House of Graphs: a database of interesting graphs

Gunnar Brinkmann^a, Kris Coolsaet^a, Jan Goedgebeur^a, Hadrien Mélot^b

^aApplied Mathematics & Computer Science Ghent University Krijgslaan 281-S9, 9000 Ghent, Belgium ^bInstitut d'Informatique Université de Mons Place du Parc, 20 7000 Mons, Belgium

Abstract

In this note we present *House of Graphs* (http://hog.grinvin.org) which is a new database of graphs. The key principle is to have a searchable database and offer – next to complete lists of some graph classes – also a list of special graphs that already turned out to be *interesting* and *relevant* in the study of graph theoretic problems or as counterexamples to conjectures. This list can be extended by users of the database.

Keywords: graph, database, invariant, generator

1. Introduction

On the web one can find several websites with lists of graphs – see e.g. the lists of Brendan McKay [1], Gordon Royle [2], Markus Meringer [3], Frank Ruskey [4] or Ted Spence [5]. In the *Atlas of Graphs* [16] one can even find hardcopy lists with lots of pictures of graphs. Graphs are given as adjacency lists, sometimes with, sometimes without additional data and in various formats. Such lists can serve as a source for intuition when one studies some conjecture and even as a possible source for counterexamples. The website ChemSpider [15] specialising in chemical structures not only

Email addresses: Gunnar.Brinkmann@UGent.be (Gunnar Brinkmann),

Kris.Coolsaet@UGent.be (Kris Coolsaet), Jan.Goedgebeur@UGent.be (Jan Goedgebeur), Hadrien.Melot@UMons.ac.be (Hadrien Mélot)

gives lists of (graph) structures but also allows several chemically motivated ways to search the database.

As the number of graphs grows very fast (see sequence A001349 in the On-line Encyclopedia of Integer Sequences [17]), even with modern computer systems one will not be able to test conjectures or study properties on all graphs up to n vertices unless n is very small. For example, the complete list of connected graphs with 14 vertices contains already 29.003.487.462.848.061 graphs - so that even the computation of simple invariants for all of these graphs is quite a challenge. If one restricts the class of graphs one wants to study or test (e.g., only regular graphs, only 3-regular graphs, etc.), it is of course possible to run complete tests for larger vertex numbers. Unfortunately this is not always possible and most restricted classes of graphs also grow exponentially fast imposing a relatively small limit on the number of vertices for which complete lists can still be tested. The main new functionality of the database presented here is to offer a list of relatively small size that still gives you a good chance to find counterexamples or obtain results with your tests that allow to judge the general situation. For these lists there is also some additional functionality that will be described later on.

Some graphs (e.g., the famous Petersen graph or the Heawood (3,6)cage on 14 vertices) or graph classes (e.g., snarks) appear repeatedly in the literature while others will probably always be just part of the huge mass. So similar to Orwell's famous words: all graphs are interesting, but some graphs are more interesting than others.

If one wants to test a conjecture on a list of graphs, the ideal case would be if one could restrict the tests to graphs that are *interesting* or *relevant* for this conjecture. Here the meaning of *interesting* and *relevant* is very vague, but this already shows how much the question whether a graph is interesting or not depends on the question one wants to study.

In this paper we will not try to give an exact definition of the terms *interesting* or *relevant* – not even in the restricted form *interesting/relevant* for a certain invariant. If you think of a specific graph, this is sufficient to separate the graph from the huge mass of other graphs, proving that the graph is interesting in some respect – and of course the database allows you to add that graph and also offers the possibility to say for which invariants the graph is especially interesting. We consider e.g. counterexamples to known conjectures and extremal graphs to be interesting.

In order to be a rich source of possible counterexamples right from the start, we already added 1570 graphs to the database. Most of these graphs

are extremal graphs found by *GraPHedron* [12], but there are also other graphs like maximal triangle free graphs that occured as Ramsey graphs for triangle Ramsey numbers [6] or graphs that occured as named graphs in the mathematical literature.

The graphs found by GraPHedron are extremal in the following sense: for a given set of p graph invariants, GraPHedron uses a polyhedral approach placing the graphs in p-dimensional space and computing the facets that bound the set. These facets determine linear inequalities between the graph invariants for the set of graphs under consideration. Extremal graphs are graphs where the corresponding point in p-space is a vertex of the polyhedron. This means that the extremal graphs determine the inequalities and in the database they are listed as interesting with respect to the invariants occurring in the inequality.

In some cases a lot of graphs are situated at the same extremal point. We call these sets of graphs *conglomerates*. Typical conglomerates are e.g. trees or complete bipartite graphs. Adding all conglomerates would increase the number of graphs dramatically and would lead to lists that are much larger than desired. All graphs in conglomerates share a specific structure that made them extremal points for the given set of invariants. But this specific structure can be represented by any element of a conglomerate. So we decided to represent conglomerates by one of their elements. Choosing a minimal set of graphs representing all conglomerates is in fact a Minimum Set Covering problem and therefore NP-complete, so we have used some greedy heuristic to determine a relatively small set of graphs representing all conglomerates that occurred during the computations.

2. Functionality of the website

A basic functionality one must expect from every database of graphs is the possibility to download some specific lists of graphs. At the moment the website *House of Graphs* offers (among others) the following lists:

- All graphs registered as interesting in the database.
- All snarks up to 34 vertices (girth 4) resp. 36 vertices (girth 5).
- All IPR-fullerenes up to 160 vertices.
- Complete lists of regular graphs for various combinations of degree, vertex number and girth.

- Vertex-transitive graphs.
- Some classes of planar graphs.

Some of these lists are physically situated on the same server as the website itself, but others are just links to other peoples websites, like those of Brendan McKay [1], Gordon Royle [2], Ted Spence [5] or Markus Meringer [3].

In some cases it is much faster to generate the graphs instead of storing the list and downloading it. *House of Graphs* offers source codes of some graph generation programs (like e.g. *snarkhunter* [9], *minibaum* [8] or *MTF* [7]) and contains links to other pages where such programs (like *genreg* [13], *geng* [11] or *FreeTree* [10]) can be downloaded.

2.1. Search functionality of the website

The list of graphs that are marked as *interesting* plays a special role in this database. For graphs in this list, a lot of invariants (like the chromatic number, the clique number, the diameter, etc.) and also embeddings (drawings) are precomputed and stored.

Furthermore this database can be searched in various ways. In this context "searching" always means that the list of all graphs in the database is reduced to the sublist of graphs that satisfy the search criterion.

It can be searched for:

- A keyword e.g. a search for "Petersen" will give a list containing the Petersen graph, but also a graph that is a Kronecker product involving the line graph of the Petersen graph as that involvement is mentioned in the text belonging to the graph.
- Graphs that are marked as interesting for a certain invariant (e.g. all graphs that are marked interesting for the matching number).
- Graphs where the value of an invariant is in a certain range (e.g. graphs for which the matching number m(G) is between 11 and 13).
- A specific graph to see whether it is already in the database and what information is given on it. The graph can either be described by uploading a file in *graph6* format or an easy text format that is described on the site. Small graphs can also be described by drawing them using a simple graph drawing applet on the site.

Future plans are to make it also possible to restrict the list to graphs that satisfy or do not satisfy some expression in the given invariants – e.g. to graphs that fulfil $m(G) \leq (|V(G)|/2) - 2$.

By applying several restriction steps, these criteria can be combined with each other.

For example, to search for the cubic 6-cage one could apply the following restriction steps: girth $6 \rightarrow$ regular \rightarrow average degree $3 \rightarrow 14$ vertices.

This results in the graph in Figure 1, which is also known as the Heawood graph. The same graph is found by searching for the keywords "Heawood" or "(3,6)-cage".

All lists – complete lists or lists that are the result of a search – can be downloaded in graph6 format or the binary multicode format which are explained on the website. They can also be downloaded in a self-explanatory human readable text format. By browsing through the lists and clicking on graphs in the list additional information on the graph is displayed – like invariant values, the name of the graph, for which invariants the graph is considered interesting or comments on the graph.



Figure 1: The Heawood graph.

2.2. Submitting graphs to the site

It is essential that the list of graphs marked as *interesting* can grow whenever graphs are discovered that turn out to be relevant in the study of some graph theoretic problem. To this end it is necessary that people can submit new graphs to the list. In order to submit a graph to the site you have to register first (which is also free). Having registered, a graph can be submitted in several ways: it can be submitted in any of the formats that are also available as download formats for the graphs. Furthermore some basic graph editor allows to draw graphs. After the graph has been inputted, it is checked whether the graph (or an isomorphic copy) is already in the list.

If the graph is new, the user submitting the graph is considered the owner of the graph and some information on the graph can be filled in, like e.g. the name of the graph, whether it is a counterexample to a conjecture, whether it is the result of a construction, or references to publications where it first occurred. Furthermore, the user can mark some invariants for which he thinks the graph must be considered interesting. In case the graph was submitted by drawing it, this drawing is used as the default visual presentation of the graph, otherwise a simple automatic drawing is computed.

If the graph was already in the list, it is still possible to add comments to the existing graph e.g. about properties not mentioned by the owner when the graph was submitted. The basic information about the graph - e.g. the name of the graph - can only be changed by the owner.

After the graph has been submitted, processes to compute the invariant values are submitted to a background queue. The routines to compute the invariants are from the graph theory environment *Grinvin* [14]. Depending on the load of the server and the difficulty of the invariant to be computed, the time until the invariant information is displayed can range from milliseconds to days. For very large graphs and NP-complete invariants the invariant value may even remain unknown. Information on known values of invariants for graphs where the computation of the invariants may take very long, can be given as a comment.

In the future it should also be possible to submit graphs by uploading e.g. pdf or jpg files of the drawing of the graph. At the moment this is not possible.

Acknowledgements

Jan Goedgebeur is supported by a PhD grant from the Research Foundation of Flanders (FWO).

References

[1] http://cs.anu.edu.au/~bdm/data/.

- [2] http://mapleta.maths.uwa.edu.au/~gordon/.
- [3] http://www.mathe2.uni-bayreuth.de/markus/reggraphs.html.
- [4] http://www.theory.cs.uvic.ca/~cos/.
- [5] http://www.maths.gla.ac.uk/~es/.
- [6] S. Brandt, G. Brinkmann, and T. Harmuth. All Ramsey numbers $r(K_3, G)$ for connected graphs of order 9. *Electronic Journal of Combinatorics*, 5(1), 1998.
- [7] S. Brandt, G. Brinkmann, and T. Harmuth. The generation of maximal triangle-free graphs. *Graphs and Combinatorics*, 16(2):149–157, 2000.
- [8] G. Brinkmann. Fast generation of cubic graphs. Journal of Graph Theory, 23(2):139–149, 1996.
- [9] G. Brinkmann, J. Goedgebeur, and B.D. McKay. Generation of cubic graphs. Discrete Mathematics and Theoretical Computer Science, 13(2):69–80, 2011.
- [10] G. Li and F. Ruskey. The advantages of forward thinking in generating rooted and free trees. pages 939–940, 1999. 10th Annual ACM-SIAM Symposium on Discrete Algorithms (SODA).
- [11] B.D. McKay. Isomorph-free exhaustive generation. Journal of Algorithms, 26:306-324, 1998.
- [12] H. Mélot. Facet defining inequalities among graph invariants: the system graphedron. Discrete Applied Mathematics, 156:1875–1891, 2008.
- [13] M. Meringer. Fast generation of regular graphs and construction of cages. Journal of Graph Theory, 30(2):137–146, 1999.
- [14] A. Peeters, K. Coolsaet, G. Brinkmann, N. Van Cleemput, and V. Fack. Grinvin in a nutshell. *Journal of Mathematical Chemistry*, 45(2):471– 477, 2009. Conference on 20 Years of Molecular Topology in Cluj.
- [15] H.E. Pence and A. Williams. Chemspider: An online chemical information resource. *Journal of Chemical Education*, (87):1123-1124, 2010. http://www.chemspider.com.

- [16] R.C. Read and R.J. Wilson. An Atlas of Graphs. Oxford Science Publications, 1998. ISBN 0-19-825650-4.
- [17] N. Sloane. The on-line encyclopedia of integer sequences. https://oeis.org/.