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Automated generation of conjectures on forbidden subgraph characterization

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ABSTRACT

Given a class of graphs $\mathcal{F}$, a forbidden subgraph characterization (FSC) is a set of graphs $\mathcal{H}$ such that a graph G belongs to $\mathcal{F}$ if and only if no graph of $\mathcal{H}$ is isomorphic to an induced subgraph of G. FSCs play a key role in graph theory, and are at the center of many important results obtained in that field. In this paper, we present novel methods that automate the generation of conjectures on FSCs. Since most classes of graphs do not have such characterization, we also describe methods to find less restrictive results in the form of necessary or sufficient conditions to characterize a class of graphs with forbidden subgraphs. Furthermore, while these methods require to explore a possibly infinite search space, we present an enumerative technique that guarantees the discovery of characterizations involving forbidden subgraphs with a limited number of vertices. Another technique, which enables the discovery of characterizations with much larger subgraphs through the use of a heuristic search, is also described. In our experiments, we use these methods to find new theorems on the characterization of well-known graph classes.

1. Introduction

Traditionally, the process of discovering new knowledge in graph theory was carried out by mathematicians, with little assistance from computers. In recent years, mathematicians in that field have turned to computers to find some very important results. A famous illustration of this is the proof of the four color conjecture, which was done in large part using computers [2,22]. Since then, computers have played an increasing role in the discovery of new knowledge in graph theory, and many tools have been proposed for this task. One of the first computer programs for this purpose was Graffiti, developed by Fajtlowicz [8], which has generated over a thousand conjectures as algebraic equations involving graph invariants. Another more recent and equally prolific tool to generate conjectures involving graph invariants is AutoGraphiX (AGX), proposed by Caporossi and Hansen [5]. This last program, which applies the Variable Neighborhood Search metaheuristic [20] to find extremal graphs, can also be used to find graphs satisfying various constraints, to find structural conjectures, to refute conjectures and to suggest proofs.

Although automating the generation of conjectures has been the aim of many works, almost all of these focused on generating conjectures in the form of relations on graph invariants. Yet, as recently suggested by Hansen et al. in [16], there are

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many interesting results in graph theory that take a different form. One of them, known as *forbidden subgraph characterization* (FSC), describes a class of graphs in terms of the subgraphs that these graphs are not allowed to have. A well known FSC, due to Chudnovsky et al. [6], characterizes perfect graphs as the graphs which do not have as induced subgraph any odd cycle containing five or more vertices, or its complement. Another important FSC, due to Beineke [3], characterizes line graphs using nine forbidden graphs, shown in Fig. 1.

In this paper, we present methods to automatically generate conjectures on FSCs. To our knowledge, these methods are the first to be proposed for this specific problem. The rest of the paper is structured as follows. We first introduce some preliminary concepts that will help to understand the rest of the paper. We then describe our methods, by considering three problems: finding sufficient conditions of a characterization involving forbidden subgraphs, finding necessary conditions also using forbidden subgraphs, and finding actual FSCs. We then show how these methods can be used in practice to generate conjectures, and illustrate this by reproducing some known results, as well as generating new ones. Finally, we end this paper with a short summary of our work.

2. Preliminary concepts and definitions

Since this work focuses specifically on characterizations involving forbidden *induced* subgraphs, to lighten the presentation, we will from now on refer to induced subgraphs simply as subgraphs.

Let $\mathcal{G}$ be the set containing all finite graphs. A class of graphs $\mathcal{F} \subseteq \mathcal{G}$ is a possibly infinite set of graphs that share a common property. This common property could be defined using a predicate function pred : $\mathcal{G} \rightarrow$ {true, false}, such that $\forall G \in \mathcal{G},\ \text{pred}(G) = \text{true} \iff G \in \mathcal{F}$. For instance, the class of perfect graphs could be expressed using the following predicate:

$$\text{pred}(G) : \text{if}, \quad \forall \text{ subgraphs } H \text{ of } G,\ \chi(H) = \omega(H) \text{ then true, else false,} \tag{1}$$

where $\chi(H)$ is the smallest number of colors needed to color the vertices of H so that no two adjacent vertices share the same color, i.e. the *chromatic number* of H, and $\omega(H)$ is the maximum order of a clique in H, i.e. its clique number.

Let $\mathcal{H}$ be a set of graphs, we say that a graph G is $\mathcal{H}$-free if there is no graph of $\mathcal{H}$ isomorphic to one of its subgraphs, and denote by $\mathcal{G}_{\mathcal{H}}$ the set of all such graphs. Using this terminology, an FSC of $\mathcal{F}$ is a set of graphs $\mathcal{H}$ such that $\mathcal{G}_{\mathcal{H}} = \mathcal{F}$. As we will see, not every class of graphs has an FSC. For classes that do not have an FSC, we are often interested in finding some weaker rules allowing us to partially characterize the graphs of these classes. These rules come in two forms: *sufficient conditions* (SFSC) and *necessary* conditions (NFSC). Let $\mathcal{F}$ be the class of graphs to characterize and $\mathcal{H}$ be a set of forbidden subgraphs. Sufficient conditions can be expressed as follows: if a graph G is $\mathcal{H}$-free, then it is in $\mathcal{F}$. Thus, a sufficient condition can be stated as $\mathcal{G}_{\mathcal{H}} \subseteq \mathcal{F}$. However, sufficient conditions need not fully describe $\mathcal{F}$. Indeed, if G is not $\mathcal{H}$-free, we cannot use this type of condition to determine if G is in $\mathcal{F}$ or not. On the other hand, necessary conditions can be expressed as follows: if a graph G is in $\mathcal{F}$ then it is $\mathcal{H}$-free or, equivalently, $\mathcal{G}_{\mathcal{H}} \supseteq \mathcal{F}$. Again, necessary conditions may offer only a partial description of $\mathcal{F}$: if G is not in $\mathcal{F}$ then it can either be $\mathcal{H}$-free or not.

Let G be a graph, and $W = \{v_1, v_2, \ldots, v_q\}$ be a subset of $V(G)$. We denote by $G[W]$ or, when the context is clear, by $\langle v_1, v_2, \ldots, v_q \rangle$ the subgraph of G induced by W. Furthermore, let H be another graph, we write $G \simeq H$ when G is isomorphic to H, and $H \subseteq G$ when H is isomorphic to a subgraph of G. The following elementary properties will be used later on to prove more complex results.

Property 1. *Let G_1, G_2, G_3 be three graphs, and $\mathcal{H}_1, \mathcal{H}_2$ be two sets of forbidden subgraphs.*

(a) *If $G_1 \subseteq G_2$ and $G_2 \subseteq G_3$ then $G_1 \subseteq G_3$.*
(b) *If $G_1 \not\subseteq G_2$ and $G_3 \subseteq G_2$ then $G_1 \not\subseteq G_3$.*
(c) *If $G_1 \not\subseteq G_2$ and $G_1 \subseteq G_3$ then $G_3 \not\subseteq G_2$.*
(d) *If $G_1 \subseteq G_2$ then $\mathcal{G}_{\{G_1\}} \subseteq \mathcal{G}_{\{G_2\}}$.*
(e) $\mathcal{G}_{\mathcal{H}_1 \cup \mathcal{H}_2} = \mathcal{G}_{\mathcal{H}_1} \cap \mathcal{G}_{\mathcal{H}_2}$.
(f) *If $\mathcal{H}_1 \subseteq \mathcal{H}_2$ then $\mathcal{G}_{\mathcal{H}_1} \supseteq \mathcal{G}_{\mathcal{H}_2}$.*
(g) *If $G_1 \subseteq G_2$ then $\mathcal{G}_{\{G_1\}} = \mathcal{G}_{\{G_1, G_2\}}$.*

3. Sufficient conditions

Formally, we write an SFSC as G is $\mathcal{H}$-free $\Rightarrow G \in \mathcal{F}$. This expression is logically equivalent to $G \in \overline{\mathcal{F}} \Rightarrow \exists H \in \mathcal{H}$ s.t. $H \subseteq G$, where $\overline{\mathcal{F}} = \mathcal{G} \setminus \mathcal{F}$ is the complement of the graph class $\mathcal{F}$. The task of finding an SFSC can thus be defined as follows: find a set of graphs $\mathcal{H}$ such that

$$\forall G \in \overline{\mathcal{F}}, \quad \exists H \in \mathcal{H} \text{ s.t. } H \subseteq G.$$

While a graph class $\mathcal{F}$ can have many SFSCs, these may not be equally useful. For instance, $\mathcal{H} = \overline{\mathcal{F}}$ is an SFSC of $\mathcal{F}$, but is as complex as the class $\mathcal{F}$ itself. Moreover, let H be the graph composed of a single vertex, $\mathcal{H} = \{H\}$ is an SFSC of $\mathcal{F}$ since H is a subgraph of all graphs of $\overline{\mathcal{F}}$. However, $\mathcal{H}$ offers no real information on $\mathcal{F}$, since each graph of $\mathcal{F}$ also has H as subgraph, i.e. $\mathcal{F} \cap \mathcal{G}_{\mathcal{H}} = \emptyset$. To find useful SFSCs, we need to introduce two partial orders that measure the *tightness* and *simplicity*. The