PHOEG Helps Obtaining Extremal Graphs

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Abstract—Extremal Graph Theory aims to determine bounds for graph invariants as well as the graphs attaining those bounds.

We are currently developing PHOEG, an ecosystem of tools designed to help researchers in Extremal Graph Theory. It uses a big relational database of undirected graphs and works with the convex hull of the graphs as points in the invariants space in order to exactly obtain the extremal graphs and optimal bounds on the invariants for some fixed parameters. The results obtained on the restricted finite class of graphs can later be used to infer conjectures. This database also allows us to make queries on those graphs. Once the conjecture defined, PHOEG goes one step further by helping in the process of designing a proof guided by successive applications of transformations from any graph to an extremal graph. To this aim, we use a second database based on a graph data model.

The paper presents ideas and techniques used in PHOEG to assist the study of Extremal Graph Theory.

1. Introduction

Graph Theory often focuses on questions about bounds for some graph invariants. A graph invariant is a function which, given a graph $G$ returns a value that only depends on the structure of $G$ — i.e., it is invariant by isomorphism. When the bounds on these invariants are tight, the graph realizing them are called extremal graph.

This is a specific research field in Graph Theory called Extremal Graph Theory. A generic problem in Extremal Graph Theory consists in finding bounds on some invariants with respect to some constraints. These constraints usually consist in fixing or restricting the value of some other invariants and/or restricting the graphs to a certain class.

One of the first results in Extremal Graph Theory is the theorem from Turán [1] in 1941 who determined the graphs that do not contain a clique of a given order $k$ and maximize the number of edges. These graphs were named the Turán graphs.

The solutions to these problems are parameterized bounds (if the value of an invariant was fixed) and the graphs realizing those bounds. Indeed, such extremal graphs are proofs that the bounds are tight.

These solutions obviously need to be true for all graphs respecting the given constraints and these graphs can be numerous. An often used constraint is to fix the order $n$ of the graphs. But even so, there are already more than a billion of graphs with 12 vertices.

This huge quantity of data creates a need for techniques to determine the extremal graphs and also, to help prove their extremality.

The first project to provide these helps, called Graph, was done by Cvetkovic et al. in 1981 [2]. This led later to a new version called newGRAPH by Brankov et al. [3]. But this tool was only the first of a kind and many other tools were developed.

In 1988, Graffiti was developed by Fajtlowicz [4] and, using heuristics and pre-computed data, was able to generate more than 7,000 conjectures in its first execution.

Later, in 2000, Caporossi and Hansen developed AutoGraphiX [5] which used the variable neighborhood search metaheuristic to determine good candidates for the extremal graphs. Digenes [6] (2013) uses genetic algorithms and provides support for directed graphs.

In 2008, Mélot presented GraPHedron [7]. This tool differs from the previous ones by its ideas. Indeed, rather than trying to find the extremal graphs, GraPHedron uses all the graphs up to some order in the invariant space and then computes the convex hull of these points. The facets of the hull can be seen as inequalities between the chosen invariants and the vertices of the convex hull as extremal graphs. Another difference from the previous tools is that GraPHedron uses an exact approach on small graphs.

While tools such as AutoGraphiX and Graffiti have evolved over the years, GraPHedron did not. This is why we started a complete overhaul of this tool.

This successor, PHOEG, contains a set of tools aimed at speeding the testing of ideas and helping raise new ones. It is mainly composed of a database of graphs enabling fast queries and computations but also of a module named TransProof whose goal is to assist finding proofs for the conjectures.

In the following sections, we present the different aspects of PHOEG and explain some of the main ideas used to help the researcher in studying Extremal Graph Theory. Section 3 describes the core library linking the different tools together. In Section 4 we explain how the database is built as well as how it can be used. Section 5 details how the convex hull is used to generate conjectures in PHOEG. Section 6 describes a module helping to conjecture a for-
banned graph characterization for a specific class of graphs. Finally, Section 7 presents the ideas used in TransProof to assist the construction of a proof by transformation. An idea of the general structure of PHOEG is presented in Figure 1.

Figure 1. General layout of PHOEG

2. Notations and definitions

Common Graph Theory concepts and notations will be used. Readers that are not familiar with these can refer to Graph Theory textbooks [8]. However, we define here some specific notions and notations used in this paper.

In our work, we consider only undirected simple graphs. We note $G \approx H$ if the two graphs $G$ and $H$ are isomorphic. In the computations, we only use one representant for each isomorphism class called the canonical form.

Definition 1. Let $\mathcal{G}$ be the set of all graphs and $G \in \mathcal{G}$ be a graph. We define the canonical form of $G$ (denoted by $C(G)$) as the result of a function $C : \mathcal{G} \rightarrow \mathcal{G}$ such that $\forall H \in \mathcal{G}, C(H) = C(G) \Leftrightarrow H \approx G$.

While this paper aims at presenting PHOEG and not theoretical results, we illustrate some ideas with the following problem concerning the eccentric connectivity index.

Problem (P). Let $\mathcal{G}$ be the set of graphs of order $n$ and size $m$, what is the graph or class of graphs, among those of $\mathcal{G}$, having the maximal eccentric connectivity index ?

The eccentric connectivity index invariant comes from Chemical Graph Theory and is already concerned by several theorems and conjectures [9]. This invariant is computed using the eccentricity and the degree of a vertex.

Definition 2. Let $v$ be a vertex of a graph $G = (V, E)$ with vertex set $V$ and edge set $E$, the eccentricity of $v$ ($ecc(v)$) is the maximal distance between $v$ and any other vertex of $G$, i.e., $ecc(v) = \max_{u \in V} dist(v, u)$.

Definition 3. Let $G = (V, E)$ be a graph with vertex set $V$ and edge set $E$, its eccentric connectivity index (denoted by $\xi^e(G)$) is defined as the sum for all vertices $v$ of the product between the eccentricity of $v$ and its degree, i.e., $\xi^e(G) = \sum_{v \in V} ecc(v) \cdot d(v)$.

In section 5, the convex hull of a set of points corresponding to graphs is used in order to produce conjectures.

Definition 4. Given a finite set $S = x_0, x_1, \ldots, x_n$ in a $p$-dimensional space, the convex hull of $S$ (denoted $conv(S)$) is the smallest convex set containing $S$, i.e., $conv(S) = \left\{ \sum_{i=1}^{n} a_i x_i | (\forall i : a_i \geq 0) \land \sum_{i=1}^{n} a_i = 1 \right\}$. When $S$ is finite, this set forms a convex polytope.

This polytope can be seen as an intersection of halfspaces. It can thus be represented as a system of linear inequalities.

The facets of the polytope are formed by intersections with halfspaces such that none of the interior points are located on the boundaries of the polytope. They are the "sides" of the polytope.

Section 7 explains ideas to prove generated conjectures with help of graph transformations.

Definition 5. Let $\mathcal{G}$ be the set of all graphs, a parameterized graph transformation is a function $\tau_{V,E} : \mathcal{G} \rightarrow \mathcal{G}$ where $V$ is a set of vertices and $E$, a set of edges respecting some constraints defined by the transformation. They usually work by removing or adding edges and vertices given as parameters.

Definition 6. Given a parameterized graph transformation $\tau_{V,E}$, one can build a graph transformation $\tau$ as a function that, given a graph, returns the set of graphs returned by $\tau_{V,E}$ for all allowed values of its parameters.

Graph transformations can be as simple as the removal or addition of an edge or as complex as replacing a subgraph by a new one, possibly with a different number of vertices.

3. Core Library

The whole PHOEG system is built on top of a core library that models graphs and invariants together with a set of tools. Since a desired feature of PHOEG is to be compatible with other graph libraries — in particular, LEMON [10] and the Boost Graph Library [11] — it is implemented as a C++ header templated library.

Although PHOEG’s core library supports graphs of any order, the modules built on top of it are designed to work on small graphs (typically up to order 10 and practically never to more than order 20). The core library consequently provides a graph representation specialized for small graphs, based on a binary encoding of the adjacency matrix. The resulting format is thus quite compact and efficient.

The library also offers implementations for more than a hundred of invariants as well as for graph transformations. Moreover, a set of utilities functions on graphs is provided to help defining new invariants and transformations e.g., iterators on shortest paths or cliques.
Also, thanks to the templates, one can use these functions on a custom graph implementation as well as providing optimized algorithms for some specific graph representation.

4. Invariants Database

While PHOEG provides implementations for invariants and tools to write new ones, many graph invariants come from NP-complete problems, e.g., the maximal clique or the chromatic number of graphs can take time to compute even with optimized algorithms.

This is especially inconvenient when there are millions of graphs to consider. This problem was tackled in GraPhEdron by only computing their values once for each graph and then storing their values in files.

As invariants are constant by isomorphism, each graph is only considered once thanks to its canonical form computed by the nauty software [12].

In PHOEG, those are stored in a PostgreSQL database (containing at least all the graphs up to order 10, that is more than 12 millions graphs, with their values for each invariant). Consequently the queries are written as SQL queries to the database. Query answering thus benefits from the database system features such as optimizations and parallelization.

An example of a PostgreSQL query, using windowing functions, is given in Figure 2. This query gives all the signatures (in the graph6 format [12]) of all the extremal graphs for the sample problem \( P \), together with their order, size and value of \( \xi \).

\[
\text{SELECT } t\text{.signature, } t\text{.n, } t\text{.m, } t\text{.eci FROM }
\text{ (SELECT n.val AS n, m.val AS m,}
\text{ eci.signature, eci.val AS eci,}
\text{ DENSE_RANK() OVER (}
\text{ PARTITION BY n.val, m.val}
\text{ ORDER BY eci.val DESC}
\text{ ) AS pos}
\text{ FROM num_vertices n}
\text{ JOIN num_edges m USING(signature)}
\text{ JOIN eci USING(signature)}
\text{ WHERE n.val <= 10}
\text{ ) } t
\text{ WHERE t.pos = 1}
\text{ ORDER BY t.n, t.m;}
\]

Figure 2. PostgreSQL query obtaining all extremal graphs of order less or equal to 10 for \( \xi \).

In addition, this data can be used in the computation of some invariants for graphs of higher order. e.g., the chromatic number of a graph can be computed using the chromatic number of a subgraph. An automatic dynamic programming module using the database as memory is currently being developed.

A work-in-progress feature to the database part is PgPhoeg, a plugin for PostgreSQL adding support for graph objects. This means adding extra datatypes for graphs plus exporting PHOEG’s graph functions, invariants and transformations to the PostgreSQL database. This allows for server-side computation of the invariants and access to graph manipulation functions in queries, leading to less client-server context transitions and easier writing of complex queries.

The goal of this tool is to be used by researchers in Graph Theory. As they are not necessarily accustomed to the writing SQL queries, the addition of a domain specific language for those kind of queries is a planned feature.

5. Convex Hull

In Extremal Graph Theory, many theorems and conjectures are expressed as inequalities between graph invariants [13], [14]. This observation was used by GraPhEdron by converting them to points whose coordinates are the values of invariants. The convex hull of these points is then computed.

This convex hull and more precisely, its facets, provides inequalities between the invariants used as coordinates. These correspond to bounds on their values that can be of use to define Extremal Graph Theory conjectures.

We note that this idea has led to several results (see e.g., [15]) including a complete answer [16] to an open problem introduced by Ore in 1962 [17]. A difference from existing softwares based on metaheuristics is that these bounds are exact for the graphs used in the convex hull.

The Figure 3 shows this polytope for the sample problem \( P \) with graphs of order 7. The points correspond to the coordinates of the graphs in the invariants space (the size \( m \) and \( \xi \)) and the multiplicity counts the number of graphs satisfying the problem constraints (connected graphs of order 7) that have the same coordinates. Those graphs coordinates and polytope are generated from the PostgreSQL queries shown in Figure 4. The convex hull is computed from the database using PostGIS (a PostgreSQL plugin adding support for geometric and geographic objects manipulation).

![Figure 3. Polytope and graph coordinates for the sample problem with \( n = 7 \).](image-url)
One of the specificity of PHOEG is that it is possible to explore the inner points of the polytope. Indeed, the access to the database and creation of temporary tables allows to query for additional information in the polytope. For example, Figure 5 shows a coloring of the graphs coordinates with the maximum diameter among all the graphs with the same coordinate.

6. Forbidden Graph Characterization

In Extremal Graph Theory, and in Graph Theory in general, classes of graphs are often described by means of a forbidden graph characterization. Such a characterization of a class $G$ of graphs is given by an obstruction set $O$ containing the forbidden graphs. A graph $G$ is a member of $G$ if and only if it has no element of $O$ as substructure (e.g., induced subgraph, graph minor). A classical example of such a characterization is given by the Kuratowski’s theorem [18]. It states that a finite graph is planar if and only if it has no $K_5$ (the complete graph of order 5) nor $K_{3,3}$ (the complete bipartite graph of order 6, see Figure 6) as topological minor.

PHOEG provides a tool addressing this matter. The substructure relations define a preorder. Given a finite class of graphs or a class membership function and a specific substructure relation, PHOEG computes the minimal graphs (not) in the class for this relation, using, e.g., the VF2 algorithm [19] for the subgraph (iso/mono)morphism relation. The output set of minimal graphs provides a proposed obstruction set for the forbidden graph characterization of the input class.

7. Transproof

After obtaining conjectures, one needs to prove them. Let $G$ be the set of graphs concerned by the conjecture and $E \subseteq G$, the set of extremal graphs, a common technique is a proof by transformation. This kind of proof works by defining a set of graph transformations (denoted by $T$) such that, for any graph in $G \setminus E$, there is a transformation returning a new graph, non isomorphic to the previous one and whose value for the studied invariant is closer to the conjectured bound. Incidentally, there exists a proof by transformation of the Turán theorem [20, p.272-273].

One of the most difficult parts of such proofs is finding good transformations. Actually, one not only wants correct transformations but also simple transformations to simplify the proof and as few as possible to avoid long and repetitive proofs (an example with more than 40 transformations can be seen in [21]). We define the simplicity of a transformation as the number of elements of the graph (vertices and edges) touched by the transformation.

Another way to represent these proofs is on the form of a directed graph. The vertices of this graph are the graphs concerned by the conjecture ($G$) and an arc from vertex $A$ to vertex $B$ means that there is a transformation from the graph $A$ to the graph $B$. We call this graph, the metagraph of transformations. With this point of view, a proof by transformation is correct if the metagraph is acyclic and all its sinks (vertices with no exiting arcs) are extremal graphs.

Definition 7. Let $G$ be a set of graphs and $T$ be a set of graph transformations. Let $M$ be the directed graph with vertex set $G$ and arc set $(G, U) \in G \times G | \exists \tau \in T \land \exists H \in \tau(G), H \simeq U$. We call this graph the metagraph of transformations for the given graph set $G$ and transformation set $T$. An example is given in Figure 7.

This idea is exploited in the TransProof module. The metagraph is pre-computed, for a given set of graphs and transformations, and stored inside a database using the graph data model (currently Neo4j [22]). This specific NoSQL database makes queries on the structure of the metagraph.
Definition 8. Let $G = (V, E)$ be a graph. Let $a, b, c$ be vertices in $V$ such that $ab \in E$ and $ac \not\in E$. The rotation on $G$ using the vertices $a, b, c$ is a parameterized graph transformation that removes edge $ab$ and adds edge $ac$.

A rotation thus consists in removing an edge and adding another one. Both these transformations are really simple ones. We can thus only define some simple transformations to be precomputed and stored in the database and use them to generate other more complex transformations by chaining them and adding constraints.

The choice of this basis of transformations requires to be able to generate all transformations from a subset of the simple ones. As an example, one can consider a path of length $l$ where each vertex is replaced by a clique of a given size $k$ and where the clique replacing the vertex in position $i$ is fully joined with the cliques replacing the vertices in position $i - 1$ and $i + 1$ if they exist. Figure 7 represents such a graph for $l = 5$ and $k = 3$. This graph has diameter 5 and one has to remove at least $k$ edges to increase it.

This means that we need not only transformations about edges but also about vertices, e.g., moving a vertex (removing its adjacent edges and adding new ones) means removing and adding a non fixed number of edges depending of the structure of the graph. We also need a way to specify how these edges will be added. We should thus add different transformations based on the ways one can add a vertex to the graph.

With this basis of transformations, we need only to compute simple transformations and store them inside the graph database. This data can then be exploited by queries to the database for more complex transformations.

To this extent, a specific language is being developed where a statement consists of a list of transformations to apply to some parts of the graph and, for each of these transformations, a set of constraints potentially empty. We can thus consider more complex transformations but, for the same reasons as evoked in Section 4, we are still limited to small graphs.

At the time of writing, the graph database contains eight simple transformations, illustrated in Figure 9:

- removing an edge.
- adding an edge.
- rotation.
- moving an edge.
- detour: given $ab$ in $E$ and $c$ in $V$ not adjacent to $a$ or $b$, we replace $ab$ by a path of length 2 joining $a$ to $b$ by going through $c$.
- shortcut: given a path of length 2 joining $a$ to $b$ by going through $c$, we replace that path by a single edge $ab$.
- two-opt: given $ab$ and $cd$ in $E$ such that $ac \not\in E$ and $bd \not\in E$, we replace $ab$ and $cd$ by the $ac$ and $bd$.
- slide: given $ab$ in $E$ and $c$ in $V$ such that $ac \not\in E$ and $bc \in E$, we replace $ab$ by $ac$. This is actually a rotation on $a$, $b$, and $c$ that conserve connectivity.

They are precomputed on all the graphs up to order 9. The number of arcs in the database for the different orders can be seen in Table 1. This data is currently being used to assist finding proofs for several conjectures.

8. Conclusion and future work

We explained how PHOEG exploits its databases to help finding conjectures in Extremal Graph Theory but also characterize classes of graphs via forbidden subgraphs and construct proofs by transformations.
PHOEG is already used for some open problems in Extremal Graph Theory but there is always room for improvement. Indeed, the PostgreSQL database can be used in a form of dynamic programming to compute invariants but also to generate graphs. This asks for ways to keep track of the partially generated classes to avoid recomputing the same graph twice.

The graph database can also be improved by introducing filters removing symmetries among transformations. This could be done by the exploitation of graph automorphism and could greatly reduce the number of arcs of the metagraph.

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