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1 A GENERAL PURPOSE ALGORITHM FOR COUNTING SIMPLE CYCLES AND SIMPLE PATHS OF ANY LENGTH[∗] 2

3 PIERRE-LOUIS GISCARD[†], NILS KRIEGE[‡], AND RICHARD C. WILSON[†]

 Abstract. We describe a general purpose algorithm for counting simple cycles and simple paths 5 of any length ℓ on a (weighted di)graph on N vertices and M edges, achieving a time complexity of $O(N+M+(\ell^{\omega}+\ell\Delta)|S_{\ell}|)$. In this expression, $|S_{\ell}|$ is the number of (weakly) connected induced 7 subgraphs of G on at most ℓ vertices, Δ is the maximum degree of any vertex and ω is the exponent of matrix multiplication. We compare the algorithm complexity both theoretically and experimentally with most of the existing algorithms for the same task. These comparisons show that the algorithm described here is the best general purpose algorithm for the class of graphs where $(\ell^{\omega-1}\Delta^{-1}+1)|S_{\ell}| \leq 11$ | Cycle_e|, with | Cycle_e| the total number of simple cycles of length at most ℓ , including backtracks $|\text{Cycle}_\ell|$, with $|\text{Cycle}_\ell|$ the total number of simple cycles of length at most ℓ , including backtracks 12 and self-loops. On Erdős-Rényi random graphs, we find empirically that this happens when the 13 edge probability is larger than circa $4/N$. In addition, we show that some real-world networks also belong to this class. Finally, the algorithm permits the enumeration of simple cycles and simple paths on networks where vertices are labeled from an alphabet on n letters with a time complexity of $O(N+M+(n^{\ell}\ell^{\omega}+\ell\Delta)|S_{\ell}|)$. A Matlab implementation of the algorithm proposed here is available for download.

18 Key words. Simple cycles; simple paths; self-avoiding walks; self-avoiding polygons; elementary 19 circuits; connected induced subgraphs; networks; graphs; digraphs; labeled graphs

20 AMS subject classifications. 68Q25, 68W40, 05C30, 05C38, 05C22

21 1. Introduction. Counting Hamiltonian cycles and, more generally, all simple 22 cycles passing through a given vertex is a $\#P$ -complete problem [41, 8]. The same 23 classification holds for the problem of counting simple paths with fixed endpoints. 24 Unsurprisingly, the best existing algorithms for counting such cycles have time com-25 plexities $O(2^N \text{poly}(N))$, which scales exponentially with the number N of vertices on 26 the graph. Under the exponential time hypothesis [23], this exponential scaling is, in $27/28$ principle, the best possible.

 Although evaluating the time complexity of an algorithm in the worst case sce- nario is of paramount importance for the classification of algorithmic performance, it is of little relevance to applications which differ significantly from this scenario. This is precisely the case when counting or enumerating simple cycles or simple paths. Real- world networks, be they from sociology, biology or chemistry, are typically very sparse. At the opposite, the worst case scenarios for this task—the complete graphs—are dense and counting or finding cycles and paths of any kind on them presents no inter- est, in particular since everything is already known analytically. An algorithm count- ing simple cycles and paths that is especially tailored for sparse graphs is therefore highly desirable. In particular, we expect the graph sparsity, or some quantity related $38₃₀$ to it, to be a relevant parameter when qualifying the complexity of such an algorithm.

41 In addition to these considerations, we observe that one rarely needs to count 42 all simple cycles or paths. Rather it is typically sufficient to count only those whose

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43 length does not exceed some maximum value ℓ , usually much smaller than the graph

44 size N. Yet, even with these restrictions, the problem of counting simple cycles or 45 simple paths is known to be difficult:

46 THEOREM 21 IN FLUM AND GROHE [16]. Counting simple cycles and simple paths 47 of length ℓ on both directed and undirected graphs, parameterized by ℓ , is $\#W[1]$ -48 complete.

49 The complexity classes $\#W[t], t \geq 1$, introduced by Flum and Grohe, are relevant for 50 parameterized counting problems corresponding to the classes of the W-hierarchy [13] 51 which, in turn, qualify the difficulty of parametrized decision problems according 52 to the type of circuits needed to determine them. Importantly, the class $\#\mathbf{W}[1]$ is 53 believed to *strictly* contain the class $\#W[0]$ of all fixed-parameter tractable (FPT) 54 counting problems. We recall that a counting problem P with input x is said to be 55 fixed-parameter tractable if there is a computable function f of the parameter k , a 56 constant c and an algorithm solving P in $f(k)$ poly $(|x|)$ steps. In this expression, $57 \mid x \mid$ designates the size of the input [16, 20]. For the sake of simplicity, an algorithm 58 achieving a $f(k)$ poly $(|x|)$ time complexity will be said to be FPT.

59

60 In this work, we describe a novel general purpose algorithm for the task of counting 61 simple cycles and simple paths of fixed length ℓ and determine its time complexity:

62 THEOREM 1 (Algorithm for cycle and path counting). Let $G = (V, E)$ be a graph, 63 possibly directed, on N vertices and M edges. Let $|S_{\ell}|$ be the number of connected 64 induced subgraphs of G on at most ℓ vertices. Let Δ be the maximum degree of any 65 vertex on G or, if G is directed, let Δ be the maximum degree of any vertex on the 66 undirected version of G . Then all the simple cycles of length up to ℓ on G can be 67 counted in time

$$
O\left(N+M+\left(\ell^{\omega}+\ell\Delta\right)|S_{\ell}|\right),\,
$$

69 and $O(N + M)$ space. The same complexity is achieved when counting the simple 70 paths of length up to ℓ or the simple cycles/paths with fixed endpoints of length up to $71 \quad \ell.$

 The important result of Theorem 1 is that the time complexity of the general 73 purpose algorithm presented here scales as $\text{poly}(\ell)|S_{\ell}|$. In comparison, we show in Section 4 that the time complexities of all other general purpose algorithms scale 75 either with N^{ℓ} , which is always larger than $|S_{\ell}|$ unless the graph is complete, or with 76 the number $|\text{Cycle}_\ell|$ of simple cycles of length at most ℓ on the graph.¹ From these observations, we expect that the algorithm presented here be the best available for graphs with less connected induced subgraphs than simple cycles,² something we both confirm and precise in Section 4. While deciding a-priori if a graph obeys this condi- tion is difficult, we will see in Section 5 that it is true for several real-world networks and most Erdős-Rényi random graphs.

¹There is one exception to this observation: by extending an approach of Merris to count Hamiltonian cycles [32], we show in Section 4 that all simple cycles can be counted with a time complexity scaling as $\ell \, t_{\rm imm}(\ell) |S_\ell|$, where $t_{\rm imm}(\ell)$ is exponential in ℓ . Hence, this extension is still not competitive with the algorithm presented here.

²Note in this context, backtracks, that is bidirected edges, count as simple cycles. Furthermore the orientation of the cycles counts as well. Thus, for exemple, the complete graph on three vertices with no self-loops, K_3 , has two simple cycles of length 3 and three of length 2.

83 REMARK 1.1. The algorithm presented here is FPT for the problem of counting 84 simple cycles or simple paths of length ℓ , parameterized by ℓ , for the class of graphs 85 where the number of connected induced subgraphs on at most ℓ vertices fulfils $|S_{\ell}| =$ 86 $O(f(\ell) poly(N))$, with f a computable function. This class is the class of bounded 87 degree graphs, for which the existence of an FPT algorithm is not surprising. Indeed, 88 the number of simple cycles / paths of length ℓ is upper bounded by the number of 89 walks of this length, which is at most $\Delta^{\ell}N = f(\ell)$ poly(N). In fact, on bounded degree 90 graphs, even a direct search of the simple cycles achieves the same complexity and 91 constitutes a FPT algorithm.

92

 We prove Theorem 1 in Section 3 using the analytical framework outlined in Section 2 below. Following the proof of Theorem 1, we compare in Section 4 the performance of the algorithm presented here with the time complexities achieved by existing algorithms for the same task. These fall in five families: i) combinatorial sieves; ii) cycle counts by zeon-algebras; iii) cycle counts from combinations of im- manants; iv) special identities for short length cycles on undirected graphs; and v) counting via enumeration. In Section 5, we present numerical experiments validating the results of Theorem 1 and the comparisons of Section 4. We then demonstrate the performance of the algorithm on real-world networks. The Matlab implementation and data sets used for these experiments is available for download at https://www- users.cs.york.ac.uk/∼plg508/. We conclude in Section 6 with an extension of the algorithm for the enumeration of simple cycles on graphs with few labels.

105

106 2. Analytical framework.

 2.1. Counting simple cycles. Our algorithm is based on a recent result from algebraic combinatorics relating the numbers of walks and of simple cycles on any (directed) graph. This result provides an explicit formula for the ordinary generating 110 function of the number $\gamma(\ell)$ of simple cycles of length ℓ multiplied ℓ [17]

111 (1)
$$
\sum_{\ell} \ell \gamma(\ell) z^{\ell} = \sum_{H \prec \text{conn } G} \text{Tr} \left((z \mathsf{A}_H)^{|H|} (1 - z \mathsf{A}_H)^{|N(H)|} \right),
$$

112 where the sum runs over all weakly connected induced subgraphs H of G. Recall 113 that a directed graph is said to be weakly connected if and only if its undirected 114 version is connected. Thus such subgraphs can be found by an algorithm for finding 115 connected induced subgraphs running over the undirected version $G_{\text{undir.}}$ of G. In 116 this expression, |H| designates the number of vertices of the subgraph H and $|N(H)|$ 117 is the number of neighbours of H in G. A neighbour of H in G is a vertex v of G 118 which is not in H and such that there exists at least one edge, possibly directed, from 119 v to a vertex of H or from a vertex of H to v. Finally, A_H is the adjacency matrix of 120 H. From the formula of Eq. (1) for the generating function of $\ell\gamma(\ell)$, we obtain $\gamma(\ell)$ 121 analytically as

$$
122 \quad (2) \quad \gamma(\ell) = \frac{(-1)^{\ell}}{\ell} \sum_{H \prec \text{conn } G} \binom{|N(H)|}{\ell - |H|} (-1)^{|H|} \operatorname{Tr} \left(\mathsf{A}_{H}^{\ell} \right).
$$

123 This explicit result forms the basis of the algorithm proposed here: counting the sim-

124 ple cycles can be achieved by evaluating Eq. (2).

125

 Any algorithmic implementation of Eq. (2) can be easily compared with the best existing combinatorial sieve for counting simple cycles, that of Bax and Franklin [5, 6], by observing that Eq. (2) involves a sum over the weakly connected induced subgraphs of the graph. In contrast, Bax and Franklin's algorithm evaluates a formula involving a sum over all the induced subgraphs, including the non-connected ones. Remarkably, in the worst case scenario—the complete graph—every induced subgraph is connected, making it look like both algorithms should have a comparable complexity. On any other graph however, there are far more induced subgraphs than connected induced subgraphs. This crucial difference means that evaluating Eq. (2) must yield a sig- nificant speed-up as compared to Bax and Franklin's algorithm. This argument is made rigorous by the proof of Theorem 1, which we present in Section 3, and see also Section 4.1. Before we proceed to this proof however, we present extensions of Eq. (2) for counting simple paths and simple cycles with fixed end points.

139

 2.2. Counting simple paths and simple cycles visiting a fixed vertex. To find all the simple paths, we rely once more on a recent result from algebraic combinatorics according to which the ordinary generating function of the number $\pi_{i\rightarrow j}(\ell)$ of simple paths of length ℓ from vertex i to j is the ij-entry of [17]

144 (3)
$$
\sum_{\ell} \pi_{i \to j}(\ell) z^{\ell} = \Big(\sum_{H \prec \text{conn } G} (z \mathsf{A} |_{H})^{|H|-1} (1 - z \mathsf{A} |_{H})^{|N(H)|} \Big)_{ij}.
$$

This expression employs the same notation as that presented in Section 2.1 with the exception of $A|_H$, which represents the adjacency matrix of G restricted to the connected induced subgraph H. That is,

$$
\left(\mathsf{A}|_{H}\right)_{ij} = \begin{cases} \mathsf{A}_{ij}, & \text{if } i, j \in H, \\ 0, & \text{otherwise}, \end{cases} i, j \in G.
$$

 This construction allows one to formally write the sum of the various terms on the right hand side of Eq. (3). Most importantly, from a computational point of view, 147 multiplying by A_H or $A|_H$ has the same time complexity $O(|H|^\omega)$. The number $\pi_{i\rightarrow j}(\ell)$ then follows analytically as

149 (4)
$$
\pi_{i \to j}(\ell) = (-1)^{\ell+1} \sum_{\substack{H \prec \text{conn } G \\ i,j \in H}} \binom{|N(H)|}{\ell+1-|H|} (-1)^{|H|} (\mathsf{A}|_H^{\ell})_{ij},
$$

150 where the sum now runs over all weakly connected induced subgraphs of G containing 151 both i and j. With the notation introduced here, we may also extend the result of 152 Eq. (2) to count only those simple cycles passing through any specified vertex i with

153 (5)
$$
\gamma_i(\ell) = (-1)^{\ell} \sum_{\substack{H \prec_{\text{conn}}^{\text{conn}} \\ i \in H}} \binom{|N(H)|}{\ell - |H|} (-1)^{|H|} (\mathsf{A}|_H^{\ell})_{ii}.
$$

154 In particular, we verify immediately that

$$
\gamma(\ell) = \frac{1}{\ell} \sum_{i=1}^{N} \gamma_i(\ell),
$$

156 as expected.

157 3. Proof of Theorem 1.

158 3.1. The Algorithm: Evaluating Equation (2). The algorithm consists sim- ply in evaluating Eq. (2), (4) or (5), depending on what one wants to count. Given 160 the similar structures of these equations it is readily apparent that of Eqs. (2) , (4) and (5), it is Eq. (2) that necessitates the greatest computational effort to be evalu- ated. This observation is best encapsulated by Eq. (6). For the sake of simplicity and to concretely illustrate our arguments, we will thus determine the time complexity explicitly only in the costliest situation: evaluating Eq. (2).

165

166 We first remark that the binomial coefficient appearing in Eq. (2) is non-zero if 167 and only if $|H| \leq \ell \leq |N(H)| + |H|$. Thus, only those weakly connected induced 168 subgraphs H of G on $|H| \leq \ell$ vertices contribute a term of Eq. (2) when calculating 169 $\gamma(\ell)$. Equivalently, all the weakly connected induced subgraphs of G such that $|H| \leq \ell$ 170 provide all the terms needed to calculate all $\gamma(k)$, $k \leq \ell$. Therefore, for an algorithm 171 based on Eq. (2) to count the simple cycles, it is sufficient for it to find weakly 172 connected induced subgraphs of bounded size. This observation leads to the following 173 result:

LEMMA 2. Let $t(|S_{\ell}|)$ be the time complexity of finding all the weakly connected induced subgraphs of G on at most ℓ vertices. Then the time complexity of determining the number $\gamma(k)$ of simple cycles of length k for all $k \leq \ell$ is

$$
O(t(|S_{\ell}|)+(\ell^{\omega}+\ell\Delta)|S_{\ell}|).
$$

174 Proof. This is straightforward from Eq. (2). First, all the weakly connected in-175 duced subgraphs on $k \leq \ell$ vertices must be found, costing $O(t(|S_{\ell}|))$ time, by defini-176 tion. Second, the terms of Eq. (2) must be evaluated, of which there are $|S_{\ell}|$ in total. 177 Each term involves counting: i) the number of neighbours $|N(H)|$ of a subgraph H 178 on the graph; and ii) the walks of length ℓ on this subgraph, its size being $|H| \leq \ell$. 179 The first step thus costs at most $|H|\Delta = O(\ell\Delta)$ time and the second step requires 180 $|H|^{\omega} = O(\ell^{\omega})$ time. \Box

 3.2. Time complexity of finding the connected induced subgraphs. As we have seen it is necessary and sufficient to find all the weakly connected induced 185 subgraphs of size at most ℓ to count simple cycles of length up to ℓ . This can be done using the standard reverse search algorithm for finding connected induced subgraphs 187 introduced by Avis and Fukuda [3], running on G_{undir} , the undirected version of the graph G. The total running time of this algorithm in our case is [39, 14]

189 (7)
$$
t(|S_{\ell}|) = O\left(N + M + \sum_{k=1}^{\ell-1} |S_{=k}| + \ell^2 |S_{=\ell}|\right) = O\left(N + M + \ell^2 |S_{\ell}|\right),
$$

190 where $M = |E|$ is the number of edges in $G_{\text{undir.}}$ and $|S_{=k}|$ designates the number 191 of connected induced subgraphs on exactly k vertices in G_{undir} . Furthermore this 192 algorithm uses $O(N + M)$ space. We also remark that thanks to reverse search, the 193 algorithm for counting simple cycles can be parallelised: indeed, the contribution of 194 each connected induced subgraph to Eq. (2) can be calculated independently of the 195 other subgraphs. Now combining Eq. (7) with Lemma 2 and noting that $\omega \geq 2$ concludes the proof of Theorem 1. 197

198 REMARK 3.1. The time complexity of the reverse search algorithm for finding the

199 connected induced subgraphs was recently improved upon by Karakashian et al. [26] and

200 then further by K. Elbassioni $\lfloor 14 \rfloor$. Elbassioni describes a polynomial delay algorithm

201 for this task yielding the following time complexity:

COROLLARY 1 IN ELBASSIONI [14]. Finding all the connected induced subgraphs of size $k \leq \ell$ in a graph with maximum degree Δ can be done in

$$
O\left(\ell^2\min\{(N-\ell),\ell\Delta\}(\log N+\Delta+\log\ell)|S_{\ell}|\right),\,
$$

202 total time.

203 Elbassioni also presents an algorithm with a slightly worse time complexity, but en-204 suring a $O(N + M)$ space complexity, see Theorem 1 in [14]. Unfortunately, imple-205 mentations of these recent algorithms have not yet been produced.

206

 3.3. Understanding the time complexity. In the worst case scenario, that 208 is the complete graphs K_N , Theorem 1 implies that the time complexity for counting *all* the simple cycles using the algorithm proposed here is $O(2^N N^{\omega})$ since all induced 210 subgraphs are connected, i.e. $|S_N| = 2^N$. This is marginally better than the com- plexities reported in [27, 5, 6, 38]. However, it is the performance of our algorithm on non-complete graphs that we want to highlight. To this end, it is helpful to recast the time complexity of the algorithm in terms of simple graph parameters.

215 We can do so by using an upper bound on the number $|S_k|$ of connected induced 216 subgraphs on k vertices that involves the maximum degree of any vertex. This result 217 is due to Uehara:

LEMMA 3 (Uehara [39]). Let Δ be the maximum degree of the undirected version $G_{undir.}$ of G. Then the number of connected induced subgraphs on exactly k vertices in $G_{undir.}$ is bounded by

$$
|S_{=k}| \le N \frac{(e\Delta)^k}{(\Delta - 1)k^2}
$$

,

with e the base of the natural logarithm. It follows that

$$
|S_{\ell}| = \sum_{k \leq \ell} |S_{=k}| = O\left(N \frac{\Delta^{\ell}}{(\Delta - 1)\ell^2}\right).
$$

218 Furthermore, on a graph with maximum degree Δ , there are at most $M \leq N\Delta$ edges,

219 so that, by Theorem 1, the time-complexity of counting all the simple cycles of length 220 $k \leq \ell$ is upper bounded by

221 (8a)
$$
O(N(\Delta + 1) + (\ell^{\omega} + \ell \Delta)N \frac{\Delta^{\ell}}{(\Delta - 1)\ell^2} = O(N\Delta + N(\ell^{-1}\Delta + \ell^{\omega - 2})\Delta^{\ell - 1}),
$$

222 (8b) $\sim O(N\ell^{-1}\Delta^{\ell}),$

$$
{}_{223}^{222} \quad (8b) \qquad \sim O(N\ell^{-1}\Delta^{\ell}),
$$

224 where we used that $\Delta/(\Delta - 1) \leq 2$ as soon as the graph has a connected component ²²⁵ with at least 3 vertices. ²²⁶

227 The bound on $|S_{\ell}|$ obtained from Uehara's work is typically very far from tight, especially on graphs that are far from regular, such as scale-free networks. Conse- quently, the time complexity predicted by Eq. (8b) is typically much larger than that observed in numerical experiments. However, Eq. (8b) simplifies the analysis of the 231 time complexity of the algorithm, which will help us compare it with other algorithms 232 for the same task. Observe also that we now easily verify the claim of Remark 1.1 that 233 the algorithm is FPT on bounded degree graphs. In fact, on such graphs $\Delta = O(1)$,

 234 consequently the time complexity scales as N , that is the algorithm is fixed parameter

235 linear.

236

237 4. Detailed comparisons with existing algorithms.

 4.1. Sieve methods. Bax and Bax and Franklin authored two articles detailing the use of combinatorial sieves to count simple cycles [5, 6], which extend previous re- sults by Karp [27] for counting Hamiltonian cycles. Similar techniques had previously been expounded by Khomenko and Golovko [28, 29] and more recently by Perepechko $^{242}_{243}$ and Voropaev [36, 37].

244 All these combinatorial sieves produce the simple cycles via sums over all the induced subgraphs of a graph, i.e. including the non-connected ones. There are $\binom{N}{\ell}$ 245 246 such subgraphs of size ℓ on a graph on N vertices. Assuming ℓ is fixed and much 247 smaller than N, the number of subgraphs is $\Omega(N^{\ell}/\ell!)$. Consequently, counting all 248 simple cycles of length up to ℓ using these sieves takes at least $\Omega(N^{\ell}/\ell!)$ time. If Δ is 249 sub-linear in N, this time complexity is much larger than that achieved by the algo-250 rithm presented here, which takes at most $O(N\Delta^{\ell}/\ell)$ time. In other terms, Eq. (2), 251 which only involves the connected induced subgraphs, yields a significant speed-up. 252 If instead $\Delta = \alpha N$, $0 < \alpha \le 1$, the algorithm presented here is still $1/\alpha^{\ell}$ faster than other combinatorial sieves.3 253

254

268

255 4.2. Zeons algebras. An algorithm for counting simple cycles based on zeon 256 algebras has been proposed by Schott and Staples in [38]. The algorithm relies on the 257 observation that if one attaches a formal variable ξ_e to each edge e of the graph, such 258 that any two such variable commute and $\xi_e^2 = 0$, then the corresponding labeled ad-259 jacency matrix $(A_{\xi})_{ij} := \xi_{ij} A_{ij}$ generates only simple cycles. In other terms, $\text{Tr}(A_{\xi}^{\ell})$ 260 is the number of simple cycles of length ℓ on G. Unfortunately, this method requires 261 formal matrix multiplications and cannot be implemented fully numerically.

263 Schott and Staples proved that the average time taken by this algorithm to count 264 simple cycles of length ℓ is $O(N^4(1 + q)^N)$ where $q \geq \ell N\Delta/(N^2 - \ell)$ [38]. In the 265 typical situation where $\Delta, \ell \ll N$, this cost is therefore at least $O(N^4 e^{\ell \Delta})$. This is 266 exponential in both ℓ and Δ and scales as the fourth power of N, hence always much 267 larger than the $O(N\Delta^{\ell}/\ell)$ bound obtained earlier.

269 4.3. Counting using immanants. In 1983, R. Merris discovered an exact for- 270 mula for counting the Hamiltonian cycles of a graph from a sum over at most N 271 of its immanants [32, 33]. On noting that any simple cycle is Hamiltonian on an 272 unique connected induced subgraph of the graph, Merris' formula is easily extended 273 to count all simple cycles of length up to ℓ via a sum over the $|S_{\ell}|$ connected induced 274 subgraphs of size at most ℓ . In this sum, each term is itself a sum over at most ℓ 275 immanants. Therefore, evaluating the formula takes $O(t(|S_\ell|) + t_{\text{imm}}(\ell)\ell|S_\ell|)$ time,

³In addition, we have empirically observed that the time complexity of the algorithm proposed here scales with an effective parameter $\Delta_{\text{eff}} \ll \Delta$. What determines Δ_{eff} remains unclear.

276 with $t(|S_\ell|)$ and $t_{\text{imm}}(\ell)$ the times taken to find the connected induced subgraphs on at 277 most ℓ vertices and to calculate the required immanants of $\ell \times \ell$ matrices, respectively.

279 In the same spirit, G. Cash described in 2007 an approach for counting simple 280 cycles by solving a system of equations involving selected immanantal polynomials of 281 the graph [9]. For length ℓ simple cycles, Cash's approach stems from the solution 282 of a system involving $p(\ell) - p(\ell - 1)$ equations, where $p(\ell)$ is the number of integer 283 partitions of ℓ . This number grows as $O(e^{x\sqrt{\ell}}\ell^{-3/2})$ with $x = \pi\sqrt{2/3} \sim 2.6$ and consequently solving the system takes $O(e^{7.7\sqrt{\ell}}\ell^{-9/2})$ time. Since the immanantal 285 polynomials of the graph take $O(t_{\text{imm}}(N))$ time to calculate, the cost of Cash's ap- $\frac{286}{286}$ proach is $O(t_{\text{imm}}(N)e^{7.7\sqrt{\ell}}\ell^{-9/2}).$ 287

288 Most importantly, we see that the time complexities of both methods are primar-289 ily influenced by the time taken to calculate the required immanants. Unfortunately, 290 these are difficult to obtain. First, as recognized by Cash, they require computing the 291 matrix of irreducible representations of the symmetric group S_x , a very costly task 292 for large x. Second, while the determinant of an $x \times x$ matrix requires only $O(x^3)$ 293 time, the second immanant d_2 already costs $O(x^c)$ with $3 < c \leq 4$ and computing 294 the last immanant, the permanent, is itself a $\#P$ -complete problem [40]. The perma-295 nent is required by both Merris' and Cash's approaches, meaning that, assuming the 296 exponential time hypothesis, $t_{\text{imm}}(x)$ grows exponentially in x. Comparing with The-297 orem 1, we observe that neither approach can compete with the algorithm proposed ²⁹⁸ here. ²⁹⁹

 In the same vein, Giscard, Rochet and Wilson showed that simple cycles can be counted via a combination of permanents and determinants summed over the set 302 of induced subgraphs of a graph [18], of which there are $\Theta(N^{\ell})$. This particular approach only requires the computation of two immanants per subgraph thereby by- passing the need for computing the matrices of irreducible representations of large symmetric groups, yet requires all induced subgraphs to be considered and thus takes a prohibitive $O(N^{\ell}t_{\text{imm}}(\ell))$ time.⁴ 306

307

308 4.4. Counting short simple cycles on undirected graphs. When only short 309 simple cycles on undirected graphs are of interest, these may be counted via a set of 310 special identities involving the adjacency matrix. This approach was pioneered by 311 Harary and Manvel in the 1970s and has remained popular ever since [21, 1, 10, 34]. 312 In particular, Alon, Yuster and Zwick presented an algorithm for evaluating these 313 identities up to $\ell = 7$ in $O(N^{\omega})$ time and $O(N^2)$ space [1]. This cost grows for longer 314 cycles, being $O(N^{\omega+1})$ when $\ell = 8$, and then $O(N^{\lfloor \ell/2 \rfloor} \log N)$ when $\ell = 9$, 10. To the 315 best of our knowledge, no special identity for counting $\ell > 10$ cycles has been found. 316 There is little doubt that these exist however. Yet, given that the formula for $\ell = 10$ 317 already involves 160 terms [36], any such identity would be extremely cumbersome.

 From this discussion, we conclude that if the graph is undirected, only short sim-320 ple cycles of length $\ell \leq 7$ are desired and $N \leq \Delta^{\frac{\ell}{\omega-1}}$, then we expect Alon, Yuster and Zwick's approach (AYZ) to be faster than the algorithm presented here. In practice, we find AYZ to be faster in many cases where this condition is not met, presumably

⁴Even if a reduction to connected induced subgraphs can be devised for this method, which would yield a $O(t(S_\ell)+t_{\text{imm}}(\ell)|S_\ell|)$ time complexity, it would only marginally improve upon Merris' approach and would still be worse than that of the algorithm presented here.

329 Finally, we note that the space required for running AYZ scales as $O(N^2)$ rather 330 than $O(N + M)$, the former being much larger than the latter on sparse graphs. We found this to be AYZ main limitation in practice,⁵ barring us from making compu- tations on networks with over 12,000 nodes. This memory cost is unavoidable since AYZ necessitates the computation of powers of the adjacency matrix A of the graph, which quickly become dense even on large sparse graphs. Recall in particular, that A^x is full for x larger than the graph diameter.

336

 4.5. Counting simple cycles via enumeration. Enumerating the simple cy- cles or simple paths of a graph, that is producing their vertex sequences, is much more time consuming than simply counting them. The best general purpose algorithm for this task is still Johnson's 1975 landmark algorithm [25, 31], which achieves a time 341 complexity of $O((N + M)(|\text{Cycle}_N| + 1)) \sim O(N\Delta |\text{Cycle}_N|)$. In this expression, $\lfloor \text{Cycle}_N \rfloor$ is the total number of simple cycles (or of simple paths) on G, including backtracks, that is simple cycles of length 2. This result was recently improved on 344 undirected graphs to $O(N (|\text{Cycle}_N| + 1) + M)$, a scaling which is optimal for this $\frac{345}{346}$ task [7].

347 In the worst case scenario, i.e. on the complete graph K_N , $|\text{Cycle}_N| = O(N!)$, that is enumerating all simple cycles takes factorial time. For this reason, counting simple cycles via enumeration has often been deemed greatly inefficient, in particular 350 in comparison with the "only" exponential cost $O(2^N \text{poly}(N))$ achieved by the algo- rithm presented here as well as other approaches [6]. This conclusion follows from a peculiarity of dense graphs however and for sparse graphs it is not so. ³⁵³

Indeed, evaluating Eq. (2) to count all the simple cycles on a graph costs $O(N^{\omega}|S_N|)$. It follows that if $N^{\omega}|S_N| \geq N\Delta |\text{Cycle}_N|$, then Johnson's algorithm and its variants can count all the simple cycles of a graph via enumeration faster than any combinatorial sieve, including the one presented here. When counting simple cycles of fixed maximum length ℓ , Johnson's algorithm takes $O(N + M + (\ell + \ell \Delta)|\text{Cycle}_\ell|)$ time, $|\text{Cycle}_\ell|$ being the total number of simple cycles of length up to ℓ . This means in order for the algorithm presented here to be faster than Johnson's the following must hold

$$
\left(\frac{\ell^{\omega-1}}{\Delta}+1\right)|S_{\ell}| \leq |\text{Cycle}_{\ell}|.
$$

354 Unfortunately, it is very difficult to estimate the ratio $|S_{\ell}|/|\text{Cycle}_{\ell}|$ in a preprocessing stage so as to decide which algorithm to use. Furthermore, the problem of charac- terising graphs for which the number of connected induced subgraphs is larger than the number of simple cycles is, to the best of our knowledge, an open mathematical question beyond the scope of this work. Rigorously, we may only conclude that for any number N of vertices, there must be a critical density above which the algorithm presented here will be faster than Johnson's. We undertake an empirical study of 361 this density in Section 5 on Erdős-Rényi random graphs and show it to be so small

⁵That is, beyond the fact that AYZ is limited to $\ell = 7$ on undirected graphs.

 that the resulting graphs are disconnected with very high probability. In addition, we also study two families of real-world networks exemplifying the interplay between connected induced subgraphs and simple cycles.

366 4.6. Relation to subgraph counting algorithms. Given a pattern graph H and a graph G, the *subgraph counting problem* is to determine the number of (induced) subgraphs of G that are isomorphic to H. This problem is well studied in undirected graphs and generalizes the problem of counting cycles. Therefore, we briefly summa- rize results on the subgraph counting problem, in particular, when parameterized by the size of the pattern graph $k = |V(H)|$.

 When G is a planar graph on N vertices the problem can be solved in time $N2^{O(k)}$ [12] improving the seminal FPT algorithm by Eppstein, which achieves $N k^{O(k)}$ 375 time [15]. Nešetřil and Ossona de Mendez introduced classes of graphs with bounded expansion, which include the planar graphs as well as the graphs of bounded degree. For these classes they have shown that the number of satisfying assignments of a Boolean query with a fixed number of free variables can be counted in time linear in N $[35,$ Theorem 18.9, which solves the subgraph counting problem for patterns of a fixed size as a special case. An improved algorithm tailored to counting subgraphs 381 was proposed by Demaine et al. [11] and achieves a time complexity of $O(6^k t^k k^2 N)$, where t is the height of a tree-depth decomposition of G. Again the approach yields a linear time FPT algorithm in graph classes of bounded expansion when parametrised by k. The running times of the above mentioned algorithms typically hide enormous constants and, to the best of our knowledge, have for this reason not been applied in practice. ³⁸⁷

 Technically related to our work is the method introduced by Amini et al. [2] to count subgraphs by homomorphisms using a combinatorial sieve. Their approach can be seen as a generalisation of the standard sieve methods for counting cycles to arbi- trary graphs, but does not overcome the drawbacks regarding running time discussed in Section 4.1.

 5. Experiments. In this section we present numerical evidence for the perfor- mance of a Matlab implementation of the algorithm presented in this work. Note that this implementation incorporates a preprocessing stage which removes all sources, sinks and isolated vertices of the graph. We compare it with both Johnson's and AYZ algorithms since, following Section 4, these are the only competitive algorithms for counting simple cycles. For the former we use Howbert's freely available Matlab im- plementation [22], while for the latter we wrote a Matlab code, available for download. All the calculations reported here have been made on a MacBook Pro laptop with 3.1 GHz Intel Core i7 processor and 8 GB of RAM running Matlab R2016a.

 5.1. Erdős-Rényi random graphs. We begin by considering undirected Erdős-405 Rényi random graphs $ER(N, p)$. These random graphs are determined by two param-406 eters: the number N of vertices and the probability p that any one undirected edge in the graph exists (with the exception of self-loops). The expected number of edges in ER(N, p) is $pN(N-1)/2$ so that the expected graph sparsity equals p.

FIGURE 1. Experimental comparison of Johnson's algorithm with the algorithm presented here. The blue dots are the observed values of the critical edge probability below which Johnson's algorithm is the fastest. The red line shows the best fit of the blue data points of the form $p_{critical}(N)$ = $a + b \log(N)/N$, which is $p_{critical}(N) = -0.27 + 3.17 \log(N)/N$. The blue line shows the best fit of the blue data points of the form $p_{critical}(N) = a + b/N$, which is $p_{critical}(N) = 8.5 \times 10^{-4} + 4.28/N$. Since the latter fit is clearly better than the former, we retain $p_{critical}(N) \simeq 4.3/N$ as model when discussing $p_{critical}$ in the text.

410 5.1.1. Comparison with Johnson's algorithm. We undertook the compari-411 son on two ranges of parameters: small graphs $5 \leq N \leq 30$, on which we compared 412 the times taken by both algorithms to count all the simple cycles; and on large graphs $413 \text{ } N \geq 1,000$, for which we counted simple cycles of length up to 5 only.

415 On small graphs, for each value of N from 5 to 22 as well as for $N = 25$ and 30, 416 we determined the critical value $p_{critical}(N)$ of p below which Johnson's algorithm is 417 the fastest by incrementing p from 0 to 1 by steps of 10^{-2} at N fixed. For each value 418 of p, we ran both algorithms 20 times and compared the averaged time taken, except 419 for $N = 25$ and 30 where we ran the algorithms only twice per value of p. The results 420 are shown on Figure 1. Empirically we observe that for small graphs, $N \leq 30$, John-421 son's algorithm is faster to count all simple cycles whenever $p \leq p_{\text{critical}}(N) \approx 4.3/N$. 422 Equivalently, this means that Johnson's algorithm can be expected to be faster than 423 the algorithm presented here whenever the average degree is close to 4 or smaller.

425 On large graphs $p_{\text{critical}}(N)$ falls further, being seemingly less than $1/N$ when 426 counting simple cycles of length up to 5 on Erdős-Rényi graphs with 20,000 vertices. 427 In any case, we remark that for $N \gg 1$ and $p < \log(N)/N$, $ER(N, p)$ is known to be 428 almost surely disconnected. Given that we observed that $p_{critical}(N) = O(1/N)$, it 429 seems that for Johnson's algorithm to be the fastest, an Erdős-Rényi random graph 430 must be so sparse as to be disconnected in many small components. 431

432 5.1.2. Comparison with AYZ. The algorithm of Alon, Yuster and Zwick is 433 almost always the fastest to count simple cycles of length only up to 7 on undirected 434 Erdős-Rényi random graphs. Indeed, we find that as soon as the graph is *denser* than 435 pcritical $\approx 1.23/N$, for $N \leq 10,000$, then AYZ is faster than the algorithm presented 436 here. The value of p_{critical} slowly increases with larger values of N and is around

437 pcritical $\simeq 1.3/N$ for $N \sim 12,000$. Unfortunately, the memory consumption of AYZ barres us from directly studying the performances of both algorithms on larger graphs. 439 Rather, an extrapolation of the increase of p_{critical} suggests that it crosses $\log(N)/N$ when N is well over 10^6 . This is widely beyond what can be reached by AYZ, and so large as to render the algorithm presented here prohibitively slow. We must thus conclude that AYZ remains the fastest algorithm on Erd˝os-R´enyi random graphs for counting simple cycles of length 7 or less.

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444
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445 5.2. Real-world networks. We applied the algorithm presented in this work as well as those of AYZ and Johnson to compare their performances on three real-world networks, two of which are undirected and one is both weighted and directed:

- ACTORS: This network represents collaborations between movie actors and was gen- erated and analysed by Barab´asi and Albert [4]. Each actor constitutes a vertex and an edge represents that the two actors were cast together in the ⁴⁵³ same movie.
- INFECTIOUS: A network representation of the face-to-face contacts between visitors of the exhibition Infectious: Stay Away held in Dublin in 2009 [24]. Each edge corresponds to face-to-face interaction lasting for at least 20 seconds.

458 All data sets were obtained from the KONECT website [30], where further information on the data sets is available. The networks are undirected and have parallel edges. In order to systematically study the effect of sparsity, we generated several instances of each network by deleting edges with multiplicity below a given threshold as follows. Starting with the graph with all edges present, we successively removed all edges 463 with multiplicity $1, 2, \ldots$. A new instance is created whenever at least 80 edge were removed from the previous instance. This results in a sequence of graphs with de- creasing density progressively retaining only the most important edges. The sequence based on the Actors network comprises 31 graphs, while the sequence based on the Infectious network comprises 8 graphs. ⁴⁶⁸

 WIKIELECTIONS: A weighted directed network representing the votes of Wikipedia users during elections to adminship [42]. Each user corresponds to a vertex, 471 and a directed edge from user u_1 to user u_2 exists if and only if u_1 voted 472 during the election of u_2 . This edge is given a $+1$ weight if user u_1 supported 473 u_2 candidacy and -1 otherwise. No pruning of the edges was operated on this network.

 The Wikielections network has 8289 vertices and 12915 directed edges. It is a scale-477 free graph with maximum out-degree $\Delta^{\text{out}} = 266$ and maximum in-degree $\Delta^{\text{in}} = 191$. Being directed, the Wikielections network cannot be studied with AYZ, which is lim- ited to undirected graphs, nor can it be studied with Howbert's implementation of Johnson's algorithm.

 In all cases, in order to accurately describe the performances of the algorithm 483 presented here, we provide, for each graph, the time τ_{ℓ} it takes for counting all simple 484 cycles of length up to ℓ , as well as the parameter governing the scaling of this time 485 with ℓ . Indeed, while τ_{ℓ} is upper bounded by $N\Delta^{\ell}/\ell$ as per Eq. (8b), empirically, 486 we find it to scale as $\tau_{\ell} \propto \Delta_{\text{eff}}^{\ell}$ with $\Delta_{\text{eff}} < \Delta$. This effective scaling parameter 487 is determined numerically by fitting τ_{ℓ} with $a \times \Delta_{\text{eff}}^{\ell} + b$, where a and b are fitted

- 488 constants. Surprisingly, we did not find any relation between Δ_{eff} and the maximum, 489 mean, or median of the vertex degrees. What determines its value in practice remains
-
- 490 unclear.

TABLE $1\,$

Counting simple cycles on some graphs of the ACTORS data set. The time taken by the algorithm presented in this work is labelled by "A", while "J" refers to the time taken by Johnson's algorithm. We report the time taken by AYZ only when simple cycles of length 7 or less are counted. Because of memory limitations, we could not run AYZ on graphs 1 to 4, which we designated by "OOM" for "out of memory".

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Counting simple cycles on the graphs of the INFECTIOUS data set. The time taken by the algorithm presented in this work labelled by ${}^{\eta}A$ ", while "J" refers to the time taken by Johnson's algorithm. We report the time taken by AYZ only when simple cycles of length 7 or less are counted.

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⁴⁹⁶ Finally, we turn to the Wikielections network which, as indicated earlier, is 497 both directed and signed. The sign of a simple cycle being the product of the signs 498 of its edges, we propose to demonstrate the algorithm capabilities by finding the 499 numbers p_ℓ and n_ℓ of positive and negative simple cycles of length $\ell \leq 6$, respectively. 500 Indeed, since it is sufficient to run the algorithm twice to obtain both p_ℓ and n_ℓ . 501 More precisely, running the algorithm once on the signed network yields $p_\ell - n_\ell$, 502 while running it on its unsigned version provides $p_\ell + n_\ell$.

TABLE 3

Number of positive and negative simple cycles of length ℓ up to 6 on the Wikielections directed network and the time taken to count them. Here $\Delta_{\text{eff}} \simeq 35$.

 6. Finding labelled simple cycles and simple paths. In some applications, such as chemoinformatics, counting the simple cycles or simple paths of a network is not sufficient. Rather, the vertices of the network may be labelled and it is then necessary to find all sequences of labels corresponding to simple cycles/paths on the network. If there are as many different labels as vertices, that is each vertex has its own label, then this task is best addressed by Johnson's algorithm discussed earlier 509 [25].

510

 In typical applications however, the number of labels is much smaller than the number of vertices. For example, on a network representing a molecule where vertices are atoms and edges are bonds, vertex labels represent the various atomic species, e.g. carbon, hydrogen, nitrogen etc. There is less than 10 such species in the vast majority of organic molecules in available data sets. In addition, in the standard representation of molecules, hydrogen vertices are omitted altogether and the label of carbon atoms is put to the default value 1 (that is no label), further reducing the number of different labels.

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520 Finding all simple cycles/paths label sequences in such situations can be done 521 with Eq. (2) , (4) or (5) with the following time complexity:

522 THEOREM 4. Let $G = (V, E)$ be a graph, possibly directed, on N vertices. Let Δ 523 be the maximum degree of any vertex on G or, if G is directed, let Δ be the maximum 524 degree of any vertex on the undirected version of G. Finally, let n be the number of 525 different labels attached to graph vertices. Then all the label sequences of simple cycles 526 of length up to ℓ on G can be found in time

$$
527 \quad (9) \qquad O\left(N + M + \left(n^{\ell} \ell^{\omega} + \ell \Delta\right) |S_{\ell}|\right)
$$

528 and $O(N(\Delta+1))$ space. The same complexities are achieved to find the label sequences 529 of all simple paths up to length ℓ or of simple cycles/paths with fixed endpoints up to 530 $length \ell$.

Proof. In the presence of labels, Eqs. (2), (4) and (5) continue to be valid and provide the label sequences of the simple cycles/paths upon replacing the adjacency matrix A by the labeled adjacency matrix W, defined by

$$
\mathsf{W}_{ij} := \mathsf{A}_{ij} w_{L(i)L(j)},
$$

531 where $L(i)$ is the label of vertex i and w is a formal variable. For example, a nitrogen-532 oxygen bond in a molecular graph would appear as w_{NO} in W. The time complexity of evaluating Eq. (2), (4) or (5) remains unchanged except for the cost of calculating 534 the traces $\text{Tr}(\mathsf{W}^{\ell}_{H})$. These can be obtained through matrix multiplications. Since the 535 entries of $W_H^{\ell-1}$ are sums of label sequences of walks of length $\ell-1$ on the subgraph 536 H and since there are at most $n^{\ell-1}$ such sequences, evaluating the trace costs at 537 most $|H|^{\omega}n^{\ell-1} = O(\ell^{\omega}n^{\ell})$ time. Replacing ℓ^{ω} with this cost in Theorem 1 yields the result. \Box

 7. Conclusion. We have presented a novel general purpose algorithm for count- ing simple cycles and simple paths of any length ℓ on any graph, including directed and weighted ones. The time complexity of this algorithm scales with the number $|S_\ell|$ of weakly connected induced subgraphs on at most ℓ vertices, making it the best 545 general purpose algorithm whenever $(\ell^{\omega-1}\Delta^{-1} + 1)|S_{\ell}| \leq |\text{Cycle}_{\ell}|$. In this expression | Cycle_{ℓ} | is the total number of simple cycles of length up to ℓ , including self-loops and 547 backtracks. Empirically, we found that this happens on Erdős-Rényi random graphs when the edge-probability exceeds circa $4/N$, as well as on some real-world networks, such as those in the Actors family of graphs. ⁵⁵⁰

 If the network under study is undirected and if counting simple cycles of length up to 7 is sufficient, then the algorithm of Alon, Yuster and Zwick is still by far the fastest. Furthermore, while we can predict that there must a graph size such that AYZ be- comes slower than the algorithm presented here, on Erd˝os-R´enyi random graphs this size seems to be much beyond what we can reach. Indeed, we could not run AYZ on 556 graphs with more than $N \gtrsim 12,000$ vertices owing to its important memory consump- tion. While this number can likely be increased with an optimised implementation of AYZ in conjunction with more memory, it is unlikely to get substantially larger as 559 the memory usage of AYZ scales with N^2 . In contrast, we could run the algorithm 560 presented here on networks with over 300,000 vertices without running out of memory.

 Finally, even though the algorithm presented here is the best general purpose al-563 gorithm on the class of graphs with $(\ell^{\omega-1}\Delta^{-1} + 1)|S_{\ell}| \leq |\text{Cycle}_{\ell}|$, the time necessary to count simple cycles of length e.g. up to 10 can be prohibitively large on large net- works. Instead, the algorithm is best used in conjunction with Monte Carlo methods. We demonstrate this procedure in a separate publication [19], where we use it in a sociological context to obtain the ratios of negative to positive simple cycles of length up to 20 on several real-world directed signed networks with up to 130,000+ vertices.

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