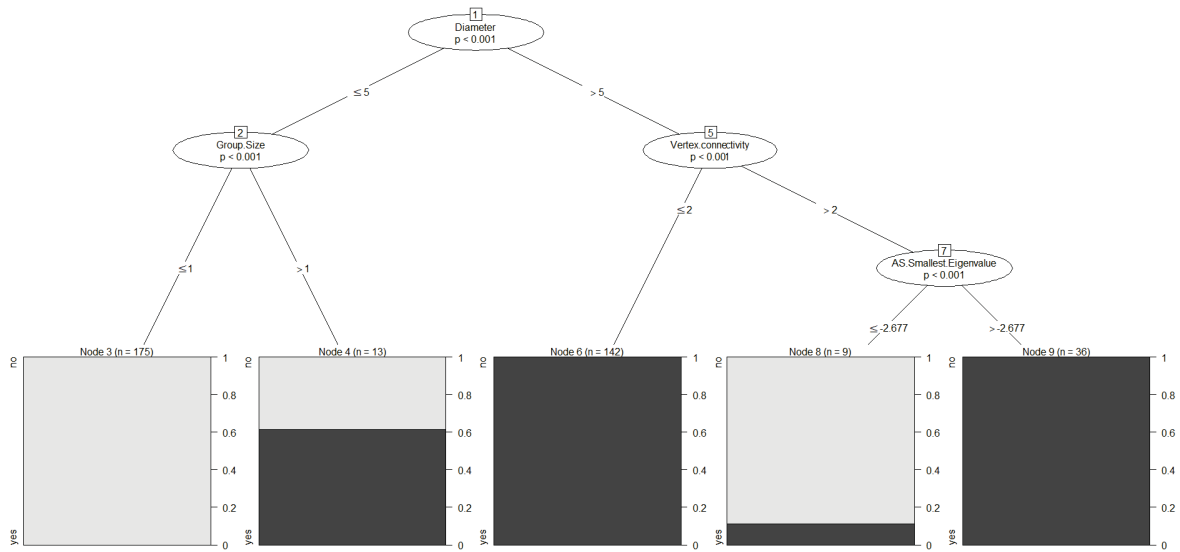


Fig. 6. Decision tree for identification of properly/improperly edge 3-colorable graphs for the dataset of 34 vertex cubic graphs

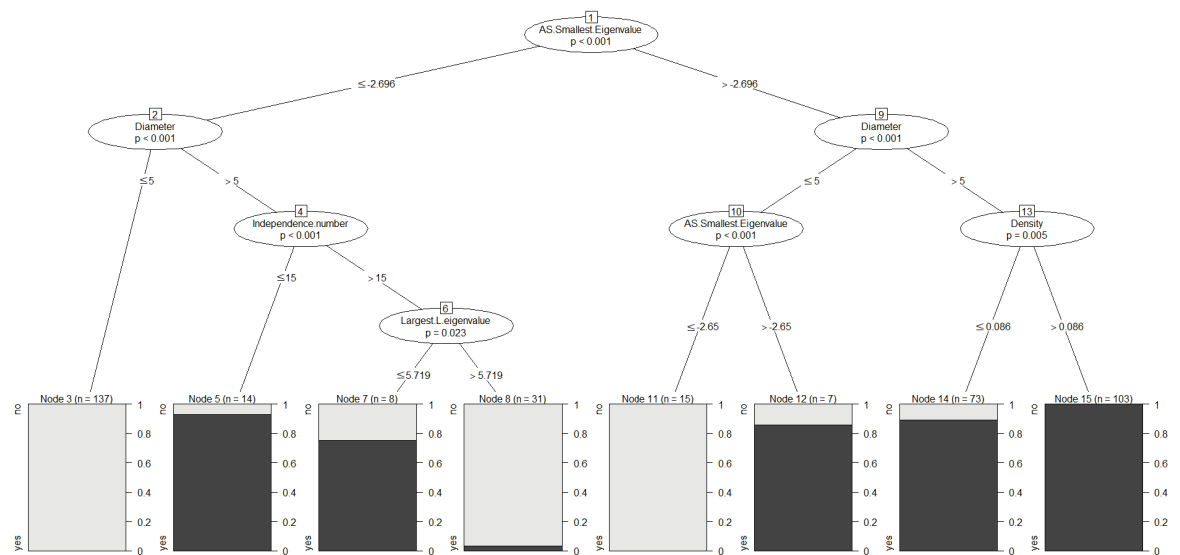


Fig. 7. Decision tree for identification of properly/improperly edge 3-colorable graphs for the dataset of 36 vertex cubic graphs

the algorithms that are used in the measurement of graph properties do not use artificial intelligence methods, this potential can be used in optimizing the measurement of graph property values.

The results presented in this work point to the possibility of applying prediction analysis techniques to accurately estimate the values of graph properties. From the research presented, we can conclude that the value of the chromatic index of a graph, which indicates the number of colors for a regular edge 3-coloring of a cubic graph, is influenced by density, second largest eigenvalue, girth, diameter, smallest eigenvalue, radius, group size, vertex connectivity, independence number and largest eigenvalue (see Fig. 4 - 7).

Future work in this area involves creating a new large dataset (approximately 800 million graphs) containing only relevant graph properties and using the findings obtained in this paper on this dataset, or modification of the created models according to the results. Another direction for future work could be a use of a neural network approach to identify snarks in a set of cubic graphs.

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TABLE III. TIME COMPLEXITY OF ALGORITHMS FOR RELEVANT GRAPH PROPERTY COMPUTATIONS [6], [15], [16]

Graph property	Time complexity
Density of graph	$O(VE)$
Girth of graph	$O(VE)$
Radius of graph	$O(VE)$
Diameter of graph	$O(V\sqrt{E})$
Edge connectivity of graph	$O(E + k^2 V \ln(\frac{V}{k}))$ for k edges
Matching number of graph	$O(VE)$
Eigenvalues of graph	$O(V)$
Edge coloring - naive backtracking	$O(2^{ E(G) })$
Edge coloring - Beigel & Eppstein	$O(2^{\frac{ V(G) }{2}})$
Edge coloring - Kowalik	$O(2^{0.427 V(G) })$

TABLE IV. CONFUSION MATRIX FOR ALL FOUR CREATED GRAPH DATASETS

Predicted value	30 vertex graphs		32 vertex graphs		34 vertex graphs		36 vertex graphs	
	False	True	False	True	False	True	False	True
False	48	2	49	7	59	4	51	5
True	5	49	1	55	0	63	3	53

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