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A new heuristic for detecting non-Hamiltonicity in cubic graphs

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A R T I C L E I N F O

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A B S T R A C T

We analyse a polyhedron which contains the convex hull of all Hamiltonian cycles of a given undirected connected cubic graph. Our constructed polyhedron is defined by polynomially-many linear constraints in polynomially-many continuous (relaxed) variables. Clearly, the emptiness of the constructed polyhedron implies that the graph is non-Hamiltonian. However, whenever a constructed polyhedron is non-empty, the result is inconclusive. Hence, the following natural question arises: if we assume that a non-empty polyhedron implies Hamiltonicity, how frequently is this diagnosis incorrect? We prove that, in the case of bridge graphs, the constructed polyhedron is always empty. We also demonstrate that some non-bridge non-Hamiltonian cubic graphs induce empty polyhedra as well. We compare our approach to the famous Dantzig–Fulkerson–Johnson relaxation of a TSP, and give empirical evidence which suggests that the latter is infeasible if and only if our constructed polyhedron is also empty. By considering special edge cut sets which are present in most cubic graphs, we describe a heuristic approach, built on our constructed polyhedron, for which incorrect diagnoses of non-Hamiltonian graphs as Hamiltonian appear to be very rare. In particular, for cubic graphs containing up to 18 vertices, only four out of 45,982 undirected connected cubic graphs were so misdiagnosed. By constrast, we demonstrate that an equivalent heuristic, when built on the Dantzig–Fulkerson–Johnson relaxation of a TSP, is mostly unsuccessful in identifying additional non-Hamiltonian graphs. These empirical results suggest that polynomial algorithms based on our constructed polyhedron may be able to correctly identify Hamiltonicity of a cubic graph in all but rare cases.

1. Introduction

The *Hamiltonian cycle problem* (HCP) is a well-known problem that features prominently in complexity theory because it is *NP-complete* [13]. The HCP can be stated simply: given a graph Γ containing N vertices, determine whether Γ contains a simple cycle of length N, or not. Such a cycle is called a *Hamiltonian cycle*. Graphs containing at least one Hamiltonian cycle are called *Hamiltonian* graphs, and those containing no Hamiltonian cycles are called *non-Hamiltonian* graphs. There are many specialised heuristics which attempt to solve HCP, which include rotational transformation algorithms, cycle extension algorithms, long path algorithms, low degree vertices algorithms, multipath search and pruning algorithms. Attempts to solve HCP have also been made by operations research or optimisation communities, such as nonlinear optimisation (e.g. see Filar et al. [10]) and importance sampling (e.g. see Eshragh et al. [9]). The HCP is also closely related to the famous Travelling Salesman Problem (TSP), which is simply the problem of finding the Hamiltonian cycle of optimal length. In the language of the TSP, Hamiltonian cycles are usually called *tours*.

A cubic graph is the one in which every vertex has degree three. The HCP is known to be NP-complete even if only undirected cubic graphs are considered. By assuming cubicity, there is much inherent graph structure that can be taken advantage of by algorithms (e.g. see Eppstein [7]). Indeed, there is still a lot of interest in special properties of not only all cubic graphs, but even special classes of cubic graphs (e.g. see Horev et al. [17]).

More generally, in literature, there have been many approaches towards developing polyhedral sets whose extreme points correspond to solutions of interest. In the case of both TSP and HCP, such a polyhedron is the convex hull of points that are in 1-to-1 correspondence to Hamiltonian cycles (or tours). Let us denote such a polyhedron by $Q:=Q(\Gamma)$ for a given graph Γ. Of course, $Q=\varnothing$ when Γ is non-Hamiltonian. In the TSP literature, some of the most successful theories and algorithms have been based on characterisations of facets of Q (e.g. see Grötschel and Padberg [14]). In the context of HCP, however, explicit identification of a Hamiltonian cycle is not necessary. Indeed, Hamiltonicity is

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equivalent to the determination that $Q \neq \emptyset$. This paper is motivated by the obvious observation that, if a set $\mathcal{P} \supset Q$ is empty, then certainly Q is empty as well. Of course, the challenge is to construct a polytope $\mathcal{P}$ that is so close to Q to increase the chances of successful detection of non-Hamiltonicity. In this paper, we construct such a set $\mathcal{P}$ – determined by a polynomially bounded number of linear constraints in continuous (relaxed) variables – that appears to possess the preceding inclusion property for a vast majority of non-Hamiltonian cubic graphs.

The approaches given in this paper differ from the more traditional approach of identifying facet-inducing cuts in that we attempt to determine *non-Hamiltonicity* by forcing $\mathcal{P}$ to become empty, rather than by seeking to eliminate subtours in an iterative fashion. Although the final approach given in this paper is an iterative procedure, none of the iterates are based upon the result of a previous iteration. Rather, for a given graph, we will outline a series of tests that can be identified in advance, and the failure of any of those tests guarantees non-Hamiltonicity.

Cubic graphs represent a natural test laboratory for this methodology, not only because HCP is still NP-complete, but also because of the availability of reliable public-domain generators (e.g. see Meringer [19]) that are capable of efficiently enumerating all nonequivalent connected cubic graphs of a given size. Our construction of the polyhedron $\mathcal{P}$ is achieved in two stages. First, we propose a base model, containing constraints which are generic for all graphs. Secondly, we add in additional constraints in an iterative fashion whenever certain structures are present in the graph. Importantly, however, these structures can be identified by preprocessing requiring only polynomial-time algorithms.

Specifically, the structures that we search for are those that identify brittle points in the graph. Recently, in Baniasadi et al. [3], it was demonstrated that the set of all connected cubic graphs can be separated into two disjoint subsets, namely *genes* and *descendants*. The key distinction between these two subsets is the presence (or absence) of special edge cut sets known as *cubic crackers*. The following two definitions are paraphrased from Baniasadi et al. [3].

Definition 1.1. In a cubic graph, a k-cracker c_k is an edge cut set of cardinality k containing no adjacent edges, such that no proper subset of c_k is also an edge cut set. A cubic cracker is a cracker with cardinality no greater than 3.

Definition 1.2. A gene is a connected cubic graph that contains no cubic crackers, and a descendant is a connected cubic graph that contains at least one cubic cracker.

In Baniasadi et al. [3], crackers were used to develop a decomposition theory for cubic graphs that exploits genes and crackers. That theory does not include any algorithmic results for identifying non-Hamiltonicity. However, the results of this paper provide strong empirical evidence that cubic crackers contain much information about the Hamiltonicity of a graph. Specifically, consideration of the cubic crackers can very often be used to detect *non-Hamiltonicity*, if it is present. The method presented in this paper either finds that a cubic graph is definitely non-Hamiltonian, or returns an inconclusive result. Since the majority of connected cubic graphs are Hamiltonian [20], the latter outcome is obviously the most common, and by itself does not provide certainty that the graph is Hamiltonian. However, we will demonstrate that the number of false positives (that is, the number of non-Hamiltonian graphs returning an inconclusive result) is extremely low whenever our iterative procedure is used. Since determining whether a polyhedron, defined by polynomially-many linear constraints in polynomially-many continuous variables is empty, can be done by linear programming, this is a problem of polynomial complexity. Hence, the results presented in this paper serve to suggest that polynomial algorithms may be able to correctly identify non-Hamiltonicity of cubic graphs in the vast majority of cases.

Since non-Hamiltonian genes, by definition, do not contain any cubic crackers, the constraints based on the latter cannot be expected to be successful for these graphs. Indeed, they return an inconclusive result in all cases tested to date. Such non-Hamiltonian genes are called *mutants*. It was conjectured in [3] that mutants are extremely rare – indeed, only three such graphs containing 18 or fewer vertices exist. Despite their rarity, their identification may still be considered important; one justification could be that the set of mutants is a superset to the more famous set of (nontrivial) *Snarks* [12]. For this reason an additional heuristic is suggested at the end of this paper that succeeds in correctly identifying two of the three aforementioned graphs as non-Hamiltonian.

A famous related approach is the, now classical, Dantzig–Fulkerson–Johnson relaxation of the TSP with subtour constraints (e.g., see Dantzig et al. [6] and Cook et al. [5]), which we will henceforth refer to as the DFJ relaxation. The constraints of that model, defined in terms of a given graph, also induce a polyhedron $\mathcal{P}_c \supset \mathcal{Q}$. Then, if the polyhedron $\mathcal{P}_c$ is empty, the graph is definitely non-Hamiltonian. Although there are exponentially many subtour constraints, it is possible to determine whether the polyhedron is empty in polynomial time using cutting plane techniques. We will compare the performance of the DFJ relaxation with the method proposed in this paper, in terms of the proportion of non-Hamiltonian graphs identified.

Three previous attempts to construct a desirable polyhedron $\mathcal{P} \supset Q$ were included in the recent Ph.D. theses of Haythorpe [15] and Eshragh [8], and in Avrachenkov et al. [1]. In Haythorpe [15], two of these polyhedra $\mathcal{P}$ in variables corresponding to arcs were constructed, it was conjectured (based on empirical evidence) that both polyhedra are empty for any cubic bridge graph. Bridge graphs are always non-Hamiltonian, and it was conjectured in [11] that, asymptotically, almost all non-Hamiltonian graphs are bridge graphs. However, no other non-Hamiltonian graphs were detected using either of the polyhedra in Haythorpe [15].

In Eshragh [8], and later in Avrachenkov et al. [1], a related but somewhat different polyhedron was constructed. New variables corresponding not only to arcs in a graph, but also to positional information, were introduced. These variables have a probabilistic interpretation – a variable $x^k_{r,ia}$ can be thought of as the probability that arc (i, a) is selected at the r-th step in a Hamiltonian cycle beginning at vertex k. By convention, if vertex a is the first vertex visited in the Hamiltonian cycle after vertex k, then arc (k, a) is said to be the 0-th step of that Hamiltonian cycle. Clearly, in a solution corresponding to a Hamiltonian cycle, the variables must either take values 0 or 1. However, to retain linearity, this binary requirement was relaxed to allow $x^k_{r,ia}$ to simply take continuous values in $[0, 1]$. The polyhedron given in these variables was again demonstrated empirically to be empty for any cubic bridge graph. In addition, a small number of non-bridge non-Hamiltonian graphs also generated empty polyhedra. These results motivated the further analysis and development of this approach, detailed in this paper.

This paper is structured as follows. In Section 2 we prove that our constructed polyhedron is empty whenever induced by a cubic bridge graph. We also demonstrate empirically that this polyhedron constitutes an LP relaxation that is at least as strong as the DFJ relaxation when induced by cubic graphs. In Section 3 we introduce additional constraints based on cubic crackers that permit us to correctly identify the Hamiltonicity of nearly all tested cubic graphs (over 40,000). By contrast, when an equivalent approach based on the DFJ relaxation was applied, very little improvement over their standard model was detected. It thus appears that the variables $x^k_{r,ia}$ can be used to capture valuable