Looking for the Hardest Hamiltonian Cycle Problem Instances

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- Keywords: Hamiltonian Cycle Problem, Evolutionary Algorithms, Plant Propagation Algorithm, Instance Hardness, NP-Complete.
- Abstract: We use two evolutionary algorithms to make hard instances of the Hamiltonian cycle problem. Hardness, or fitness, is defined as the number of recursions required by Vandegriend-Culberson, the best known exact backtracking algorithm for the problem. The hardest instances, all non-Hamiltonian, display a high degree of regularity and scalability across graph sizes. These graphs are found multiple times through independent runs and in both algorithms, suggestion the search space might contain monotonic paths to the global maximum. The one-bit neighbourhoods of these instances are also analyzed, and show that these hardest instances are separated from the easiest problem instances by just one bit of information. For Hamiltonian-bound graphs, the hardest instances are less uniform and substantially easier than their non-Hamiltonian counterparts. Reasons for these less-conclusive results are presented and discussed.

1 INTRODUCTION

The Hamiltonian cycle problem involves deciding whether an undirected and unweighted graph contains a path that visits every vertex exactly once and returns to the first vertex, closing the loop. In stark contrast to the closely related Euler cycle problem, which is easy, the Hamiltonian cycle problem is notoriously hard, and even has an entry (number 10) on Richard Karp's infamous list of NP-complete problems (Karp, 1972). Under the common assumption that the classes of P and NP are not equal, being NP-complete means that the Hamiltonian cycle problem has no subexponential solving algorithm, but candidate solutions can still be verified in polynomial time (Garey and Johnson, 1990)(Cook, 1971). NP-complete problems are in some sense 'at the summit of NP': if a polynomial time algorithm is found for just one of these problems, the class of NP-complete problems disappears. Unfortunately, such an algorithm is not known for any of the myriad problems in this class, which are therefore intractable even at very small instance sizes.

But the exponential runtime increase for solving algorithms¹ is not as crippling as it might appear on

first sight. As it turns out, there are substantial differences in instance hardness for many NP-complete problems, and literature on the subject is widely available (Cheeseman et al., 1991). One example is graph colorability, for which Daniel Brélaz' algorithm performs significantly better than the problem's exponential upper bound on many instances (Brélaz, 1979)(Turner, 1988). For the satisfiability problem (SAT), which could be considered 'the root of all NPcompleteness', the hardness of individual instances, measured in computational effort required for solving, critically depends on the ratio of clauses to variables in the formula (Larrabee and Tsuji, 1993)(Selman et al., 1996). Instances of SAT with many variables and relatively few clauses are generally speaking easy to decide, because they have many solutions. On the other hand, instances with few variables and many clauses are *also* easy to decide, because they can be quickly asserted to be unsolvable. But right in the middle, around the clause-to-variable ratio of $\alpha \approx 4.26$, where a randomly generated formula has 50 % chance of being solvable, is where the hardest instances occur² (Cheeseman et al., 1991)(Hutter et al., 2014). In this sense, the clause-to-variable ratio α functions as an 'order parameter', or 'predictive data analytic', indicating where to expect the worst

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¹Whenever we say 'solvers' or 'solving algorithms', we always mean *exact* or *complete* algorithms, and never their heuristic or non-deterministic counterparts.

 $^{^{2}}$ For further refinement on solver performance around the phase transition in SAT, see (Coarfa et al., 2000)(Aguirre and Vardi, 2001)

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Figure 1: The hardest instances of the Hamiltonian cycle problem are all non-Hamiltonian, highly structured, and maximally dense. Graphs were found with evolutionary algorithms, and the fitness measured in recursions needed for the Vandegriend-Culberson algorithm, the most efficient backtracker available. The dominant configuration of a 'wall' (left hand side) and a fully connected clique was reached multiple times in independent runs and in both algorithms.

runtimes when solving instances of randomly generated SAT-formulas.

For the Hamilton cycle problem, such an order parameter also exists, and it is again related to the solvability of the individual instance. For any randomly generated graph of V vertices and E edges, the probability of being Hamiltonian is given by

$$P_{Hamiltonian}(V,E) = e^{-e^{-2c}}$$
(1)

which is a strictly increasing function on any finite interval, and in which c depends on E as

$$E = \frac{1}{2} V \cdot ln(V) + \frac{1}{2} V \cdot ln(ln(V)) + cV \quad (2)$$

following the results of János Komlós and Endre Szemerédi (Komlós and Szemerédi, 1983). In this equation, $P_{Hamiltonian}(V,E)$ has its steepest derivative at c = 0, where E = 1/2 V ln(V) + 1/2 V ln(ln(V)). Although this 'threshold point' happens to be at $e^{-1} \approx$ 0.368, rather than a more intuitive 0.5 like in SAT³, this 'Komlós-Szemerédi bound' is considered as the central point for the hardest Hamiltonian problem instances. The number of edges (or equivalently: vertex degree) is consequentially proposed as its order parameter (Cheeseman et al., 1991)(van Horn et al., 2018). For a numerical example: randomly generated undirected graphs of 120 vertices, the hardest Hamiltonian cycle problem instances would occur around 381 edges, where the probability of being Hamiltonian is $\approx 37\%$. Far more edges make for much easier problems instances, as dense graphs contain many Hamiltonian cycles, and one is quickly found. Graphs with far fewer edges are also easy, because they can be qualified as unhamiltonian (i.e. not having a Hamiltonian cycle) relatively fast.

In an attempt to find the absolute hardest of the hardest problem instances, (Sleegers and van den Berg, 2020) used evolutionary algorithms to generate graphs requiring maximum computational effort for the best known bactracking algorithm. Starting off from the Komlós-Szemerédi bound where traditionally the hardest problem instances were found, a stochastic hillclimber and plant propagation algorithm (PPA) produced graphs that required ever more recursions for the Vandegriend-Culberson (henceforth 'Vacul') algorithm, the most efficient backtracking algorithm for the problem known to date (Culberson and Vandegriend, 2011). But NP-completeness

³The origin of this specific value is that the threshold function becomes ever steeper exactly around e^{-1} as graph size increases, approaching a step function as $V \to \infty$.



Figure 2: The hardest instances of the Hamiltonian cycle problem that *do* contain a Hamiltonian cycle. Structure is much less obvious than for the non-Hamiltonian instances, although some premature tendencies towards cliquing might be discerned.

had not surrendered all of its suprises yet: the resulting graphs were found nowhere near the Komlós-Szemerdi bound. They were much denser, and sported a high degree of structural regularity, which might be expressed as low Kolmogorov complexity (Li et al., 2008). The authors hypothesized that exactly for this reason, these very hard problem instances had never shown up in the large randomized ensembles of the aforementioned research endeavours. But the study raised more questions than answers: had the evolutionary algorithms actually converged? Are these almost-regular graphs really the hardest problem instances? And why are they all non-Hamiltonian? What do the hardest Hamiltonian graphs look like? And does the number of edges of the initial graph influence the outcome?

In this study, we will answer some of these questions, and further our knowledge into the problem. First, we will explain the algorithms involved: Vacul's algorithm for solving problem instances, the stochastic hillclimber and the plant propagation algorithms for evolving graphs. Then, the experiment is described; we significantly extend the scope of graph sizes, runs, starting points, and evaluations. We also conduct a 'Hamiltonian-bound' experiment, in which evolving graphs are *forced* to be Hamiltonian, to see how hard these instances can possibly be. Hard, but not nearly as hard as the non-Hamiltonian graphs, as we will shortly see. The paper concludes with a discussion of the results, outlining future research directions and acknowledging the reviewers' efforts.

2 ALGORITHMS

2.1 Hamiltonian Cycle Problem Solver

Over the last century, a great number of deterministic exact solving algorithms have been developed for the Hamiltonian cyle problem. Rooted in dynamic programming, the Help-Karp algorithm is quite memory intensive, but by $O(n^2 \cdot 2^n)$ still holds the lowest time complexity (Held and Karp, 1962). Later algorithms by Frank Rubin (1974), Martello's 'Algorithm 595' (1983), Cheeseman's (1991), Vandegriend & Culberson's (1998) and Van Horn's (2018) are all exact backtracking algorithms, and therefore have a theoretical upper runtime bound of O(v!), but perform significantly better on large ensembles of random graphs due to clever optimization strategies (Rubin, 1974; Martello, 1983; Cheeseman et al., 1991; Culberson and Vandegriend, 2011; van Horn et al., 2018). Still, the hardest graphs for all these depthfirst based algorithms are found around the Komlós-Szemerédi bound, where the probability of a random graph being Hamiltonian goes from almost zero to almost one as *E* increases (eqs.1 and 2).

non-Hamiltonicity checks. The more the better, it seems, as Vacul's algorithm, containing all three techniques, significantly outperforms all the others – even though its hardest instances are *still* near the Komlós-Szemerédi bound (Komlós and Szemerédi, 1983). It is this algorithm, the best backtracker available, that we use for measuring the hardness of Hamiltonian cycle problem instances.

Vacul's algorithm is a depth-first search algorithm that uses pruning, non-Hamiltonicity checks and employs a low-degree first ordering while recursing over the vertices. Techniques for edge pruning and non-Hamiltonicity checks are employed both before and during recursion. The pruning subroutine removes edges that cannot be in any Hamiltonian cycle, based on 'required edges' that must be in a Hamilton cycle, given a problem instance has one. An edge is required if it is connected to a vertex with degree two. The algorithm then uses two pruning methods; the first method seeks out vertices that have a degree higher than two and are connected to two required edges, rendering all other edges removable. The second method looks for paths of required edges that do not (yet) form a Hamilton cycle. If an edge exists that would close such a path prematurely, it should be removed.

The checks for non-Hamiltonicity examine whether the graph cannot contain a Hamilton cycle based on two global properties: having a vertex with degree smaller than two, or the graph being disconnected. Third, the algorithm checks whether the graph is 1-connected, using Tarjan's algorithm (Tarjan, 1972). If any of these three conditions are met, the graph cannot be Hamiltonian and the recursive process can be skipped or be backtracked upon.

2.2 Evolutionary Algorithms

The evolutionary algorithms used for making hard problem instances are a stochastic hillclimber and an implementation of the plant propagation algorithm, adapted from an earlier application to the traveling salesman problem (Selamoğlu and Salhi, 2016)(Geleijn et al., 2019). By applying mutations to the edges of a graph, both algorithms try to iteratively increase its fitness, measured in number of recursions required by the Vacul-algorithm to solve the instance. The more recursions are required, the harder the problem instance, and the fitter the graph. The evolutionary algorithms use three mutation types with equal probability: to **insert** an edge at a random unoccupied place in the graph, to randomly **remove** an existing edge from the graph, and to **move** and edge, which is effectively equal to a remove mutation followed by an insert mutation (on a *different* unoccupied place). In the hillclimber algorithm, one mutation is chosen at random after which the graph is reevaluated. The mutation is reverted iff the resulting graph is unfitter than its parent, and kept otherwise. This process is repeated for a predetermined number of evaluations (or iterations, for this algorithm).

Table 1: The number and mutability of offspring produced by PPA's individuals are based on its fitness rank (1 = fittest).

Rank	1	2	3	4	5	6 - 10
#offspring	6	5	4	3	2	1
#mutations	1	2	5	5	10	20

The plant propagation algorithm is a populationbased algorithm that tries to balance exploration and exploitation by letting the fitter individuals in the population produce many offspring with few mutations, and unfitter individuals in the population few offspring with many mutations. It can be applied to a broad spectrum of continuous, discrete and mixed objective landscapes in scientific, industrial and even artistic optimization problems (Salhi and Fraga, 2011)(Selamoğlu and Salhi, 2016)(Geleijn et al., 2019)(Vrielink and van den Berg, 2019)(Paauw and Van den Berg, 2019). A most recent investigation suggested that one version of the algorithm might be largely parameter independent (de Jonge and van den Berg, 2020).

The implementation of the plant propagation algorithm used in this experiment is closely related to a discrete adaptation that was earlier applied to the traveling salesman problem and the university timetabling problem (Selamoğlu and Salhi, 2016)(Geleijn et al., 2019). Each generation, the population is sorted on fitness after which each individual produces offspring by first copying itself, and then applying a number of mutations to the offspring. If any of a parent's offspring is fitter, it replaces the parent; if multiple offspring are fitter, the *fittest* replaces the parent. The exact numbers of offspring and mutations are predetermined for all ranks in the sorted population (see Table 1). In this study, the population size is 10 and therefore the number of evaluated offspring is 25 in all PPA-runs. These parameters are chosen intuitively, as they abide strongly by PPA's philosophy of balancing the powers of exploration and exploitation, but more efficient parameter settings are ceratinly not unthinkable. The algorithm's source code can be accessed



Figure 3: Recursions required for the hardest graph on the right-side vertical axis versus their corresponding graph size on the horizontal axis. The left graph shows results of the experiment without restrictions on edge mutation, the right graph shows the results of the experiment in which graphs forcibly retained an unmutable Hamiltonian cycle at all times. The bars represent the number of multiple times a graph of maximum recursions was found.

through a public GitHub repository⁴.

3 EXPERIMENT

To obtain the hardest Hamiltonian cycle problem instances, we evolve 560 graphs of sizes $8 \le V \le 14$ in runs of 3000 evaluations. The investigation is split in tow parts: an 'unbound' experiment, in which the evolutionary algorithms are free to modify all the edges, and a 'Hamiltonian-bound' experiment in which the evolutionary algorithms are free to modify all the edges *except* the edges $\{(1,2), (2,3)...(v-1,v), (v,1)\}$, thereby enforcing the presence of a Hamiltonian cycle in the graph at all times.

For the hillclimber runs, twenty randomly generated graphs were evenly dispersed in terms of edge density, ranging from 0 to $1/2V \cdot (V-1)$ edges, corresponding to edge densities $\in \{0\%, 5\%, 10\%...100\%\}$. For the PPA runs, twenty initial populations were made along the same edge density intervals, with all graphs in one population having the same edge density. It should be noted that these densities are fixed only upon initialization, as the evolutionary algorithms are free to insert and remove edges from graphs at every step of a run. The rationale behind these choices however, is that earlier results could have been biased from the initialization on the Komlós-Szemerédi bound. Besides, this approach would cover more of the state space, at least as seen from the initial conditions. In the end, it didn't make much of a difference.

From these evely distributed initial positions, both algorithms ran for 3000 function evaluations. This means 3000 iterations for the stochastic hillclimber, but 120 generations of PPA, which produces 25 offspring, and therefore performs 25 evaluations per generation (see Table 1). These numbers might look small, as do the numbers of vertices in the graphs used, but the number of recursions required for Vacul's solving algorithm in every function evaluation can still easily run in the millions (see Figure 3). And as we are actively pushing towards the maximum, the entire unbound experiment of 280 runs (7 graph sizes with 20 starting points for two evolutionary algorithms) with 3000 function evaluations still took approximately 45 days on 16 cores of the LISA cluster computer at Amsterdam's Science Park⁵. The 280 runs of 3000 evaluations for the Hamiltonianbound experiment took significantly less time, possibly because the Hamiltonian-bound instances require significantly fewer recursions to decide. Hamiltonian instances are *easier*, generally speaking. But if you want to see for yourself, all the experiment's resources are publicly available through a repository⁶.

⁴https://github.com/Joeri1324/evolving-hard-hamiltoncycles

⁵https://userinfo.surfsara.nl/systems/lisa

⁶https://github.com/Joeri1324/evolving-hard-hamilton-cycles

Table 2: The smallest distance between the hardest and easiest problem instances for the Hamiltonian cycle problem is just one bit: inserting an edge on either of the two possible insertion point types makes the hardest (non-Hamiltonian) instance trivially Hamiltonian. Removing an edge from either of the three possible types will make for a (just slightly) easier non-Hamiltonian instance. Only five one-bit operations are possible, due to the highly structured nature of the results. Instance hardness is measured in number of recursions required by Vacul's algorithm.

Graph size	8	9	10	11	12	13	14
Most difficult	67	785	1,673	25,061	61,051	1,139,785	3,091,141
Insert wall #1	8	9	10	11	12	13	14
Insert wall #2	8	-	10	-	12	-	14
Remove clique-clique	63	717	1,577	23,261	57,799	1,071,037	2,943,549
Remove wall-wall	49	-	1,081	-	47,655	-	2,016,877
Remove wall-clique	25	529	1,015	18,561	43,513	894,861	2,387,791

4 RESULTS

4.1 Unbound Experiment

The results of the unbound experiment clearly show the hardest problem instances are all non-Hamiltonian. Both evolutionary algorithms produced structurally similar graphs consisting of a 'clique' and a 'wall' for all vertex numbers (See Figure 1). The clique is a fully connected subset consisting of $V_{c(odd)} = \frac{V-1}{2}$ vertices in odd-sized graphs, and $V_{c(even)} = \frac{V-2}{2}$ vertices in even-sized graphs. Every graph of size V is a subgraph of size V + 1, even though the exact addition of edges differs from odd to even graphs. The edge number of these graphs is consequently given by:

$$(V - V_c) \cdot V_c + 1/2V_c \cdot (V_c - 1)$$
 (3)

with $V_c = V_{c(odd)}$ if V is odd, and

$$(V - V_c) \cdot V_c + 1/2V_c \cdot (V_c - 1) + 1$$
 (4)

with $V_c = V_{c(even)}$ if V is even. These quadratic results suggest that the larger the graph, the further away the hardest instances are from the Komlós-Szemerédi bound, which only increases (double) logarithmically in V. It should be noted that these results strongly contradict earlier findings that find the hardest instances close to the bound (Cheeseman et al., 1991)(Culberson and Vandegriend, 2011). This might be due to the random nature of the test sets, but for the related SAT-problem, two studies led by Moshe Vardi suggest that the hardness peak *itself* might also move, depending on the specific solver used in the experiments (Coarfa et al., 2000)(Aguirre and Vardi, 2001).

On the lognormal scale of Figure 3, the number of recursions roughly follows a straight line with an inclination of 0.78, indicating that for wall-and-clique graphs of size V, the number of recursions increases exponentially as approximately $O(c^{0.78V})$, in which c > 1. The number of required recursions wobbles a bit in V, which is possibly due to discrepancy between odd- and even-sized graphs. In the odd-sized graphs, there are slightly more vertices in the clique, which results in a higher edge density, and possibly more required recursions.

In the unbound experiment, both the plant propagation algorithm and the stochastic hillclimber converged multiple times to the same graph. Hillclimber between 4 and 16 out of 20 runs for each V, averaging at about 11,3 (See the bars in Figure 3, left). In its operation, the stochastic hillclimber is prone to get stuck in local maxima, but the plant propagation algorithm is well equipped for navigating large nonconvex search spaces with its highly mutative offspring at the bottom of the population. Maybe that's why the algorithm did solidly better however, with an average of 14.9 out of 20 runs converging to the (same) wall-and-clique graph, with all values between 11 and 18. It should be noted though, that PPA only outperforms the hillclimber only after approximately 2000 evaluations, an effect that was also witnessed in other problems (Geleijn et al., 2019). Because of the consistent convergence through independent runs of both algorithms, and the insensitivity of PPA to local maxima, it seems possible that the wall-and-clique graphs are indeed the hardest instances of the Hamiltonian cycle problem for Vacul's algorithm. Moreover, this maximum appears to be connected through a state path of monotonically increasing fitness values, but this yet awaits further verification. A slightly eyebrow raising observation is that both algorithms converge somewhat better for even numbers of V.

4.2 One-bit Neighbourhood

As an added bonus, the highly structured results of the unbound experiment allow for an exhaustive mapping of the one-bit neighbourhood of the most diffi-

Table 3: The edge-independent search space increases faster than exponential in the number of vertices, but the percentage of Hamiltonian instances increases also. This results in an ever denser volume of Hamiltonian graphs, which might explain a possible lack of convergence in the evolutionary algorithms for the Hamiltonian-bound experiment. Numbers are rounded.

Vertices	8	9	10	11	12	13	14
Graphs	$2.68 \cdot 10^8$	$6.87 \cdot 10^{10}$	$3.52 \cdot 10^{13}$	$3.60 \cdot 10^{16}$	$7.38 \cdot 10^{19}$	$3.02 \cdot 10^{23}$	$2.48 \cdot 10^{27}$
Hamiltonian	57.9%	66.5%	74.4%	81.0%	86.3%	90.4%	93.4%

cult instances. For the odd-sized graphs, there is only one possible graph type resulting from edge insertion. For the even-sized graphs there are two neighbouring graph types from inserting an edge, due to the extra edge in the wall. Both these edge insertions immediately make the graph Hamiltonian and decidable within V recursions (Table 2). It is a remarkable finding, that the hardest non-Hamiltonian instances and the easiest Hamiltonian instances are separated by just one bit of information.

Removal of an edge can create two one-bit neighbouring graph types in odd-sized graphs, either from removal inside the clique, or removal of a wall-clique edge. In even-sized graphs, a third removal is possible, from the single wall-wall edge. All edge removal operations lower the number of recursions needed to decide the graph, but the effect is much less dramatic than for inserting edges. Even though the number of recursions from edge removal drops between 6% and 63% for the smallest instances, the difference is only between 5% and 33% for the largest instance in this study, and is expected to become ever smaller for larger instances, simply because larger graphs have more edges, so the removal of one could have a smaller impact on recursion.

These neighbourhood results do show however, that the wall-and-clique graphs are at the very least a local maximum of instance hardness. But since both algorithms repeatedly and independently converged to the same graph, and PPA is not sensitive to local maxima, it might well be that these graphs are the hardest instances of the Hamiltonian cycle problem (for Vacul's algorithm). These results could be taken as a suggestion that harder problem instances for the Vandegriend-Culberson algorithm do not exist, but more extensive testing could substantially (dis)confirm this hypothesis.

4.3 Hamiltonian-bound Experiment

For the Hamiltonian-bound experiment, results are much less unisono than for the unbound experiment. The hardest Hamiltonian graphs found by the evolutionary algorithms are still roughly a magnitude easier than the non-Hamiltonian graphs (See Figure 3, right), with the number of recursions increasing as approximately $O(c^{0.62V})$, in which c > 1. Again, this exponent is a fit on only seven data points, needs fu-

ture refinement, but still serves as a rough indication.

The structural resemblance between graphs of different sizes is also much lower (Figure 2). For graphs of size V = 8, the maximum number of recursions was identical in two graphs, reached in 10 out of 40 runs. For V = 9, only 7 out of 40 runs reached any of 4 graphs with maximum recursions, and for larger V, the hardest Hamiltonian instance was unique among 40, with just a single PPA run producing that graph. These results suggest that the hardest possible Hamiltonian instances might not yet have been found, and that harder graphs are still possible. A neighbourhood mapping was not done for these graphs, as the lack of structure makes it relatively cumbersome, and results inconclusive.

5 DISCUSSION

If the problem instances found in the unbound experiment are indeed global maxima, it could indicate that the problem space is largely convex, since the stochastic hillclimber acquires similar results to the PPA. In this sense, The wall-and-clique graph might be sitting on the top of mount hardness, with very easy Hamiltonian instances and very hard non-Hamiltonian instances in its immediate vicinity. For the Hamiltonian-bound experiment, such observations are less expedient, because convergence of the algorithms appears unlikely. So what makes these algorithms perform so bad on the Hamiltonian-bound problem instances? Surely, less freedom from fixing unmutable edges would make a problem easier, right? The converse might actually be true, and the argument is a somewhat bewildering and counterintuitive numerical elaboration resulting from Komlós and Szemerédi early results and some basic combinatorics.

As presented in Equation 1, the probability of a random graph being Hamiltonian sigmoidally depends on the number of edges. But for a complete edge independent search space such as ours, this probability might also be seen as a *frequency*. As a numerical example: for V = 8 and E = 14, Komlós and Szemerédi's equations predict an approximate 61% chance of Hamiltonicity. Equivalently, one could say that 61% of all existable graphs with V = 8 and E = 14 are Hamiltonian. Now the *number* of graphs is equivalent to the number of options for placing the *E* edges between *V* vertices:

$$\binom{1/2 \cdot V \cdot (V-1)}{E} \tag{5}$$

which for V = 8 and E = 14, amounts to 40,116,600 graphs. Of these, approximately 61%, or 24,274,846 gaphs are Hamiltonian, the remaining 39%, or 15,841,754 graphs, are non-Hamiltonian. Summing these results over all possible values of E for a given V gives us the number (or percentage) of Hamiltonian graphs in the entire edge-independent search space (Table 3).

As it turns out, the number of Hamiltonian instances ever more outweigh the number of non-Hamiltonian instances as graphs get larger, possibly making the state space harder to navigate for our evolutionary algorithms, which have identical numbers of evaluations for all V. This observation might also account for the slightly deminishing returns in both experiments for both algorithms as Vincreases. But contrarily, these numbers do not account for graph isomorphism which might be quite influential, but whose detection is a notorious problem in itself (McKay and Piperno, 2014). It is an interesting and non-trivial question to see whether other (meta)heuristic algorithms such as a properly parameterized simulated annealing (Kirkpatrick et al., 1983)(Dahmani et al., 2020) or genetic algorithms (Bäck et al., 1997) do better for this problem. It is also plausible that metaheuristic parameter tuning and/or control might set some serious sods to the dyke, as the problem space clearly changes rapidly as V increases.

On a final note, these graphs might be difficult for Vacul's solving algorithm because its efficiency heavily depends on pruning off edges that cannot be in any Hamilton cycle, which only occurs when a vertex is connected by two required edges. Because of the compact structure of the wall-and-clique graph, this will only happen near the full depth of the search tree, when all but two vertices of the maximum clique are included in a partial solution. But just the ubiquity of pruning techniques throughout history doesn't spell much good for other exact algorithms either when it comes to these graphs. The non-Hamiltonian instances in this study might thereby actually be the hardest around, but more evidence, or perhaps even a proof, is needed to soldify this conjecture.

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